Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(lecture rooms H 0104, H 2053, H 3005, H 3010, BH 243 and BH 334 ; Poster Area B)

Invited Talks

(except focused sessions, see below for the focused session program)

TT 14.1	Mon	16:45–17:15	H 3005	**Multiferroicity in an organic charge-transfer salt: Electric-dipole-driven magnetism** — •Peter Lunkenheimer
TT 17.10	Tue	12:00–12:30	H 2053	**Magnetism and Superconductivity: A new era of convergence in condensed matter physics** — •Piers Coleman
TT 19.8	Tue	11:30–12:00	H 3010	**Interactions and disorder in topological quantum matter** — •Simon Trebst
TT 20.1	Tue	9:30–10:00	BH 243	**Making and manipulating Majorana fermions for topological quantum computation** — •Felix von Oppen
TT 30.1	Wed	15:00–15:30	H 3005	**Bose-Einstein condensation of Photons** — •Martin Weitz
TT 20.5	Tue	11:00–11:30	BH 243	**Distinguishing quantum and classical transport through nanostructures** — •Clive Emary
TT 29.7	Wed	16:45–17:15	H 2053	**Novel Josephson effect in triplet Josephson junctions: the story begins** — •Dirk Manske
TT 30.8	Wed	17:15–17:45	H 3005	**Topological superfluids confined in a regular nano-scale slab geometry** — •John Saunders
TT 38.8	Thu	11:30–12:00	H 3010	**Emergent electrodynamics of skyrmions in chiral magnets** — •Christian Pfleiderer

Invited and Topical Talks in the Focused Session "Resonant Inelastic X-ray Scattering on Magnetic Excitations"

TT 7.1	Mon	15:00–15:40	H 0104	**RIXS Studies of Strongly Correlated Electron Systems** — •John Hill
TT 7.2	Mon	15:40–16:20	H 0104	**RIXS in the soft X-ray range: applications and perspectives** — •Lucio Braicovich
TT 7.3	Mon	16:40–17:20	H 0104	**The theory of resonant inelastic x-ray scattering on valence excitations** — •Michel van Veenendaal
TT 7.4	Mon	17:20–18:00	H 0104	**Excitons as a probe for low-energy spin fluctuations in cuprate chains** — •Jochen Geck
TT 7.5	Mon	18:00–18:40	H 0104	**Fractionalization of electronic degrees of freedom in low-dimensional cuprates** — •Justine Schlappa

Invited and Topical Talks in the Focused Session "Charge and Spin Transport through Junctions at the Nanometre Scale"

TT 35.1	Thu	9:30–10:10	H 0104	**The information is the noise: shot noise a tool for investigating atomic and molecular nanowires** — •Jan van Ruitenbeek
TT 35.2	Thu	10:10–10:50	H 0104	**Electronic transport and magnetism in one-atom contacts** — •Carlos Untiedt

TT 35.3	Thu	10:50–11:30	H 0104	**Metallic atomic-size contacts: The role of absorbed noble gas atoms and anisotropic magnetoresistance** — •Juan Carlos Cuevas
TT 35.4	Thu	11:40–12:20	H 0104	**Spin transport through organic molecules** — •Wulf Wulfhekel
TT 35.5	Thu	12:20–13:00	H 0104	**Spin-current manipulation of atomic-scale magnets using SP-STM** — •Stefan Krause

Invited and Topical Talks in the Focused Session "Cryogenic Detectors"

TT 41.1	Thu	15:00–15:30	H 2053	**Performance and Understanding of Transition-Edge Sensor Microcalorimeters** — •Simon Bandler
TT 41.2	Thu	15:30–16:00	H 2053	**Kinetic Inductance Detectors** — •Jochem Baselmans
TT 41.3	Thu	16:15–16:40	H 2053	**Magnetic calorimeters for x-ray and particle detection** — •Andreas Fleischmann
TT 41.4	Thu	16:40–17:05	H 2053	**Readout of TESs and MCCs with SQUID current sensors** — •Jörn Beyer
TT 41.5	Thu	17:05–17:30	H 2053	**Direct Dark Matter Search with the CRESST II Detector** — •Jean-Côme Lanfranchi

Invited talks of the joint symposium SYTI

See SYTI for the full program of the symposium.

SYTI 1.1	Tue	9:30–10:00	H 0105	**Search for Majorana fermions in topological insulators** — •Carlo Beenakker
SYTI 1.2	Tue	10:00–10:30	H 0105	**Cooper Pairs in Topological Insulator Bi_2Se_3 Thin Films Induced by Proximity Effect** — •Jinfeng Jia
SYTI 1.3	Tue	10:30–11:00	H 0105	**Gate tunable normal and superconducting transport through a 3D topological insulator** — •Alberto Morpurgo
SYTI 1.4	Tue	11:00–11:30	H 0105	**Weyl Metal States and Surface Fermi Arcs in Iridates** — •Sergey Savrasov
SYTI 1.5	Tue	11:30–12:00	H 0105	**Engineering a Room-Temperature Quantum Spin Hall State in Graphene via Adatom Deposition** — •Marcel Franz

Invited talks of the joint symposium SYNM

See SYNM for the full program of the symposium.

SYNM 1.1	Wed	15:00–15:30	H 0105	**Mechanical resonators in the quantum regime** — •Andrew N. Cleland
SYNM 1.2	Wed	15:30–16:00	H 0105	**Quantum optomechanics: exploring the interface between quantum physics and gravity** — •Markus Aspelmeyer
SYNM 1.3	Wed	16:00–16:30	H 0105	**Integrated transduction and coherent control of high Q nanomechanical systems using dielectric gradient forces** — •Eva M. Weig
SYNM 1.4	Wed	16:30–17:00	H 0105	**Cavity optomechanics with microwave photons** — •John Teufel
SYNM 1.5	Wed	17:00–17:30	H 0105	**Optomechanical crystals** — •Oskar Painter

Sessions

TT 1.1–1.14	Mon	9:30–13:15	H 0104	**Correlated Electrons: Low-dimensional Systems - Models 1**
TT 2.1–2.13	Mon	9:30–13:00	H 2053	**Superconductivity: Fe-based Superconductors - 1111, LiFeAs & As-free Pnictides**
TT 3.1–3.14	Mon	9:30–13:15	H 3005	**Correlated Electrons: Heavy Fermions**
TT 4.1–4.13	Mon	9:30–13:00	H 3010	**Transport: Topological Insulators 1 (jointly with HL and MA)**
TT 5.1–5.12	Mon	9:30–12:45	BH 243	**Transport: Quantum Coherence and Quantum Information Systems 1 (jointly with MA and HL)**
TT 6.1–6.13	Mon	9:30–13:00	BH 334	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1**

TT 7.1–7.5	Mon	15:00–18:40	H 0104	**Focused Session: Resonant Inelastic X-ray Scattering on Magnetic Excitations**
TT 8.1–8.13	Mon	15:00–18:30	H 2053	**Superconductivity: Fe-based Superconductors - 122 Part 1**
TT 9.1–9.6	Mon	15:00–16:30	H 3005	**Transport: Topological Insulators 2 (jointly with HL and MA)**
TT 10.1–10.12	Mon	15:00–18:15	H 3010	**Correlated Electrons: (General) Theory 1**
TT 11.1–11.9	Mon	15:00–17:30	BH 243	**Transport: Quantum Coherence and Quantum Information Systems 2 (jointly with MA and HL)**
TT 12.1–12.6	Mon	15:00–16:30	BH 334	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2**
TT 13.1–13.54	Mon	15:00–19:00	Poster B	**Transport: Poster Session**
TT 14.1–14.4	Mon	16:45–18:00	H 3005	**Matter At Low Temperature: Multiferroics (jointly with MA, DF, DS, KR**
TT 15.1–15.5	Mon	16:45–18:00	BH 334	**Correlated Electrons: Quantum Impurities, Kondo Physics 1**
TT 16.1–16.14	Tue	9:30–13:15	H 0104	**Correlated Electrons: Low-dimensional Systems - Models 2**
TT 17.1–17.10	Tue	9:30–12:30	H 2053	**Superconductivity: Fe-based Superconductors - 122 Part 2 & Theory**
TT 18.1–18.12	Tue	9:30–12:45	H 3005	**Correlated Electrons: Quantum Impurities, Kondo Physics 2**
TT 19.1–19.12	Tue	9:30–13:00	H 3010	**Correlated Electrons: (General) Theory 2**
TT 20.1–20.8	Tue	9:30–12:15	BH 243	**Transport: Quantum Coherence and Quantum Information Systems 3 (jointly with MA and HL)**
TT 21.1–21.13	Tue	9:30–13:00	BH 334	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3**
TT 22.1–22.13	Wed	9:30–13:00	H 0104	**Correlated Electrons: Low-dimensional Systems - Materials 1**
TT 23.1–23.7	Wed	9:30–11:15	H 2053	**Superconductivity: Fe-based Superconductors - Fe(Se/Te)**
TT 24.1–24.12	Wed	9:30–12:45	H 3005	**Nanomechanics**
TT 25.1–25.12	Wed	9:30–12:45	H 3010	**Correlated Electrons: Quantum-Critical Phenomena 1**
TT 26.1–26.13	Wed	9:30–13:00	BH 334	**Transport: Topological Insulators 3 (jointly with HL and MA)**
TT 27.1–27.7	Wed	11:30–13:15	H 2053	**Superconductivity: Cuprate Superconductors**
TT 28.1–28.13	Wed	15:00–18:30	H 0104	**Correlated Electrons: Low-dimensional Systems - Materials 2**
TT 29.1–29.12	Wed	15:00–18:30	H 2053	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 1**
TT 30.1–30.12	Wed	15:00–18:45	H 3005	**Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 1**
TT 31.1–31.5	Wed	15:00–16:15	H 3010	**Correlated Electrons: Quantum-Critical Phenomena 2**
TT 32.1–32.9	Wed	15:00–17:30	BH 334	**Transport: Nanoelectronics III - Molecular Electronics 1**
TT 33.1–33.74	Wed	15:00–19:00	Poster B	**Superconductivity, Measuring Devices, Matter at Low Temperature: Poster Session**
TT 34.1–34.6	Wed	16:30–18:00	H 3010	**Correlated Electrons: Metal-Insulator Transition 1**
TT 35.1–35.5	Thu	9:30–13:00	H 0104	**Focused Session: Charge and Spin Transport through Junctions at the Nanometre Scale**
TT 36.1–36.10	Thu	9:30–12:15	H 2053	**Superconductivity: Cryodetectors**
TT 37.1–37.13	Thu	9:30–13:00	H 3005	**Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 2**
TT 38.1–38.12	Thu	9:30–13:00	H 3010	**Correlated Electrons: Spin Systems and Itinerant Magnets 1**
TT 39.1–39.13	Thu	9:30–13:00	BH 334	**Transport: Graphene 1 (jointly with MA, HL, DY, DS, O)**
TT 40.1–40.12	Thu	15:00–18:15	H 0104	**Correlated Electrons: Low-dimensional Systems - Materials 3**
TT 41.1–41.5	Thu	15:00–17:30	H 2053	**Focused Session: Cryogenic Detectors**
TT 42.1–42.11	Thu	15:00–18:00	H 3005	**Superconductivity: Fabrication, Properties, Electronic Structure**
TT 43.1–43.10	Thu	15:00–17:45	H 3010	**Correlated Electrons: Metal-Insulator Transition 2**
TT 44.1–44.8	Thu	15:00–17:15	BH 334	**Transport: Nanoelectronics III - Molecular Electronics 2**
TT 45.1–45.111	Thu	15:00–19:00	Poster B	**Correlated Electrons: Poster Session**
TT 46.1–46.8	Thu	17:45–20:00	H 2053	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 2**
TT 47.1–47.12	Fri	9:30–12:45	H 0104	**Correlated Electrons: Spin Systems and Itinerant Magnets 2**

TT 48.1–48.13	Fri	9:30–13:00	H 2053	**Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Vortices**
TT 49.1–49.9	Fri	9:30–12:00	H 3005	**Correlated Electrons: Low-dimensional Systems - Materials 4**
TT 50.1–50.10	Fri	9:30–12:15	H 3010	**Superconductivity: (General) Theory**
TT 51.1–51.9	Fri	9:30–12:00	BH 243	**Transport: Nanoelectronics II - Spintronics and Magneto-transport (jointly with HL and MA)**
TT 52.1–52.12	Fri	9:30–12:45	BH 334	**Transport: Graphene 2 (jointly with MA, HL, DY, DS, O)**

Annual General Meeting of the Low Temperature Physics Division

Thursday 20:15 H 3005

TT 1: Correlated Electrons: Low-dimensional Systems - Models 1

Time: Monday 9:30–13:15 Location: H 0104

TT 1.1 Mon 9:30 H 0104

Lithium purple bronze: strong renormalization of the perpendicular hopping — •L. Dudy[1,2], J. Denlinger[3], J. He[4], and J.W. Allen[1] — [1]Randall Laboratory, University of Michigan, Ann Arbor, MI, USA — [2]Julius-Maximilians-Universität Würzburg, Germany — [3]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [4]Clemson University, Clemson, SC, USA

An interesting topic in condensed matter physics is the question of whether one dimensional (1d) behavior of the electronic structure can be realized in our 3d world. In the case of a network (or bundle) of one-dimensional chains, in the framework of the Tomonaga Luttinger model, it is found in theory that movement of electrons between neighboring chains, the "perpendicular hopping", can be greatly suppressed by the 1d behavior, although at a sufficiently low temperature a crossover to 3d is nonetheless expected. We will present results from angle resolved photoemission spectroscopy on single crystals of the quasi-1d lithium purple bronze ($Li_{0.9}MoO_{17}$) measured at a temperature of 6K on the Merlin beam line at the Advanced Light Source. We will show that the hopping parameter has to be extremely renormalized down from its LDA value in order to explain the experiment. Therefore, there might even be the rare possibility that the superconductivity of this material (at about 1.9K) evolves out of a 1d normal state.

TT 1.2 Mon 9:45 H 0104

Low-energy local spectral weights of the one-dimensional Hubbard chain — Stefan Söffing[1], Imke Schneider[2], and •Sebastian Eggert[1] — [1]TU Kaiserslautern and Research Center OPTIMAS — [2]TU Dresden

The Hubbard model in one dimension is a proto-typical model for a quantum wire with separate spin and charge excitations. We now examine the local spectral weights along a finite wire with the numerical Density Matrix Renormalization group in order to find signatures of strongly correlated excitations in the low-energy tunneling density of states. The resulting level structureis remarkably rich in space and energy. Comparing with the predictions from bosonization, we observe strong corrections from higher order operators and boundary effects.

TT 1.3 Mon 10:00 H 0104

Ballistic expansion of interacting fermions in one-dimensional optical lattices — •Stephan Langer[1], Martin Schuetz[3], Ian McCulloch[2], Ulrich Schollwöck[1], and Fabian Heidrich-Meisner[1] — [1]LMU München — [2]University of Queensland, Brisbane, Australia — [3]MPQ Garching and LMU München

In most quantum quenches, no net particle currents arise. Access to studying transport properties can be gained by letting a two-component Fermi gas that is originally confined by the presence of a trapping potential expand into an empty optical lattice. In recent experiments, this situation was addressed in 2D and 3D optical lattices [1]. We focus on the 1D case in which an exact numerical simulation of the time-evolution is possible by means of the DMRG method. Concretely, we study the expansion in the 1D Hubbard model with repulsive interactions, driven by quenching the trapping potential to zero, and we concentrate on the most direct experimental observable, namely density profiles [2]. In the strict 1D case, we identify conditions for which the expansion is ballistic, characterized by an increase of the cloud's radius that is linear in time. This behavior is found whenever initial densities are smaller or equal to one, both for the expansion from box and harmonic traps. We make quantitative predictions for the expansion velocity as a function of on-site repulsion and initial density that can be probed in experiments.

[1] Schneider et al., arXiv:1005.3545
[2] Langer et al., arXiv:1109.4364

TT 1.4 Mon 10:15 H 0104

Local density of states of the one-dimensional spinless fermion model — •Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate the local density of states of the one-dimensional half-filled spinless fermion model with nearest-neighbor hopping $t > 0$ and interaction V in its Luttinger liquid phase $-2t < V \leq 2t$. The bulk density of states and the local density of states in open chains are calculated over the full band width $\sim 4t$ with an energy resolution $\leq 0.08t$ using the dynamical density-matrix renormalization group (DDMRG) method. We also perform DDMRG simulations with a resolution of $0.01t$ around the Fermi energy to reveal the power-law behaviour $D(\epsilon) \sim |\epsilon - \epsilon_F|^\alpha$ predicted by the Luttinger liquid theory for bulk and boundary density of states. The exponents α are determined using a finite-size scaling analysis of DDMRG data for lattices with up to 3200 sites. The results agree with the exact exponents given by the Luttinger liquid theory combined with the Bethe Ansatz solution. The crossover from boundary to bulk density of states is analyzed. We have found that boundary effects can be seen in the local density of states at all energies even far away from the chain edges [1].

[1] E. Jeckelmann, arXiv:1111.6545v1 [cond-mat.str-el]

TT 1.5 Mon 10:30 H 0104

Relaxation and thermalization in the 1d Hubbard model — •Tilman Enss[1] and Jesko Sirker[2] — [1]TU München, Germany — [2]TU Kaiserslautern, Germany

The time evolution of a 1d quantum system after a quench is a challenging many-body problem which can be studied, e.g., numerically using time-dependent density matrix renormalization group (DMRG) techniques. As shown by Lieb and Robinson, information spreads at a finite velocity resulting in an effective "light cone". In my talk I will present a very efficient DMRG algorithm based on this light cone structure. With the help of the DMRG data I will discuss the relaxation and thermalization of doublon states in the fermionic Hubbard model.

TT 1.6 Mon 10:45 H 0104

Fractionalization of electron's spin and orbital degrees of freedom in 1D — •Krzysztof Wohlfeld[1], Maria Daghofer[1], Satoshi Nishimoto[1], Giniyat Khaliullin[2], and Jeroen van den Brink[1] — [1]IFW Dresden, Germany — [2]MPI-FKF Stuttgart, Germany

We show that electron's spin and orbital degrees of freedom can fractionalize in 1D antiferromagnets: although the orbital excitations are inherently coupled to spinons in antiferromagnetic Mott insulators, in 1D they separate into a *pure* orbiton and a single spinon. This is similar to the spin-charge separation in 1D but corresponds to an exotic regime where spinons are faster than holons [1]. The resulting large dispersion of the *pure* orbiton can be detected in e.g. quasi-1D cuprates [2].

[1] K. Wohlfeld, M. Daghofer, S. Nishimoto, G. Khaliullin, and J. van den Brink, Phys. Rev. Lett. **107**, 147201 (2011).
[2] J. Schlappa *et al.*, to be published (2011).

TT 1.7 Mon 11:00 H 0104

Fractionalization of Fractionalized Charges in the 1D t-J Model — •Alexander Moreno and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart, Germany

On the basis of the density matrix renormalization group (DMRG) we study the ground-state phase diagram [1] of the model and the excitation content of each phase. The real time dynamics of a low-energy electron added to the system can be described by right and left propagating fractional excitation predicted by the Luttinger Liquid theory (LL) [2]. However, at higher energies the dynamics reveals one more level of fractionalization of the already fractional LL excitation. This new kind of fractionalization is also visible in the one-particle spectral function obtained in a previous quantum Monte Carlo simulation [3] where the branches were assigned to a spinon, a holon, and an antiholon, as in the supersymmetric t-J model with $1/r^2$ exchange [4]. By switching an electric field, we aim at identifying the charge of the fractionalized elementary excitations that result from the electron.

[1] A. Moreno, A. Muramatsu and S. Manmana, Phys. Rev. B **83**, 205113 (2011).
[2] K.-V. Pham, M. Gabay, and P. Lederer, Phys. Rev. B **61**, 16397(2000).
[3] C. Lavalle, M. Arikawa, S. Capponi, F. F. Assaad, and A. Muramatsu, Phys. Rev. Lett. **90**, 216401 (2003).
[4] M. Arikawa, Y. Saiga, and Y. Kuramoto, Phys. Rev. Lett. **86**, 3096 (2001).

15 min. break.

TT 1.8 Mon 11:30 H 0104

Entanglement spectrum in two dimensional systems — •Vincenzo Alba[1], Masud Haque[1], and Andreas Lauchli[2] — [1]Max Planck Institute for the Physics of the Complex Systems, Dresden, Germany — [2]University of Innsbruck, Innsbruck, Austria

We studied the entanglement spectrum of several two dimensional systems (2D Bose-Hubbard, XXZ, tight binding systems with staggered chemical potential). We found a physical description of the low part of the entanglement spectrum in terms of effective hamiltonians (entanglement hamiltonians). For the 2D Bose Hubbard we also characterized the behavior of the entanglement spectrum in the superfluid phase where we found that the entanglement hamiltonian shows clear signatures of the condensate wavefunction.

TT 1.9 Mon 11:45 H 0104

Robustness of the two-dimensional cluster phase in an external magnetic field — •Henning Kalis, Daniel Klagges, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The cluster state represents a highly entangled state which is one central object for measurement-based quantum computing. Here we study the robustness of the cluster state on the two-dimensional square lattice at zero temperature in the presence of external magnetic fields by means of high-order series expansions. Interestingly, the phase diagram contains a self-dual line in parameter space allowing many precise statements about the fate of the cluster phase at finite fields. We provide strong evidences for first- and second-order phase transitions between the cluster phase and polarized phases.

TT 1.10 Mon 12:00 H 0104

Quantum paramagnetism in the Kagomé transverse field Ising model — •Michael Powalski[1], Kris Cöster[1], Roderich Moessner[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

We study the intriguing interplay of strong geometrical frustration and of quantum fluctuations. Using perturbative continuous unitary transformations to study the high-field phase, we have calculated the one-magnon excitation spectrum as a high-order series expansion for both Kagomé and for the triangular lattices. Most interestingly, the one-particle gap for the Kagomé transverse field Ising model shows no tendency to close for any finite magnetic field suggesting that the disordered quantum paramagnet is adiabatically connected to the low-field limit. In contrast, for the triangular lattice we find a quantum phase transition which is compatible with the 3dXY universality class. The different behaviour of both lattices can be traced back to the existence of an (almost) dispersionless lowest-energy band for the Kagomé lattice which is exactly flat up to order seven in perturbation theory. This behaviour is understood in terms of a local mode. Furthermore, we can understand the occurrence and the properties of such local modes for any lattice by the corresponding graph expansion.

TT 1.11 Mon 12:15 H 0104

Anomalous criticality near semimetal-to-superfluid quantum phase transition in a two-dimensional Dirac cone model — •Benjamin Obert[1], So Takei[2], and Walter Metzner[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Department of Physics, The University of Maryland College Park, MD 20742, USA

We analyse a two-dimensional Dirac Cone model which undergoes a quantum phase transition between a semimetal and a superfluid. The model consists of attractively interacting electrons with a linear dispersion around a single Dirac point. We compute the renormalization group flow for the model and study both ground state and finite temperature properties. The electrons and the order parameter fluctuations exhibit power-law scaling with anomalous scaling dimensions. The quasiparticle weight and the Fermi velocity vanish at the quantum critical point. The order parameter correlation length turns out to be infinite everywhere in the semimetallic ground state.

[1] P. Strack, S. Takei, and W. Metzner, Phys. Rev. B **81**, 125103 (2010).

[2] B. Obert, S. Takei, and W. Metzner, Ann. Phys. (Berlin) **523**, No.8-9, 621-628 (2011)

TT 1.12 Mon 12:30 H 0104

Robustness of a Z(3) topological phase — •Marc Daniel Schulz[1,4], Sébastien Dusuel[2], Roman Orùs[3], Julien Vidal[4], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany — [4]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

Kitaev's toric code model is an exactly solvable lattice model, whose ground state(s) are topologically ordered. We study the robustness of a generalized version of this model with Z(N) degrees of freedom in the presence of local perturbations. For N = 2, this model reduces to the conventional toric code in a uniform magnetic field. A quantitative analysis is performed for the perturbed Z(3) toric code by applying a combination of high-order series expansions and variational techniques. We provide strong evidences for first- and second-order phase transitions between topologically-ordered and polarized phases. Most interestingly, our results also indicate the existence of topological multi-critical points in the phase diagram.

TT 1.13 Mon 12:45 H 0104

Magnetocaloric effect in Suzuki models. — Myroslava Topilko[1], Oleg Derzhko[1], and •Vadim Ohanyan[2] — [1]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Street, L'viv-11, 79011, Ukraine — [2]Department of Theoretical Physics, Yerevan State University, Al. Manoogian 1, 0025 Yerevan, Armenia

We consider the exactly solvable general spin-1/2 XX chain in an external (transverse) magnetic field with the multiple-spin(long range) interactions of the XZ...ZX+YZ...ZY and XZ...ZY-YZ...ZX types. The model can be mapped on the free spinless fermion system by means of Jordan-Wigner transformation. We focus on the magnetocaloric effect and entropic properties of the system. The simplest case of three-spin interaction which is equivalent to zigzag ladder is investigated in details. The plots of the adiabatic cooling rate are obtained. We examine the effect of coupling constants on the features of magnetocaloric effect. The main result is that tuning the parameters one can shift the position of magnetocaloric anomaly, but the magnitude of effect depends only on the properties of corresponding quantum phase transition. As the system under consideration possessed a quantum triple point, the maximal enhancement of magnetocaloric effect occurs at the quantum triple point.

TT 1.14 Mon 13:00 H 0104

(De)coherence in two-electron quantum dots — •Sebastian Schröter[1], Paul-Antoine Hervieux[2], Giovanni Manfredi[2], Johannes Eiglsperger[3], Moritz Schönwetter[1,4], and Javier Madroñero[1] — [1]TU München — [2]CNRS, IPCMS Strasbourg — [3]Universität Regensburg — [4]MPI PKS, Dresden

The coherence of a system can be evaluated by the quantum fidelity (QF). Investigations of many-body systems, based on a mean-field approach, have shown an unusual behaviour [1] of the QF decay. As an exactly treatable model, which exhibits all relevant features of the investigated many-body systems, we study a planar two-electron quantum dot with an anharmonic confining potential. It becomes apparent, that the behaviour of the QF strongly depends on the level distribution and the degree of mixing of the states, a property, which is closely connected to the chaoticity of the underlying classical analogue. For simple linear combinations of eigenstates the QF decay can be computed from static properties of the system, while for complex wave packets sophisticated numerical algorithms for the propagation of the time-dependent Schrödinger equation [2,3] are needed. We compare analytical and numerical results and address the question if the unusual behaviour gives physical insight into the decoherence of a strongly interacting system or if it is merely an artefact of the mean-field approximation.

[1] G. Manfredi, P.-A. Hervieux, New J. Phys. **11** (2009), 013050. – PRL **100** (2008), 050405. – PRL **97** (2006), 190404.

[2] J. Madroñero, B. Piraux, Phys. Rev. A **80** (2009), 033409.

[3] A. Hamido, *et al.*, Phys. Rev. A **84** (2011), 013422.

TT 2: Superconductivity: Fe-based Superconductors - 1111, LiFeAs & As-free Pnictides

Time: Monday 9:30–13:00 Location: H 2053

TT 2.1 Mon 9:30 H 2053

NMR evidence for spin fluctuations in underdoped $LaO_{1-x}F_xFeAs$ — •Franziska Hammerath[1], Hans-Joachim Grafe[1], Guillaume Lang[1], Dalibor Paar[2], Günter Behr[1], Jochen Werner[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Department of Physics, Faculty of Science, University of Zagreb

We present ^{75}As Nuclear Magnetic Resonance (NMR) measurements on the iron-based superconductor $LaO_{1-x}F_xFeAs$ with $0 \leq x \leq 0.1$, covering a broad range of the phase diagram from magnetically-ordered to optimally-doped superconducting samples [1]. For underdoped samples ($x = 0.05$, $x = 0.075$) the ^{75}As NMR spin-lattice relaxation rate $(T_1T)^{-1}$ shows a Curie-Weiss-like increase at intermediate temperatures, indicating the slowing down of spin fluctuations. However, a simple Curie-Weiss fit fails to describe $(T_1T)^{-1}(T)$ above 250 K and the occurrence of a peak in $(T_1T)^{-1}$ slightly above T_c. Instead, the data can be well described by considering a BPP-model for fluctuating magnetic fields in combination with a doping-independent linear temperature dependence at high temperature. At optimal doping ($x = 0.1$) spin fluctuations are suppressed and only the linear contribution to $(T_1T)^{-1}$ is left. This stands in contrast to other pnictides, such as $Ba(Fe_{1-x}Co_xAs)_2$ and $Ba(FeAs_{1-x}P_x)_2$. Our analysis is consistent with charge carrier localization in underdoped $LaO_{1-x}F_xFeAs$ as seen by means of resistivity measurements [2].

[1] H. Luetkens et al. Nature Materials **8**, 306 (2009).
[2] C. Hess et al., Eur. Phys. Lett. **87**, 17005 (2009).

TT 2.2 Mon 9:45 H 2053

^{75}As NQR investigations of charge inhomogeneities in $CeFe_{1-x}Co_xAsO$ — •Eva Maria Brüning, Guillaume Lang, Hans-Joachim Grafe, Louis Veyrat, Sabine Wurmehl, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

In the iron pnictides superconductors, carrier doping plays a crucial role in the appearance of superconductivity, whereas the magnetic and the structural phase transitions are suppressed. This is for example the case in $LaFeAsO_{1-x}F_x$ [1]. NQR measurements on $LnFeAsO_{1-x}F_x$ (Ln = La, Sm) showed in the underdoped region the coexistence of two charge environments at the nanoscale; they point to local electronic order in the iron layers [2]. Surprisingly, in LaFeAsO and SmFeAsO, superconductivity could be successfully induced by cobalt substitution in place of iron which shows that in-plane disorder is highly tolerated in these compounds [3], as in 122 pnictides. This is in high contrast to the cuprate high-Tc superconductors where replacing Cu by other transition metals (Zn, Ni) leads to a suppression of superconductivity. We report on ^{75}As NQR investigations of $CeFe_{1-x}Co_xAsO$ (x=0.03, 0.05, 0.07) and the comparison of in-plane Co-doping and out-of-plane F-doping.

[1] Y. Kamihara. al., Chem. Soc. **130**, 3296 (2008)
[2] G. Lang et. al., Phys Rev. Lett. **104**, 097001 (2010)
[3] C. Wang et. al., Phys Rev. B **79**, 054521 (2009)

TT 2.3 Mon 10:00 H 2053

Physics of defect induced local moments in pnictide superconductors — •Vadim Grinenko[1], Stefan-Ludwig Drechsler[1], Konstatin Kikoin[2], Mahmoud Abdel-Hafiez[1], Saicharan Aswartham[1], Anja Wolter-Giraud[1], Christian Hess[1], Manoj Kumar[1], Sabine Wurmehl[1], Guenter Fuchs[1], Konstantin Nenkov[1], Franziska Hammerath[1], Guillaume Lang[1], Hans-Joachim Grafe[1], Bernhard Holzapfel[1], Jeroen van den Brink[1], Bernd Buechner[1], and Ludwig Schultz[1] — [1]IFW-Dresden, D-01171 Dresden, Germany — [2]School of Physics and Astronomy, Tel-Aviv University , Tel-Aviv, Israel

Many unusual physical properties of Fe-pnictide superconductors are related to the presence of local magnetic moments induced by point-defects, e.g. As-vacancies. In the La-1111 system they improve the superconducting properties as compared with As-stoichiometric samples enhancing T_c and the $-dH_{c2}/dT$ at T_c. But they also enhance strongly the spin susceptibility, which governs the Pauli limiting behavior of the As-deficient La-1111. In heavily hole doped K-122 superconducting single crystals the local moments leads to a complex phase diagram with a Griffith and a spin glass phase. The local moments picture explains also the observed non-Fermi-liquid behavior and the large effective mass enhancement of the quasi-particles in K-122. In Co-doped Ba-122 superconducting single crystals the local moments form also a spin glass state and lead to a strong Pauli limiting behavior.

TT 2.4 Mon 10:15 H 2053

Critical current scaling and anisotropy in oxypnictide superconductors — Martin Kidszun[1], Jens Hänisch[1], Bernhard Holzapfel[1], Tom Thersleff[1,2], and •Silvia Haindl[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O.Box 270116, 01171 Dresden, Germany — [2]Department of Engineering Sciences, University of Uppsala, Box 534, 751 21 Uppsala, Sweden

Having succeeded in the fabrication of epitaxial superconducting La-1111 thin films we performed an extensive study of electrical transport properties [1]. We found that the anisotropic Ginzburg-Landau scaling approach can be applied to the angular dependent critical current densities and results in temperature dependent γ-values between 3 and 5. Originally, the anisotropic Ginzburg-Landau scaling approach was developed for a single band superconductor where γ denotes the mass anisotropy. In multiband superconductors the scaling parameter, γ, varies with temperature, however its interpretation as an effective mass anisotropy remains subtle. According to the temperature dependence of the upper critical field we present an explanation using two dominating electronic bands.

[1] M. Kidszun et al., Phys. Rev. Lett. 106 (2011) 137001

TT 2.5 Mon 10:30 H 2053

Effects of correlation in LiFeAs — •Johannes Ferber, Kateryna Foyevtsova, Roser Valenti, and Harald 0. Jeschke — Institut für theoretische Physik, Universität Frankfurt, Germany

We discuss the role of correlations in the iron pnictide LiFeAs by studying the effects on band structure, mass enhancements, and Fermi surfaces in LDA+DMFT. For LiFeAs, seemingly contradictory results from angle-resolved photoemission spectroscopy (ARPES) and de Haas-van Alphen (dHvA) measurements have been reported. Whereas dHvA observes good agreement with LDA results, ARPES reports strongly altered Fermi surfaces, possibly as a result of electronic correlations. In our calculations we find the hole pockets of the Fermi surface to be affected more strongly by correlations. Based on this observation, we give a suggestion for how to reconcile the experimental findings and assess the importance of correlations in this compound.

TT 2.6 Mon 10:45 H 2053

Spin fluctuations in the FeAs-based superconductors — •N. Qureshi[1], Y. Sidis[2], S. Wurmehl[3], I. Morozov[3], S. Aswartham[3], L. Harnagea[3], C. Nacke[3], B. Büchner[3], P. Steffens[4], and M. Braden[1] — [1]University of Cologne — [2]LLB, Saclay (France) — [3]IFW Dresden — [4]ILL, Grenoble (France)

We have performed inelastic neutron scattering (INS) studies on two undoped compounds: superconducting paramagnetic LiFeAs and non-superconducting antiferromagnetic (AF) $BaFe_2As_2$. INS using LiFeAs single crystals revealed clear evidence for AF fluctuations at an incommensurate Q-vector, which vanish at low energies. The excitations clearly responds to the opening of the superconducting gap by a redistribution of spectral weight. Applying more sophisticated methods like polarized neutron scattering with longitudinal polarization analysis to $BaFe_2As_2$ single crystals revealed anisotropic fluctuations, where the out-of-plane mode lies lower than the in-plane mode. This finding is astonishing as the static moment aligns along the FeAs layers. The fit of a J_1-J_2 model [1] using the coupling constants of $SrFe_2As_2$ [2] and taking into account the instrumental resolution yielded the single-ion anisotropies responsible for both gaps. In comparison to theoretical values [3] we find that the order of the gaps is reversed and that the spin-orbit coupling is underestimated in the calculations.

[1] D.-X. Yao and E. W. Carlson, Front. Phys. China 5, 166 (2010)
[2] R. Ewings et al., Phys. Rev. B 83 214519 (2011)
[3] A. N. Yaresko et al. Phys. Rev. B 79, 144421 (2009)

TT 2.7 Mon 11:00 H 2053

Anisotropic Energy-Gaps of Iron-Based Superconductivity from Intra-Band Quasiparticle Interference in LiFeAs —

•A.W. Rost[1,2], M.P. Allan[1,2,3], A.P. Mackenzie[2], Y. Xie[3], J.C. Davis[1,2,3,4], K. Kihou[5], C.-H. Lee[5], A. Iyo[5], H. Eisaki[5], and T.-M. Chuang[1,3,6] — [1]LASSP, Department of Physics, Cornell, Ithaca, NY 14853, USA — [2]SUPA, School of Physics and Astronomy, Univ. of St Andrews, St Andrews, Fife KY16 9SS, UK — [3]CMPMS Department, Brookhaven National Laboratory, Upton, NY 11973, USA — [4]Kavli Institute at Cornell for Nanoscale Science, Cornell, Ithaca , NY 14853, USA — [5]AIST, Tsukuba, Ibaraki 305-8568, Japan — [6]Inst. of Physics, Academica Sinica, Nankang, Taipei 11529, Taiwan

Cooper pairing in the Fe-based superconductors is thought to occur due to the projection of the antiferromagnetic interactions between iron atoms onto the complex momentum-space electronic structure. A key consequence is that distinct anisotropic energy gaps $\Delta_i(k)$ with specific relative orientations should occur on the different electronic bands i. To determine this previously unresolved gap structure high-precision spectroscopy is required. Here we introduce the STM technique of intra-band Bogoliubov quasiparticle scattering interference (QPI) to iron-based superconductor studies, focusing on LiFeAs. We identify the QPI signatures of three hole-like dispersions and, by introducing a new QPI technique, determine the magnitude and relative orientations of corresponding anisotropic $\Delta_i(k)$. Intra-band Bogoliubov QPI therefore yields the spectroscopic information required to identify the mechanism of superconductivity in Fe-based superconductors.

15 min. break.

TT 2.8 Mon 11:30 H 2053

Defect dependent influence on the superconducting gap of LiFeAs — •Danny Baumann, Torben Hänke, Ronny Schlegel, Sabine Wurmehl, Rico Pohle, Martha Scheffler, Luminita Harnagea, Christian Hess, and Bernd Büchner — IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

We have performed scanning tunneling spectroscopy measurements on the stoichiometric iron pnictide superconductor LiFeAs. After cleaving single crystalline samples, we observe a flat sample surface which can be imaged with atomic resolution by scanning tunneling microscopy. In addition, the surface contains a small amount of defects.

Here we will report on the dependence of the spectroscopic signature of LiFeAs on the occurring defects. Furthermore, we will present an analysis of the structure and symmetry of the observed defects and the influence on the density of the state of LiFeAs.

TT 2.9 Mon 11:45 H 2053

Temperature dependency of the superconducting gap in LiFeAs probed by STM — •Martha Scheffler, Rico Pohle, Torben Hänke, Ronny Schlegel, Danny Baumann, Steffen Sykora, Luminita Harnagea, Sabine Wurmehl, Christian Hess, Jeroen van den Brink, and Bernd Büchner — IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

We present temperature depending scanning tunneling spectroscopy measurements on the iron pnictide superconductor LiFeAs. At temperatures T $\sim$ 15K we see that the superconducting gap vanishes. Independent on the temperature we observe an asymmetry in the spectra with additional features near the Fermi energy and 50mV above E_F.

The good agreement of our results with model calculations for the tunneling conductance allows us to draw conclusions about the low energy properties of the superconducting system.

TT 2.10 Mon 12:00 H 2053

Electronic Transport Properties of LiFeAs in comparision to Ni-doped and Li-deficient LiFeAs — •Dirk Bombor, Anne Bachmann, Luminita Harnagea, Claudia Nacke, Saicharan Aswaratham, Sabine Wurmehl, Christian Hess, and Bernd Büchner — Leibnitz Institute for Solid State and Materials Research, IFW Dresden, Germany

Electronic transport properties of the unconventional 111-superconductor LiFeAs in comparison with Ni-doped and Li-deficient LiFeAs have been studied. Unlike in other iron arsenide superconductors the stoichiometric LiFeAs doesn't show any nesting of the Fermi surface and therefore exhibits no spin density wave but even the undoped compound becomes superconducting below 18 K. In contrast to other iron arsenide superconductors we find that doping by substitution of iron with Ni as well as Li-deficiency suppresses superconductivity. Beside this Li-deficient samples show ferromagnetic ordering below 160 K which leads to an enhancement of the unusual negative magnetoresistance. All compounds show a non-monotonic temperature dependence of the Hall coefficient which is discussed.

TT 2.11 Mon 12:15 H 2053

Ferromagnetic resonance in $Li_{1-\delta}Fe_{1-x}Ni_xAs$ single crystals — •A. Alfonsov, V. Kataev, C. Nacke, S. Aswartham, L. Harnagea, S. Wurmehl, A. U. B. Wolter, and B. Büchner — IFW Dresden, D-01169 Dresden, Germany

The magnetization measurements on $Li_{1-\delta}Fe_{1-x}Ni_xAs$ samples reveal a spontaneous magnetization below a critical temperature $T_c \sim 140 - 160$ K. In the electron spin resonance spectra measured at the X-band (9.5 GHz) frequency a strong ferromagnetic resonance (FMR) signal appears below T_c. Its behavior is similar in all samples. The temperature dependence of the resonance position of this signal corresponds to that of the spontaneous magnetization. The angular dependence of the position and of the linewidth of the signal, measured at low temperatures, suggests that the ferromagnetic magnetization is aligned in the FeAs plane. We discuss the properties of FMR signals in $Li_{1-\delta}Fe_{1-x}Ni_xAs$ samples.

TT 2.12 Mon 12:30 H 2053

As-free pnictide $LaNi_{1-x}Sb_2$ thin films grown by Reactive Molecular Beam Epitaxy — •Reiner Retzlaff, Alexander Buckow, Jose Kurian, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

We use reactive molecular beam epitaxy (RMBE) as synthesis technique for the search of arsenic free pnictide superconductors. Epitaxial thin films of $LaNi_{1-x}Sb_2$ were grown on (100) MgO substrates from elemental sources by simultaneous evaporation of high purity La, Ni and Sb metals by e-gun. The $LaNi_{1-x}Sb_2$ thin films grow epitaxially and are (00l) oriented with high crystalline quality, as evident from RHEED and X-Ray diffraction studies. The Ni deficient $LaNi_{1-x}Sb_2$ thin films show metallic behavior with a room temperature resistivity of 110 $\mu\Omega$cm, while the stoichiometric compound is a semiconductor/insulator [1]. The isostructural compound with Bi as pnictide shows a superconducting transition with a $T_C(0)$ of 3.1 K.

[1] R. Retzlaff *et al.* Submitted.

TT 2.13 Mon 12:45 H 2053

Synthesis of As-free pnictide superconductors $RENi_{1-x}Bi_2$ (RE = La, Ce) using Molecular Beam Epitaxy — •Alexander Buckow, Reiner Retzlaff, Jose Kurian, and Lambert Alff — FB Materialwissenschaft, TU Darmstadt, Deutschland

We have used reactive molecular beam epitaxy (RMBE) as synthesis technique for the search for arsenic free pnictide superconductors. High quality epitaxial thin films of $LaNiBi_2$, which was reported recently [1], were successfully grown on (100) MgO substrates by RMBE. The films were (00l) oriented and the epitaxial nature of the films was confirmed by RHEED and X-ray diffraction measurements. The a-axis of $LaNiBi_2$ is 45° rotated with respect to the MgO lattice. The c-axis lattice constant was determined to be 9.79 Å and the in-plane lattice constant is 4.565 Å. Ni deficient films show a $T_C(0)$ of 3.1 K, while the stoichiometric compound is semiconducting [2]. Furthermore, we report on the substitution of La by Ce demonstrating the capability of MBE as material screening tool.

[1] H. Mizoguchi *et al.*, Phys. Rev. Lett. **106**, 057002 (2011)
[2] A. Buckow *et al.* (to be published)

TT 3: Correlated Electrons: Heavy Fermions

Time: Monday 9:30–13:15 Location: H 3005

TT 3.1 Mon 9:30 H 3005

Elusive Fulde-Ferrell-Larkin-Ovchinnikov state: Evolution of quasi-particle entropy in high-field superconducting phase in $CeCoIn_5$ — •Yoshi Tokiwa — I. Physik. Institut, Georg-August Universität Gottingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We have performed a "smoking gun" experiment for Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state for $CeCoIn_5$. Entropy as a function of field is expected to show a steep increase at the transition field from BCS to FFLO superconducting (SC) state, because of the additional quasi-particles in the nodal parts of FFLO SC gap structure. We obtained electronic entropy of $CeCoIn_5$ by measuring magnetocaloric effect and specific heat at low temperatures down to 100mK and high fields up to 12T. In the high-field SC state for the field along [100], we observed a reduction of entropy, $\sim$8 mJ/mol·K, which is consistent with a spin density wave (SDW) order without the formation of FFLO state. The anomaly for the SDW transition in magnetocaloric effect and specific heat disappears, when the field is tilted 18° towards [001] from [100] in agreement with the neutron scattering experiment. Our experiment shows negative results for the formation of FFLO state in $CeCoIn_5$ for all the studied field directions, $H \parallel$[100], 18° and [001]. Although the numerous efforts for the experimental realization of FFLO state have been made since its prediction 40 years ago, an unambiguous observation in a solid state system still remains as a challenge in the field of condensed matter physics. This work is done by the collaboration with P. Gegenwart and E. Bauer and supported by DFG through research unit 960 (Quantum phase transitions).

TT 3.2 Mon 9:45 H 3005

Superconducting gap symmetry from the quasiparticle interference in the heavy fermion superconductor $CeCoIn_5$ — •Alireza Akbari[1], Peter Thalmeier[1], and Ilya Eremin[2] — [1]Max Planck Institute for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, 44780, Bochum, Germany

One of the most difficult issues in the heavy Fermion superconductors like the 115 compounds $CeMIn_5$ (M = Co, Ir, Rh) is the identification of the symmetry of superconducting order parameter. The ambiguity between d_{xy} and $d_{x^2-y^2}$ symmetry remained from earlier specific heat and thermal transport investigations has been resolved in favor of the latter by the observation of a spin resonance that can occur only in $d_{x^2-y^2}$ symmetry. However these methods are all indirect and depend considerably on theoretical interpretation. We presented the theory for the quasiparticle interference (QPI) in the heavy Fermion superconductor $CeCoIn_5$ as a direct method to confirm the d-wave gap symmetry. We calculate the QPI pattern for both magnetic and nonmagnetic impurities. By comparing the effect of the possible d-wave superconducting order parameters on QPI, the characteristic differences are found which may be identified by STM method. Our results propose that quasiparticle interference (QPI) and scanning tunneling microscopy (STM) can give a direct fingerprint of the superconducting gap in real space which may lead to a definite conclusion on its symmetry for $CeCoIn_5$ and related 115 compounds.

[1] A. Akbari, P. Thalmeier, I. Eremin, Phys. Rev. B 84, 134505 (2011).

TT 3.3 Mon 10:00 H 3005

Resonant magnetic exciton mode in the heavy-fermion antiferromagnet CeB_6 — G. Friemel[1], Y. Li[1], A. V. Dukhnenko[2], N. Y. Shitsevalova[2], N. E. Sluchanko[3], A. Ivanov[4], V. B. Filipov[2], B. Keimer[1], and •D. S. Inosov[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany. — [2]Institute for Problems of Material Sciences, Kiev, Ukraine. — [3]General Physics Institute, Moscow, Russia. — [4]Institut Laue-Langevin, Grenoble, France.

Resonant magnetic excitations are widely recognized as hallmarks of unconventional superconductivity in copper oxides, iron pnictides, and heavy-fermion compounds. Model calculations have related these modes to the microscopic properties of the pair wave function, but the mechanisms of their formation are still debated. Here we report the discovery of a similar resonant mode in the non-superconducting antiferromagnetic heavy-fermion metal CeB_6. Unlike conventional magnons, the mode is non-dispersive and is sharply peaked around a wave vector separate from those characterizing the antiferromagnetic order. The magnetic intensity distribution rather suggests that the mode is associated with a coexisting antiferro-quadrupolar order parameter, which has long remained "hidden" to the neutron-scattering probes. The mode energy increases continuously below the onset temperature for antiferromagnetism, in parallel to the opening of a nearly isotropic spin gap throughout the Brillouin zone. These attributes bear strong similarity to those of the resonant modes in unconventional superconductors, indicating the dominance of itinerant spin dynamics in the ordered low-temperature phases of CeB_6.

TT 3.4 Mon 10:15 H 3005

Lattice dynamical Properties of the non-centrosymmetric Superconductor $CePt_3Si$ — •Sven Krannich[1], Frank Weber[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Daniel Lamago[1,2], Ludwig Klam[3], Dirk Manske[4], and Hilbert von Löhneysen[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA-Saclay, Gif sur Yvette Cedex, France — [3]ETH Zürich, Institute for Theoretical Physics, Zürich, Switzerland — [4]Max Planck Institute for Solid State Research, Department Metzner, Stuttgart, Germany — [5]Karlsruhe Institute of Technology, Physics Institute, Karlsruhe, Germany

The order parameter of superconductors is usually classified as either a spin singlet (even parity) or a spin triplet (odd parity) by the Pauli exclusion principle. A necessary prerequisite for such a classification is, however, the existence of an inversion center. Something of a stir has been caused by the discovery of bulk superconductivity in $CePt_3Si$ which lacks inversion symmetry. In such systems the existence of an antisymmetric potential gradient causes a parity-breaking antisymmetric spin-orbit coupling (ASOC) that leads to a splitting of the Fermi surface and, moreover, gives rise to the unique possibility of having admixtures of spin-singlet and spin-triplet pairing states. Model calculations including ASOC predict anomalous lattice dynamics even in the non-superconducting state. Here we report on first measurements of the phonon dispersion using inelastic neutron scattering at T= 10 K. Experimental results are compared to DFT calculations including the Ce 4f electrons.

TT 3.5 Mon 10:30 H 3005

Resistivity, specific heat, and pressure dependent magnetization of multiple-transition antiferromagnet $CeAu_2Ge_2$ — •Chien-Lung Huang[1,2], Veronika Fritsch[1], Wolfram Kittler[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76031 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

The resistivity and specific heat of a $CeAu_2Ge_2$ single crystal grown from Au-Ge flux were measured between 1.8 and 200 K. Two transitions were observed in the specific heat at 11.5 and 14.5 K, confirming our recent susceptibility results[1]. We observe three field-induced transitions in the magnetoresistance measured at 1.6 K in accordance with the $B-T$ phase diagram constructed from magnetization. In addition, we have measured the magnetization under pressure. The antiferromagnetic transition temperature T_N is linearly enhanced by pressure with a small rate of 0.067 K/kbar, which suggests that, if attributed to a pure volume effect, this compound is close to the maximum transition temperature of the Doniach phase diagram. The transition fields B_M between the field-induced phases increase linearly upon applying pressure. The comparable Grüneisen parameters of T_N and B_M indicate that the energy scale depending on the sample's volume is determined by the antiferromagnetic correlations.

[1] V. Fritsch, P. Pfundstein, P. Schweiss, E. Kampert, B. Pilawa, and H. v. Löhneysen, Phys. Rev. B 84, 104446 (2011).

TT 3.6 Mon 10:45 H 3005

Superconductivity in an intermediate valence Ce compound with a quasi-two-dimensional structure — •Thomas Gruner[1], Miss. Anupam[2], Zakir Hossain[2], and Christoph Geibel[1] — [1]MPI for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics, IIT Kanpur, 208016, Kanpur, India

Binary rare earth - transition metal metallographic phase diagrams show a large immiscibility gap for early transition metals (i.e. from the left side of the periodic table). As a result, no binary compound forms

and only very few ternary compounds have been reported. Among them $CeRe_4Si_2$ presents an interesting structure: a stacking of Re_2Si and Ce layers results in a quasi-two-dimensional character. The preparation of this compound is challenging because of the high melting point of Re (3180 °C) and the fact that $CeRe_4Si_2$ likely forms in a solid-state reaction. We developed an appropriate synthesis process and obtained almost phase pure polycrystalline samples. Results of electrical resistivity, magnetic susceptibility and specific heat measurements show that Ce is in an intermediate valence state and that the compound becomes superconducting below $T_c \approx 3.2$ K. $CeRe_4Si_2$ is thus one of the very few intermediate valence Ce-based superconductors. The properties of this superconducting state will be discussed.

TT 3.7 Mon 11:00 H 3005

Shubnikov-de Haas Oscillations in $LuRh_2Si_2$ — •Sven Friedemann[1], Swee K Goh[1], F Malte Grosche[1], Zachary Fisk[2], Michael Sutherland[1], Patrick Rourke[3], and Gertrud Zwicknagl[4] — [1]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, CB3 0HE Cambridge, United Kingdom — [2]Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575, USA — [3]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, UK — [4]Institute for Mathematical Physics, TU Braunschweig, Mendelssohnstrasse 3, 38106 Braunschweig, Germany

We present measurements of the Shubnikov-de Haas effect on $LuRh_2Si_2$ in conjunction with electronic band structure calculations. These electronic structure investigations can help understand the peculiar temperature dependence of the Hall effect. In addition, $LuRh_2Si_2$ represents the non-magnetic reference compound to $YbRh_2Si_2$, a prototypical heavy-fermion system featuring an unconventional quantum critical point. In $YbRh_2Si_2$, an orbitally selective Mott transition occurs from a large Fermi surface configuration including f electrons to a small configuration with conduction electrons only. $LuRh_2Si_2$ resembles the small Fermi surface configuration of $YbRh_2Si_2$. We detect oscillations of the resistivity with a large number of frequencies and discuss the angular dependency. We compare the detected orbits with those predicted for the three sheets by band structure calculations and discuss implications for the interpretation of quantum oscillation measurements on $YbRh_2Si_2$.

15 min. break.

TT 3.8 Mon 11:30 H 3005

Ferromagnetic correlations in Yb based heavy fermions probed by NMR relaxation: $YbNi_4P_2$ vs. $Yb(Rh,Ir)_2Si_2$ — •M. Baenitz, R. Sarkar, P. Khuntia, C. Krellner, C. Geibel, and F. Steglich — Max - Planck Institute of Chemical Physics of Solids, 01187 Dresden, Germany.

Intersite correlations in Ce-based heavy fermion systems close to the quantum critical point separating the magnetic ordered state from the paramagnetic Kondo lattice are in almost all cases predominantly antiferromagnetic (AFM) in nature. The NMR relaxation of these systems show an evolution from localized fluctuations with $1/T_1$ nearly constant above the Kondo temperature T_K, to a linear in T Korringa- like behavior with a constant and enhanced $(1/T_1T)$- value below T_K. We report on ^{31}P-NMR results on the ferromagnetic (FM) quantum critical system $YbNi_4P_2$ over a wide range in temperature (2-300 K) and field (0.2 - 9 T). Here, $^{31}(1/T_1T)(T)$ does not show such a signature at T_K, instead a continuous increase of $(1/T_1T)$ down to lowest T is observed. A similar behavior has been reported for $YbRh_2Si_2$, which also exhibits strong FM correlations evidenced by ^{29}Si - NMR and an enhanced Wilson ratio. Furthermore, in CeFePO, which is likely unique among Ce-based quantum critical system because of its strong FM correlations, $(1/T_1T)$ also diverges continuously for $T \longrightarrow 0$. This suggests that the difference in the relaxation between most of the Ce systems and the Yb systems is predominantly related to a change from AFM to FM intersite correlations. NMR-results (shift, line width, T_1) are analyzed and discussed in diffrent models (Korringa, Moriya).

TT 3.9 Mon 11:45 H 3005

High-field thermoelectric transport in $YbRh_2Si_2$ — R. Daou, •H. Pfau, M. Brando, C. Krellner, C. Geibel, and F. Steglich — MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany

The heavy fermion compound $YbRh_2Si_2$ has attracted much interest providing an example of an unconventional quantum critical point that can be approached using very small magnetic fields. However, there are also anomalous features at higher fields that have not been well explored, and these may give us further insights into the electronic state of this unusual material. We report thermopower measurements on the best available single crystals of $YbRh_2Si_2$ at temperatures down to 0.1 K and magnetic fields up to 12 T applied along the ab-plane. We find two step-like features in the field dependence at 9 T and 11 T, the region where a suppression of the heavy fermion state was reported [1]. Additionally, another step appears at 3.5 T. These steps in thermopower correspond to features found in electrical transport [2]. The experimental results are supported by recently published renormalized bandstructure calculations [3] which show two features in the field dependent quasiparticle density of states at around 4 T and at 10 T. In these calculation, the anomalies at 10T in various quantities are caused by a van-Hove-type singularity below the Fermi energy. However, the separation into two features in thermopower and in resistivity remains unexplained as well as the origin of the clear 3.5 T-signature.

[1] P. Gegenwart et al., New. J. Phys. **8**, 171 (2006).
[2] HR. Naren et al., *This conference*.
[3] G. Zwicknagl, J. Phys.: Condens. Matter **23**, 094215 (2011).

TT 3.10 Mon 12:00 H 3005

High-field study of the heavy-fermion material URu_2Si_2 — •Gernot Werner Scheerer[1], William Knafo[1], Dai Aoki[2], Geraldine Ballon[1], Cyril Jaudet[1], Alain Mari[3], Cyril Proust[1], David Vignolles[1], and Jacques Flouquet[2] — [1]Laboratoire National des Champs Magnétiques Intenses, UPR 3228, CNRS- UJF-UPS-INSA, Toulouse, France — [2]Institut Nanosciences et Cryogénie, SPSMS, CEA-Grenoble, France — [3]Laboratoire de Chimie de Coordination, Toulouse, France

URu_2Si_2 is known for its "hidden-order" state below T_0=17.5 K, where the order parameter is still not identified [1]. A magnetic field along the **c**-axis induces a cascade of low-temperature phase transitions between 35 and 39 T from the "hidden order" to a polarized paramagnetic state. We have performed electrical transport and magnetization measurements in pulsed magnetic fields on ultra clean URu_2Si_2 samples. We established the H-T-phase diagram for $\mathbf{H} \parallel c$ in extended scales up to 60 T and 60 K. The vanishing of a high-temperature crossover at around 40-50 K, presumably related to intersite electronic correlations, precedes the polarization of the magnetic moments, as well as the destabilization of the "hidden-order" phase. Strongly sample-quality dependent magnetoresistivity confirms the Fermi surface reconstructions in a high magnetic field along **c** and at T_0 [2,3]. Shubnikov-de Haas quantum oscillations will also be presented.

[1] J. A. Mydosh and P. M. Oppeneer, arXiv:1107.0258
[2] E. Hassinger et al.: Phys. Rev. Lett. **105** (2010) 216409
[3] M.M. Altarawneh et al.: Phys. Rev. Lett. **106** (2011) 146403

TT 3.11 Mon 12:15 H 3005

Fermi surface and magnetic order in UPt_2Si_2 — •Zübeyir Cakir and Gertrud Zwicknagl — Institut f. Mathemat. Physik, TU Braunschweig, Germany

U intermetallic compounds exhibit highly complex phase diagrams at low temperatures with unusual and often enigmatic orders. The high sensitivity with respect to variations in external parameters like pressure or magnetic field reflect the strong correlations within the U 5f-shell. The present contribution focusses on the tetragonal compound UPt_2Si_2. We calculate the magnetic-field dependence of the Fermi surface for itinerant and partially localized U 5f-electrons and discuss consequences for field-induced instabilities.

TT 3.12 Mon 12:30 H 3005

Finite-temperature spectra and quasiparticle interference in Kondo lattices: From light electrons to coherent heavy quasiparticles — •Adel Benlagra[1], Thomas Pruschke[2], and Matthias Vojta[1] — [1]Institut für theoretische physik, TU Dresden, Germany — [2]Institut für theoretische physik, Universität Göttingen, Germany

Recent advances in scanning tunneling spectroscopy performed on heavy-fermion metals provide a window onto local electronic properties of composite heavy-electron quasiparticles. Here we theoretically investigate the energy and temperature evolution of single-particle spectra and their quasi- particle interference caused by point-like impurities in the framework of a periodic Anderson model. By numerically solving dynamical-mean-field-theory equations, we are able to access all temperatures and to capture the crossover from weakly interacting c and f electrons to fully coherent heavy quasiparticles. Remarkably, this crossover occurs in a dynamical fashion at an energy-dependent

crossover temperature. We study in detail the associated Fermi-surface reconstruction and characterize the incoherent regime near the Kondo temperature. Finally, we link our results to current heavy-fermion experiments.

TT 3.13 Mon 12:45 H 3005

Metamagnetism and Lifshitz transitions in models for heavy fermions — •Martin Bercx and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg

We investigate metamagnetic transitions in models for heavy fermions by considering the metallic Kondo lattice model in two dimensions. Results are obtained within the framework of dynamical mean field and dynamical cluster approximation. Universal magnetization curves for different temperatures and Kondo couplings develop upon scaling with the lattice coherence temperature. Furthermore, the coupling of the local moments to the magnetic field is varied so as to take into account the different g-factors between localized and itinerant electrons. Competition between lattice coherence scale and Zeeman energy scale allow for two interpretations of the metamagnetism in heavy fermions: Kondo breakdown or Lifshitz transitions. By tracking the single particle residue through the transition and showing that it does not vanish at the transition, we can uniquely conclude in favour of the Lifshitz transition scenario.

TT 3.14 Mon 13:00 H 3005

Ring Exchange Periodic Anderson Model for Bilayer ^{3}He — •Jan Werner and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Deutschland

A unique feature of experiments on bilayer ^{3}He[1] is that the second layer starts growing before the first solidifies. The fermions in the first layer close to solidification are thus slow, whereas the fermions in the second layer are light. This combination of slow and light fermions which can hybridize with each other is the basic ingredient of the Anderson model, and the experiment has been interpreted in terms of heavy fermion physics. However in contrast to the Anderson model, magnetism in the 3He first layer is dominated by three body ring exchange. We present a simple model, which captures all above features, including an independent scale for the ring exchange and the strict constraint of no double occupancy in the first layer. We solve this model using CDMFT with a hybridization expansion CT-QMC algorithm as impurity solver. Our results show remarkable similarities with the experiments: a suppression of the coherence temperature upon approaching the solidification point of the first layer accompanied by the onset of ferromagnetic correlations within the first layer.

[1] M. Neumann, J. Nyeki, B. Cowan, und J. Saunders, Science 317, 1356 (2007)

TT 4: Transport: Topological Insulators 1 (jointly with HL and MA)

Time: Monday 9:30–13:00 Location: H 3010

TT 4.1 Mon 9:30 H 3010

Quantum point contact as a probe of a topological superconductor — •Michael Wimmer, Anton Akhmerov, Jan Dahlhaus, and Carlo Beenakker — Instituut-Lorentz, Universiteit Leiden, The Netherlands

We calculate the conductance of a ballistic point contact to a superconducting wire, produced by the s-wave proximity effect in a semiconductor with spin-orbit coupling in a parallel magnetic field. The conductance G as a function of contact width or Fermi energy shows plateaus at half-integer multiples of $4e^2/h$ if the superconductor is in a topologically nontrivial phase, supporting Majorana fermions. In contrast, the plateaus are at the usual integer multiples in the topologically trivial phase (without Majorana fermions). Disorder destroys all plateaus except the first, which remains precisely quantized, consistent with previous results for a tunnel contact. The advantage of a ballistic contact over a tunnel contact as a probe of the topological phase is the strongly reduced sensitivity to

TT 4.2 Mon 9:45 H 3010

Interaction and trapping effects on a 2D topological insulator in an optical lattice. — •Daniel Cocks[1], Peter P. Orth[2], Michael Buchhold[1], Stephan Rachel[3], Karyn Le Hur[4,3], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie — [3]Department of Physics, Yale University, New Haven — [4]Center for Theoretical Physics, École Polytechnique, Palaiseau

We investigate effects of interaction, disorder and trapping of a 2D system that exhibits topologically insulating phases in an optical square lattice using both real-space dynamical mean-field theory (R-DMFT) and analytical techniques. The tunability of this system allows for a large degree of freedom, and by adjusting the size of the magnetic unit cell, along with the strength of a spin-orbit coupling that does not preserve the S_z spin component and a staggered super-lattice potential, topologically non-trivial regions have been identified.

Using R-DMFT, we determine the interacting phase diagram as a function of Hubbard U. We observe interaction driven transitions between the topological and normal insulating phase, as well as dependence of transitions to magnetically ordered phases on the flux parameter. We also analyze trapping effects that are relevant to experimental conditions and identify ideal trapping potentials that preserve the topological phases. This system is realizable (Goldman et al. PRL 105, 255302, 2010) as an effective Hamiltonian by generating a synthetic non-Abelian gauge field on the surface of an atom chip.

TT 4.3 Mon 10:00 H 3010

Phonon induced backscattering in helical edge states — •Patrik Recher[1], Jan C. Budich[2], Fabrizio Dolcini[3], and Bjoern Trauzettel[2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [3]Dipartimento di Fisica del Politecnico di Torino, I-10129 Torino, Italy

A single pair of helical edge states as realized at the boundary of a quantum spin Hall insulator is known to be robust against elastic single particle backscattering as long as time reversal symmetry is preserved. However, there is no symmetry preventing inelastic backscattering as brought about by phonons in the presence of Rashba spin orbit coupling. In this talk, we show that the quantized conductivity of a single channel of helical Dirac electrons is protected even against this inelastic mechanism to leading order. We further demonstrate that this result remains valid even when Coulomb interaction is included in the framework of a helical Tomonaga Luttinger liquid.

TT 4.4 Mon 10:15 H 3010

Electromagnetically induced topological charge on the surface of a topological insulator due to magnetization dynamics — •Flavio Nogueira and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany

A topologically non-trivial solution of the Landau-Lifshitz-Gilbert equation is obtained. Such a solution induces electric and magnetic fields and implies a topological current at the surface of a topological insulator which is proportional to $\mathbf{E}\cdot\mathbf{B}$. The values of the topological charge in our solution are $Q=-1,0,1$. The spin current density plays in this scenario the role of a non-Abelian gauge field and the topological charge is reminiscent of the 't Hooft-Polyakov construction of the magnetic monopole. We discuss the physical consequences of our theory, including the role of topological spin transport on the surface of a topological insulator.

TT 4.5 Mon 10:30 H 3010

Interplay of bulk and edge states in transport of topological insulators — •Rolf W. Reinthaler and Ewelina M. Hankiewicz — Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

We study ballistic transport in two-terminal metal/quantum spin-Hall insulator (QSHI)/metal junctions within the effective four band model (conduction/heavy hole bands) [1, 2]. We show that the conductance signals originating from the bulk and the edge contributions are not additive. While for a long junction the transport is determined by the

edge states contribution, for a short junction, the conductance signal is built from both, bulk and edge states, in the ratio which depends on the width of the sample. Further, the conductance for short junctions shows a non-monotonic behavior as a function of the sample lenght in topological insulator regime [3]. Suprisingly this non-monotonic behavior of conductance can be traced to the formation of an effectively propagating solution which is robust against scalar disorder. Our predictions should be experimentally verifiable in HgTe QWs and BiSe thin films.

We acknowledge the financial support of the German DFG Grant HA5893/1-2 .

[1] B. A. Bernevig et al., Science, 314(5806):1757, 2006.
[2] D G Rothe et al., New Journal of Physics, 12(6):065012, 2010.
[3] E. G. Novik et al., Phys. Rev. B, 81(24):241303, 2010.

TT 4.6 Mon 10:45 H 3010

Landau levels in a topological insulator — •Peter Schwab and Michael Dzierzawa — Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Two recent experiments successfully observed Landau levels in the tunneling spectra of the topological insulator Bi_2Se_3. To mimic the influence of a scanning tunneling microscope tip on the Landau levels we solve the two-dimensional Dirac equation in the presence of a localized electrostatic potential. We find [1] that the STM tip not only shifts the Landau levels, but also suppresses for a realistic choice of parameters the negative branch of Landau levels.

[1] P. Schwab and M. Dzierzawa, arXiv:1107.0827

TT 4.7 Mon 11:00 H 3010

Surface flat bands in gapless topological phases — •Andreas Schnyder — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

In this talk we discuss a classification of Fermi surfaces, Fermi lines and Fermi points, as well as nodal lines and nodal points in superconductors in terms of discrete symmetries and Fermi surface codimension. By use of a bulk-boundary correspondence, we determine the types of topologically protected zero-energy states that appear at the boundary of these gapless topological systems. As concrete examples we examine the polar state of 3He, the nodal non-centrosymmetric superconductor Li2Pt3B, and the ferromagnetic superconductor URhGe. For the latter two systems, we examine the signatures of the protected surface states in tunneling-conductance measurements and in Fourier transformed scanning tunneling spectra. Furthermore, we study the appearance of gapless modes located on topological defects in gapless topological phases.

15 min. break.

TT 4.8 Mon 11:30 H 3010

Weak antilocalization in HgTe quantum wells and topological surface states: Massive versus massless Dirac fermions — •Ewelina Hankiewicz and Grigory Tkachov — Wuerzburg University

HgTe quantum wells and surfaces of three-dimensional topological insulators support Dirac fermions with a single-valley band dispersion. In this work we conduct a comparative theoretical study of the weak antilocalization in HgTe quantum wells (QWs) and topological surface states. The difference between these two single-valley systems comes from a finite band gap (effective Dirac mass) in HgTe quantum wells in contrast to gapless (massless) surface states in topological insulators. The finite effective Dirac mass implies a broken internal symmetry, leading to suppression of the weak antilocalization in HgTe quantum wells and transition to the weak localization regime as a function of the gap or carrier density. Further we show how the difference in the behavior of the weak localization corrections for HgTe QWs allows to distinguish topological versus normal insulators. On the other hand, the topological surface states exhibit specific weak-antilocalization magnetoconductivity in a parallel magnetic field due to their exponential decay in the bulk. The relevant experiments will be discussed.

We acknowledge the financial support of the German DFG Grant HA5893/1-2 .

TT 4.9 Mon 11:45 H 3010

Coulomb blockade signatures of the topological phase transition in semiconductor-superconductor nanowires — •Björn Zocher[1,2], Mats Horsdal[1,3], and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Max Planck Institut für Mathematik in den Naturwissenschaften, Leipzig, Germany — [3]Max Planck Institut für Festkörperforschung, Stuttgart, Germany

In semiconductor-superconductor hybrid structures a topological phase transition is expected as a function of chemical potential or magnetic field strength. We show that signatures of this transition can be observed in nonlinear Coulomb blockaded transport through a ring shaped structure. In particular, for a fixed electron parity of the ring, the flux periodicity of the neutral excitation spectrum changes from the usual $h/2e$-periodicity to a characteristic h/e-periodicity when tuning the system from the topologically trivial to the nontrivial phase. We relate the h/e-periodicity to the recently predicted 4π-periodicity of the Josephson current across a junction formed by two topological superconductors.

TT 4.10 Mon 12:00 H 3010

Tuning the Fermi velocity of Dirac cones: Towards an anomalous quantum Hall effect on the surfaces of topological insulators? — •Lars Fritz, Matthias Sitte, and Achim Rosch — Universität zu Köln, Institut für theoretische Physik, Zülpicher Strasse 77, 50937 Köln

Long-range Coulomb interaction can trigger an instability of two-dimensional Dirac fermions, the so-called chiral symmetry breaking. Three-dimensional topological insulators host two-dimensional helical Dirac fermions on their surfaces. We investigate whether long-range Coulomb interaction, controlled by the dimensionless coupling constant $\alpha = e^2/(\hbar\epsilon_r\epsilon_0 v_F)$, can induce surface ferromagnetism thereby gapping the surface metal. This is accompanied by an anomalous quantum Hall effect *without* explicit breaking of time-reversal invariance by an external magnetic field. We find that the prerequisite for observing this effect is to reduce the Fermi velocity v_F of the surface Dirac fermions while keeping the bulk dielectric constant ϵ_r finite. We discuss under which conditions this can be achieved.

TT 4.11 Mon 12:15 H 3010

Supersymmetry and Ballistic Transport in Topological Insulators with Ferromagnetic Domain-walls — •Christian Wickles and Wolfgang Belzig — Universität Konstanz, Fachbereich Physik, 78457 Konstanz, Germany

We consider the surface Dirac Fermions of a topological insulator with a proximity induced ferromagnetic domain wall (DW). We present an exact analytical treatment to discuss the spectrum, bound states and the ballistic conductance of the system with a DW in the in-plane and out-of-plane configuration. In the latter case of the "mass" DW, we find oscillations in the conducatance as a function of the wall width and we find for certain widths the DW to be completely reflectionless. We will use the language of supersymmetry to reveal that the dispersion of the surface Dirac Fermions together with the specific DW profile gives rise to these interesting features.

TT 4.12 Mon 12:30 H 3010

Aspects of electron-electron interactions and spin-conservation in topological insulators — •Stephan Rachel — Department of Physics, Yale University, New Haven, CT 06520, USA

We consider topological insulators on the honeycomb lattice and investigate the effect of electron-electron interactions and breaking of S_z spin-symmetry. We compare (i) non-interacting bandstructures with and without conserved spin, (ii) the regime of moderate interactions as well as (iii) the corresponding spin models. We find in all interaction-regimes qualitative differences between conserved and broken S_z spin-symmetry. The origin of these differences is explained. Eventually we discuss which of the effects are generic and which are specific for the honeycomb lattice.

TT 4.13 Mon 12:45 H 3010

Luttinger Liquid Physics and Spin-Flip Scattering on Helical Edges — •Martin Hohenadler and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Deutschland

We investigate electronic correlation effects on edge states of quantum spin Hall insulators within the Kane-Mele-Hubbard model by means of quantum Monte Carlo simulations. In accordance with Luttinger liquid theory, we find dominant transverse spin fluctuations with an interaction dependent power law and the expected doping dependence.

For strong electronic correlations, bulk states become important, and high-energy spectral features beyond Luttinger liquid theory emerge. Inelastic spin-flip scattering leads to graphene-like edge state signatures, and transfers spectral weight from low to high energies causing a suppression of charge transport.

TT 5: Transport: Quantum Coherence and Quantum Information Systems 1 (jointly with MA and HL)

Time: Monday 9:30–12:45 Location: BH 243

TT 5.1 Mon 9:30 BH 243

Coherence in a transmon qubit with epitaxial tunnel junctions — •Martin Weides[1,4], Jeffrey Kline[1], Michael Vissers[1], Martin Sandberg[1], David Wisbey[1,2], Blake Johnson[3], Thomas Ohki[3], and David Pappas[1] — [1]National Institute of Standards and Technology, Boulder, Colorado 80305, USA — [2]Saint Louis University, St. Louis, Missouri 63103, USA — [3]Raytheon BBN Technologies, Cambridge, Massachusetts 02138, USA — [4]Karlsruhe Institute of Technology, Germany

Transmon qubits based on epitaxial tunnel junctions and interdigitated capacitors were developed. This multileveled qubit, patterned by use of all-optical lithography, is a step towards scalable qubits with a high integration density. The relaxation time T_1 is $.72-.86$ μsec and the ensemble dephasing time T_2^* is slightly larger than T_1. The dephasing time T_2 (1.36 μsec) is nearly energy-relaxation-limited. Qubit spectroscopy yields weaker level splitting than observed in qubits with amorphous barriers in equivalent-size junctions. The qubit's inferred microwave loss closely matches the weighted losses of the individual elements (junction, wiring dielectric, and interdigitated capacitor), determined by independent resonator measurements.

TT 5.2 Mon 9:45 BH 243

Single atom lasing of a dressed flux qubit — •Gregor Oelsner[1], Pascal Macha[1], Miroslav Grajcar[2], Oleg Astafiev[3], Boris Ivanov[1], Evgeni Il'ichev[1], Uwe Hübner[1], Solveig Anders[1], and Hans-Georg Meyer[1] — [1]Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany — [2]Department of Solid State Physics, Comenius University, SK-84248 Bratislava, Slovakia — [3]NEC Nano Electronics Research Laboratories. Tsukuba, Ibaraki, 305-8501, Japan

We study a strongly driven superconducting flux qubit coupled to a high-quality coplanar waveguide resonator. In the frame of the dressed state approach, the energy of the Rabi splitting depends on the amplitude of the microwave field and the detuning between the qubit and the microwave frequency, which also controls the level occupation. If, for a certain detuning and amplitude, this splitting is in resonance with the fundamental mode of the resonator, a lasing (damping) effect is expected. Indeed we experimentally observe an increase in the transmission amplitude as well as line width narrowing, which proofs the predicted phenomena.

TT 5.3 Mon 10:00 BH 243

Gradiometric persistent current flux qubit with tunable tunnel coupling — •Manuel Johannes Schwarz[1,2], Jan Goetz[1,2], Zhaohai Jiang[1,2], Frank Deppe[1,2], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching — [2]Physik Department, TU München, Garching

The persistent current flux qubit is a Josephson junction based superconducting circuit exhibiting strong anharmonicity and excellent coherence time of more than 10 μs. However, quantum coherence deteriorates drastically away from an optimal operation point. Moreover, a controlled adjustment of the transition frequency at the optimal point requires excellent stability of the fabrication process. Here, we present the spectroscopic analysis of a gradiometric flux qubit, where the minimal transition frequency, the qubit gap, can be tuned in situ while staying at the point of optimal coherence. We show a tunability of the qubit gap from a few hundreds of megahertz to several gigahertz, making the system suitable for future experiments with coupled qubit-resonator systems.

This work is supported by the DFG via SFB 631 and by the German Excellence Initiative via NIM.

TT 5.4 Mon 10:15 BH 243

Four-level lasing in the two-qubit system — •Sergey Shevchenko[1,2], Simon van der Ploeg[2], Miroslav Grajcar[2,3], Evgeniy Temchenko[1], Alexandr Omelyanchouk[1], Evgeniy Il'ichev[2], and Hans-Georg Meyer[2] — [1]Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine — [2]Institute of Photonic Technology, Jena, Germany — [3]Comenius University, Bratislava, Slovakia

The system of two coupled qubits can be described as a quantum four-level system. To make it useful for applications, e.g. for lasing, the hierarchy of relaxation times is needed. Such a situation occurs naturally in a case of two coupled superconducting qubits [1]. We have studied both experimentally and theoretically resonant excitation and relaxation in this system [1,2]. Two types of the multi-photon transitions were demonstrated: the direct and the ladder-type ones. This can be used for the creation of the inverse population, which was discussed in relation to the possibility of three- and four-level lasing in the system [2].

[1] E. Il'ichev, S.N. Shevchenko, S.H.W. van der Ploeg, M. Grajcar, E.A. Temchenko, A.N. Omelyanchouk, and H.-G. Meyer, Phys. Rev. B 81, 012506 (2010).
[2] E. A. Temchenko, S. N. Shevchenko, A. N. Omelyanchouk, Phys. Rev. B 83, 144507 (2011).

TT 5.5 Mon 10:30 BH 243

Observation of the Geometric Phase of a Harmonic Oscillator in Circuit Quantum Electrodynamics — •Stefan Filipp, Marek Pechal, Simon Berger, Abdufarrukh A. Abdumalikov, and Andreas Wallraff — ETH Zurich, Department of Physics, 8093 Zurich, Switzerland

Transporting a quantum harmonic oscillator state along a closed path in Hilbert space leads to a path-dependent geometric phase. However, the linearity of the system precludes its observation without a nonlinear quantum probe. We therefore make use of a superconducting qubit serving as an interferometer to measure the geometric phase of a harmonic oscillator realized as an on-chip transmission line resonator [1]. We demonstrate the proportionality of the geometric phase to the enclosed area for a variety of path shapes. At the transition to the non-adiabatic regime, we analyze corrections to the geometric phase and show how entanglement between the two-level system and the harmonic oscillator leads to dephasing. This system provides a versatile tool to study adiabatic and non-adiabatic geometric phases in open quantum systems and as a resource for quantum information processing.

[1] M. Pechal, S. Berger, A.A. Abdumalikov, A. Wallraff and S. Filipp, arxiv:1109.1157 [quant-ph] (2011)

TT 5.6 Mon 10:45 BH 243

High cooperativity in a microwave resonator coupled to YIG — Hans Huebl[1], •Johannes Lotze[1], Christoph Zollitsch[1,2], Fredrik Hocke[1], Sebastian T. B. Goennenwein[1], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

Understanding the coupling of magnetic moments (spins) to light fields (photons) on a quantum level is of fundamental interest. Recent work [1,2] on paramagnetic samples coupled to superconducting resonators has shown coherent coupling between microwave photons and electron spins. This coupling is enhanced compared to a single spin by a factor of $\sqrt{N}$, where N is the number of spins in the ensemble. Here, we study a bulk ferrimagnetic Ga-doped yttrium iron garnet (YIG) crystal coupled to a superconducting niobium resonator operating at 6 GHz. Measuring the transmission through the resonator in a magnetic field, we observe an anticrossing of the spin and photon dispersions with a splitting of 450 MHz. Analyzing the magnetic field dependence of the resonance linewidths in this system in the interaction regime, we find that the coupling clearly dominates the intrinsic loss rates of the

spin system and the resonator, an important requirement for studying the magnon-photon interaction in the strong coupling regime. The impact of microwave power and system temperature will be critically discussed.
[1] D. I. Schuster *et al.*, Phys. Rev. Lett. **105**, 140501 (2010)
[2] Y. Kubo *et al.*, Phys. Rev. Lett. **105**, 140502 (2010)

15 min. break.

TT 5.7 Mon 11:15 BH 243

Measurement scheme for the Lamb shift in a superconducting circuit with broadband environment — •Vera Gramich[1], Paolo Solinas[2,3], Mikko Möttönen[2,3], Jukka Pekola[3], and Joachim Ankerhold[1] — [1]Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Department of Applied Physics/COMP, Aalto University, P.O. Box 14100, FI-00076 Aalto, Finland — [3]Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 Aalto, Finland

Motivated by recent experiments on quantum mechanical charge pumping in a Cooper pair sluice [1], we present a measurement scheme for observing shifts of transition frequencies in two-level quantum systems induced by broadband environmental fluctuations. In contrast to quantum optical and related setups based on cavities, the impact of a thermal phase reservoir is considered. The experimental protocol to measure the Lamb shift in experimentally feasible superconducting circuits is analyzed in detail and supported by numerical simulations [2]. Therefore, we turn our attention to a brief description of the actual setup followed by an analysis of the detection proposal.
[1] A. O. Niskanen, J. P. Pekola, and H. Seppä, Phys. Rev. Lett. 91, 177003 (2003).
[2] V. Gramich, P. Solinas, M. Möttönen, J. P. Pekola, and J. Ankerhold, Phys. Rev. A 84, 052103 (2011).

TT 5.8 Mon 11:30 BH 243

Lasing, trapping states, and multistability in circuit quantum electrodynamical analog of a single-atom injection maser — •Michael Marthaler[1], Juha Leppäkangas[1,2], and Jared Cole[1,3] — [1]Institut für Theoretische Festkörperphysik and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Applied Quantum Physics Laboratory, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden — [3]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne 3001, Australia

We study a superconducting single-electron transistor (SSET) which is coupled to a LC oscillator via the phase difference across one of the Josephson junctions. This leads to a strongly anharmonic coupling between the SSET and the oscillator. The coupling can oscillate with the number of photons, which makes this system very similar to the single-atom injection maser. However, the advantage of a design based on superconducting circuits is the strong coupling and existence of standard methods to measure the radiation field in the oscillator. This makes it possible to study many effects that have been predicted for the single-atom injection maser in a circuit quantum electrodynamics setup.

TT 5.9 Mon 11:45 BH 243

Towards photon quantum gates in circuit qed — •Lukas Neumeier, Martin Leib, and Michael Hartmann — TU München, Munich,Germany

Quantum information processing can be decomposed into quantum channels and quantum gates. Photons are well suited for transferring information whereas stationary qubits offer better perspectives for implementing gates. Traditionally in circuit qed quantum gates are therefore realized by interactions between stationary superconducting qubits. As opposed to this we analyze a circuit qed setup where itinerant microwave photons, confined to two one dimensional transmission-lines, interact at a localized superconducting qubit. We provide results for reflection and transmission spectra and photon measurement probabilities for both waveguides which depend on the incoming single or two-photon pulses.

TT 5.10 Mon 12:00 BH 243

Bose-Hubbard dynamics in a chain of nonlinear superconducting transmission-line resonators — •Martin Leib and Michael J. Hartmann — TU München,Munich,Germany

Quantum mechanical many body physics offers many interesting phenomena and its simulation in well controlable experimental setups is therefore attracting increasing attention. We propose a superconducting circuit setup where microwave photons in an array of transmission line resonators interact due to an intrinsic nonlinearity of the resonators. We show that a transmission line resonator which is intersected by a Josephson junction can be approximatly described as a harmonic oscillator with a Kerr nonlinearity, making the whole array of resonators a quantum simulator for a Bose-Hubbard Hamiltonian. Strong nonlinearities and long coherence times can be easily achieved in superconducting circuits and in addition individual readout and control of resonators can be realized with current state of the art experimental techniques.

TT 5.11 Mon 12:15 BH 243

Backaction of Microwave Photon Detection by a Strongly Coupled Josephson Junction — •Emily Pritchett[1], Luke Govia[2], Seth Merkel[3], and Frank Wilhelm[1] — [1]Saarland University, Saarbrucken, Deutschland — [2]University of Waterloo, Waterloo, Canada — [3]IBM Watson Research Center, Yorktown Heights, USA

We analyze the functionality of on-chip Josephson junctions as single microwave photon detectors, as has been demonstrated recently [1]. The Josephson junction device, which we refer to as a Josephson Photomultiplier (JPM), acts as a nearly perfect binary detectors of microwave photons by undergoing an observable switching event when there are one or more photons in an incident cavity. We analyze the backaction of this switching event on the state of incident light, including the energy dissipation and dephasing affecting an imperfect JPM. This analysis improves the efficiency and fidelity with which a JPM reconstructs the state of light in an incident transmission line 'cavity', which are commonly used to store and transfer quantum states in implementations of circuit-QED.
[1] Chen et al., arXiv:1011.4329

TT 5.12 Mon 12:30 BH 243

Time-resolved qubit readout via nonlinear Josephson inductance — •Georg Michael Reuther[1], Peter Hänggi[1], and Sigmund Kohler[2] — [1]Institut für Physik, Universität Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC) C/Sor Juana Inés de la Cruz 3, Cantoblanco 28049 Madrid, Spain

We propose a generalization of dispersive qubit readout which provides the time evolution of a flux qubit observable. Our proposal relies on the non-linear coupling of the qubit to a harmonic oscillator with high frequency, representing a dc-SQUID. Information about the qubit dynamics is obtained by recording the oscillator response to resonant driving and subsequent lock-in detection. We simulate this measurement process for the example of coherent qubit oscillations and, in doing so, we corroborate the underlying measurement relation. In addition, we derive a quantum master equation for the qubit alone. With this at hand, we investigate the dependence of qubit dephasing on the measurement backaction that is induced by the oscillator driving [1].
[1] Georg M. Reuther, David Zueco, Peter Hänggi, and Sigmund Kohler, New J. Phys. 13, 093022 (2011)

TT 6: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1

Time: Monday 9:30–13:00 Location: BH 334

TT 6.1 Mon 9:30 BH 334

Transport through multiple quantum dots coupled to superconducting leads — •Sebastian Pfaller and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We present a microscopic theory of transport through quantum dot set-ups coupled to superconducting leads. We derive a master equation for the reduced density matrix to lowest order in the tunneling Hamiltonian and focus on quasi-particle tunneling. In particular, we

apply the theory to a quantum double dot with independently gated dots; considering the dots in series as well as in parallel configuration. Negative differential conductance, as well as the expected gap of the Coulomb diamonds proportional to the superconducting gap, are observed. Moreover, a current flows in the Coulomb blockade region due to thermally excited quasiparticles. These thermal excitations can be used to identify transitions through excited states in the "honeycomb" shaped stability diagrams.

TT 6.2 Mon 9:45 BH 334

Geometric phases in adiabatically driven, interacting quantum dots out of equilibrium — •Hernan L. Calvo[1,2], Janine Splettstoesser[1,2], and Maarten R. Wegewijs[1,2,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Geometric phases arise in the quantum state of a system whose parameters are slowly varied along a closed contour, e.g. a quantum dot in a rotating magnetic field. In this work, we present a novel, generally applicable quantum transport theory for adiabatically driven, strongly interacting nanosystems characterized by non-trivial geometric phases in their dynamics. We account exactly for the local many-body interaction and applied non-linear voltages on a general type of quantum dot. We develop a perturbation theory in the tunnel coupling to the electrodes where the crucial ingredient is the time-dependent modulation of both the quantum energies (dynamical phases) as well as the wave functions (inducing geometric phases), both in the quantum dot and / or the reservoirs. We discuss the transport properties of such devices where the experimental signatures of geometric phases appear in the charge and spin pumping induced by the time-dependent parameters.

TT 6.3 Mon 10:00 BH 334

Influence of Coulomb interaction on the Aharonov-Bohm effect in an electronic Fabry-Pérot interferometer — •Stéphane Ngo Dinh[1] and Dmitry Bagrets[2,3] — [1]Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

We study the role of Coulomb interaction in an electronic Fabry-Pérot interferometer (FPI) realized with chiral edge states in the integer quantum Hall regime in the limit of weak backscattering.

Assuming that a compressible Coulomb island in a bulk region of the FPI is formed, we develop a capacitance model which explains the plethora of experimental data on the flux and gate periodicity of conductance oscillations. It is also shown that a suppression of finite-bias visibility stems from a combination of weak Coulomb blockade and a nonequilibrium dephasing by the quantum shot noise.

TT 6.4 Mon 10:15 BH 334

Single-particle interference versus two-particle collisions — •Stefan Juergens[1], Janine Splettstoesser[1], and Michael Moskalets[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [2]Department of Metal and Semic. Physics, NTU "Kharkiv Polytechnical Institute", Ukraine

In mesoscopics the particle- and wave-like nature of the electrons usually appears in separate setups. The discreteness of the charge leads e.g. to the well-known Coulomb blockade effect in quantum dots, while the wave-like behavior of an electron is manifested in the single-particle interference leading to Aharonov-Bohm (AB) oscillations of the current through a ring. Recently, tunable single-electron sources, supplying particles one by one, have been realized in the QHE regime [1]. Here we make use of these sources in order to propose and theoretically discuss a mesoscopic circuit in which the particle- and wave-like nature of electrons can be observed in the same setup. It comprises of two sources emitting particles into a Mach-Zehnder interferometer penetrated by a magnetic flux [2]. We show that when synchronizing the sources, on one hand the time-resolved current always shows an interference pattern, indicating the wave-like behavior of electrons. In contrast, whether the detected charge shows the AB effect depends on the occurrence of collisions between particles, emitted from the two different sources, at the interferometer's output. This ability to collide allows for an interpretation based on the particle nature of electrons.

[1] G. Fève et al, Science 316, 1169 (2007)
[2] S. Juergens, J. Splettstoesser, M. Moskalets, EPL 96, 37011(2011)

TT 6.5 Mon 10:30 BH 334

Finite size effects on transport coefficients for models of atomic wires coupled to phonons — •Christian Bartsch — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig

We consider models of quasi-1-d, planar atomic wires consisting of several, laterally coupled rows of atoms, with mutually non-interacting electrons. This electronic wire system is coupled to phonons, corresponding, e.g., to some substrate. We aim at computing diffusion coefficients in dependence on the wire widths and the lateral coupling. To this end we firstly construct a numerically manageable linear collision term for the dynamics of the electronic occupation numbers by following a certain projection operator approach. By means of this collision term we set up a linear Boltzmann equation. A formula for extracting diffusion coefficients from such Boltzmann equations is given. We find in the regime of a few atomic rows and intermediate lateral coupling a significant and non-trivial dependence of the diffusion coefficient on both, the width and the lateral coupling. These results, in principle, suggest the possible applicability of such atomic wires as electronic devices, such as, e.g., switches.

TT 6.6 Mon 10:45 BH 334

Even-odd effect in the thermopower of superconducting single-electron transistors — •Jens Siewert[1,2] and Christopher Eltschka[3] — [1]Departamento de Química Física, Universidad del País Vasco, 48080 Bilbao, Spain — [2]Ikerbasque, Basque Foundation for Science, 48011 Bilbao, Spain — [3]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We study charge and heat transport in single-electron transistors with a superconducting island and normal-conducting leads (NSN SET). Below a crossover temperature T^* the transport properties of this device depend on the parity of the island charge number, *i.e.*, whether *all* electrons are paired in Cooper pairs or whether there is a single unpaired electron [1]. While this effect has been described for the current-voltage characteristics of NSN SET, we show that even-odd effects manifest themselves also in the thermopower. Our results can be understood by applying an idea due to Matveev [2]. A particularly interesting finding is that the thermoelectric efficiency ZT may grow dramatically (up to 10^3 for realistic parameters) for such devices.

[1] M.T. Tuominen, J.M. Hergenrother, T.S. Tighe, and M. Tinkham, Phys. Rev. Lett. **69**, 1997 (1992).
[2] K.A. Matveev, Statistical and Dynamical Aspects of Mesoscopic Systems. Proceedings of the XVI Sitges Conference on Statistical Mechanics (2000).

15 min. break.

TT 6.7 Mon 11:15 BH 334

Zero-frequency noise in adiabatically driven quantum systems — •Roman-Pascal Riwar[1,2], Janine Splettstoesser[1,2], and Jürgen König[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Theoretische Physik, Duisburg-Essen and CeNIDE, D-47048 Duisburg, Germany

We investigate current-current correlations of adiabatic quantum pumps, taking into account Coulomb interaction. We make use of a real-time diagrammatic approach within a perturbative expansion in the tunnel coupling to the reservoirs and extend a treatment of adiabatic time dependence (Splettstoesser et al., PRB 2006) to the calculation of current noise.

We consider the case of a single-level quantum dot coupled to two leads where charge pumping arises by applying two out-of-phase time-dependent parameters, such as the energy levels, the bias or the tunnel couplings. While the instantaneous contribution to the noise confirms the results of the stationary case (Thielmann et al., PRL 2005), new properties are found in the adiabatic correction, i.e., the pumping noise. If the leads are at equilibrium at any time, the adiabatic correction of the Fano factor has a stable shape independently of the choice of the pumping parameters, also beyond the sequential tunneling regime. It provides additional information on the tunnel-coupling and the electron-hole symmetric point. When including a time-dependent finite bias, we find that there can be pumping noise even if there is zero pumped charge, due to a finite tunnel coupling asymmetry.

TT 6.8 Mon 11:30 BH 334

Influence of interaction-induced dephasing on the ac-

conductivity of disordered metals — •Martin Schäffer, Maximilian Treiber, Oleg Yevtushenko, and Jan von Delft — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany

We consider the influence of electron-interactions on the weak-localization (WL) correction to the ac-conductivity of disordered metals. It is well known that both an external ac-frequency and an interaction induced dephasing rate can govern the infrared behavior of the WL, but their interplay has never been studied in detail. One reason for this is that previous calculations had to employ a self-consistent regularization scheme which may lead to inaccurate results. Here, we adopt the diagrammatic approach developed in Ref.[1], which is free of both infrared and ultraviolet divergences since it includes so-called vertex diagrams. We analyze how this approach is modified at finite ac-frequencies and determine the leading cross- contributions for metals of arbitrary dimensionality. Furthermore, we discuss the effect of a finite system size (including the crossover to the so-called 0D regime of dephasing) on the interplay.

TT 6.9 Mon 11:45 BH 334

Bunching and anti-bunching in electronic transport — •Christina Pöltl, Clive Emary, Alexander Carmele, Julia Kabuss, Andreas Knorr, and Tobias Brandes — Institut für Theoretische Physik, Hardenbergstr. 36, TU Berlin, D-10623 Berlin, Germany

Current noise has long-since been established as an important tool for studying the physics of transport through mesoscopic and nano-scale conductors. The character of the current noise is typically assessed by considering the Fano factor, the ratio of the zero-frequency noise to the steady state current, and comparing with a Poisson process for which the Fano factor is equal to one. Systems with $F < 1$ are described as sub-Poissonian and systems which have $F > 1$ are called super-Poissonian. The standard physical interpretation of this comparison is that super-Poissonian Fano factors indicate a bunching of electrons which tunnel out of the conductor, whereas sub-Poissonian values indicates anti-bunching.

We directly investigate bunching and anti-bunching in electronic transport as a phenomenon in the time domain through the introduction of a second-order correlation function $g^{(2)}(\tau)$, analogous to that found in quantum optics. Our analysis shows that the simple picture relating super-Poissonian Fano factors to bunching and sub-Poissonian ones to anti-bunching is an oversimplification. Timescales can be found for which the electrons bunch, even though the Fano factor is sub-Poissonian and conversely.

TT 6.10 Mon 12:00 BH 334

Highly efficient Cooper pair splitting with carbon nanotube quantum dots — •Jens Schindele, Andreas Baumgartner, and Christian Schönenberger — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

An elegant idea for the creation of entangled electrons in a solid-state device is to split spin-singlet Cooper pairs by coupling a superconductor to two parallel quantum dots (QDs) in a Y-junction geometry [1]. Such Cooper pair splitting (CPS) was successfully detected in recent transport experiments on devices based on InAs nanowires [2,3] and Carbon nanotubes (CNTs) [4].

Here we present experiments on a CNT based Cooper pair splitter device with low inter-dot tunnel coupling. We find an unprecedented splitting efficiency, often much larger than 50

A high CPS efficiency is a prerequisite for Bell state measurements, a clear way of proving that Cooper pairs can be extracted coherently and lead to spatially separated entangled electron pairs.

[1] Recher et al., Phys. Rev. B 63, 165314 (2001)
[2] Hofstetter et al., Nature 461, 960-963 (2009)
[3] Hofstetter et al., Phys. Rev. Lett. 107, 136801 (2011)
[4] Herrmann et al., Phys. Rev. Lett. 104, 026801 (2010)
[5] Burset et al., Phys. Rev. B 84, 115448 (2011)

TT 6.11 Mon 12:15 BH 334

Carbon nanotubes with metallic contacts: energy and spin-orbit dependence of the tunneling rates — •Magdalena Marganska and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany

A microscopic approach to evaluate tunneling rates between a carbon nanotube and a metallic lead is presented. We show that the magnitude of the tunneling rate not only depends on the energy of the tunneling electron, but also on specific carbon nanotube features, such as its chiral angle and size. The latter in turn determine its curvature and the strength of the spin-orbit coupling. As a consequence, we predict different tunneling rates when tunneling in or out of the spin-orbit-split doublet states.

TT 6.12 Mon 12:30 BH 334

Coherence of single-electron sources from Mach-Zehnder interferometry — •Geraldine Haack[1], Michael Moskalets[2], Janine Splettstoesser[3], and Markus Buettiker[1] — [1]University of Geneva, Geneva, Switzerland — [2]Kharkiv Polytechnic Institute, Kharkiv, Ukraine — [3]RWTH Aachen University, Aachen, Germany

A new type of single electron sources (SES) has emerged which permits to inject single particles in a controllable manner into an electronic circuit. Multiparticle exchange, two-particle interference effects and entanglement have already been proposed [1]. Here we determine the coherence length of the single-particle states analyzing the decay of Aharonov-Bohm oscillations as a function of the imbalance of a Mach-Zehnder interferometer connected to an SES [2]. This single-particle coherence length is of particular importance as it is an intrinsic property of the source in contrast to the dephasing length.

[1] J. Splettstoesser, M. Moskalets, M. Buettiker, PRL 103, 076804 (2009).
[2] G. Haack, M. Moskalets, J. Splettstoesser, M. Buettiker, PRB 84, 081303(R) (2011).

TT 6.13 Mon 12:45 BH 334

Inhomogeneous Spin Chains and Luttinger Liquids — •Nicholas Sedlmayr, Jan Ohst, Jesko Sirker, and Sebastian Eggert — University of Kaiserslautern, Germany

We consider a one-dimensional spin chain with inhomogeneous coupling, which can also be modeled as an inhomogeneous Luttinger liquid. The Luttinger liquid paradigm has proved a very successful theoretical tool for investigating one-dimensional wires. However, there remain open questions about what happens when such a system becomes inhomogeneous. The mapping between the spin chain and the Luttinger liquid allows us to use a variety of methods in analyzing the problem. Of particular interest is the case where the Luttinger liquid is attached to external leads, as is necessary for example when measuring the conductance of the wire. In this paper we use an abrupt shift in the parameters of the Luttinger liquid to model these connections and see how this affects its behavior. In particular we analyze the relevant back-scattering perturbations at the connections, and identify a case where this relevant operator can be tuned to zero within an otherwise still inhomogeneous system. This of course has consequences not only for transport in the Luttinger liquid system but also for the magnetic susceptibility of the spin chain.

TT 7: Focused Session: Resonant Inelastic X-ray Scattering on Magnetic Excitations

Time: Monday 15:00–18:40 Location: H 0104

Invited Talk TT 7.1 Mon 15:00 H 0104

RIXS Studies of Strongly Correlated Electron Systems — •John Hill — Dept. of Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, USA

Resonant Inelastic X-ray Scattering (RIXS) has undergone enormous theoretical and experimental development in recent years - to the point where the technique is now able to observe all the relevant low energy excitations, including phonons, magnons, orbital excitations, charge transfer excitations, etc. As a result it is now able to make significant contributions to many of the current hardest problems in condensed matter physics. Here I provide an overview of the technique, and its development, focusing on the hard x-ray regime. In particular, I review work on the cuprates, the observation of two-magnon scattering and the very recent work on the low energy excitations of the iridates

including the observation of mixed spin and orbital excitations. Finally I conclude with a brief discussion of the exciting prospects for the future of this technique.

Invited Talk TT 7.2 Mon 15:40 H 0104

RIXS in the soft X-ray range: applications and perspectives — •Lucio Braicovich — Dip. di Fisica, Politecnico Milano 20133 Italy

After a brief introduction some recent results on RIXS in the soft x-ray range will be presented. The aim is to show the possibilities of the method and to explore the future growth areas. In particular we will discuss: (i) The measurement of the dispersion of magnons in undoped and in doped cuprates, (ii) the study of stripes in high Tc superconductors, (iii) the study of phonons, (iv) the measurement of the polarization of the radiation scattered by the sample, and (v) the peculiar aspects of RIXS at the FEL sources.

Finally we will present the RIXS project at the new soft x-rays beamline under consruction at the ESRF-Grenoble.

20 min. break.

Topical Talk TT 7.3 Mon 16:40 H 0104

The theory of resonant inelastic x-ray scattering on valence excitations — •Michel van Veenendaal — Department of Physics, Northern Illinois University, De Kalb IL 60115, USA — Argonne National Laboratory, 9700 S Cass Avenue, Argonne IL 60439, USA

The coupling between resonant inelastic x-ray scattering (RIXS) and valence excitations is discussed. The concepts of direct and indirect RIXS are described setting the framework for the interpretation of the RIXS cross section. The various mechanism how RIXS couples to dd-transitions, (bi)magnon excitations and phonons are discussed. It is shown how RIXS couples to the dynamic structure factor at the K-edge. At the L-edge, RIXS can be expressed in terms of effective transition operators drawing parallels to optical spectroscopy. Furthermore, selection rules in RIXS are discussed. Finally, the promise of RIXS in the future is discussed, in particular, in connection with X-ray free-electron lasers.

Topical Talk TT 7.4 Mon 17:20 H 0104

Excitons as a probe for low-energy spin fluctuations in cuprate chains — •Jochen Geck[1], Valentina Bisogni[1], Claude Monney[2], Kejin Zhou[2], Roberto Kraus[1], Jiri Malek[1], Stefan-Ludwig Drechsler[1], and Thorsten Schmitt[2] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Paul Scherrer Institute, Villigen, Switzerland

High-resolution RIXS provides outstanding capabilities for studying the spin, charge and orbital dynamics in correlated electron materials. Focussing on one-dimensional cuprates, a short overview of recent experiments will be presented, which illustrates that soft RIXS is a unique probe for collective spin and orbital excitations in such systems. However, low-energy excitations below 10meV are currently not directly accessible with this technique, due to the limited energy resolution of about 100meV. In this talk, we will present an experimental approach that circumvents this limitation. Using a charge transfer exciton as a probe, we show that local spin fluctuations at excitation energies of the order of 1meV can be detected with great sensitivity. Two prototypical edge-sharing cuprate chain materials with different magnetic intra-chain order have been studied in this way, namely $CuGeO_3$ (AFM) and Li_2CuO_2 (FM). For the latter, the FM intra-chain spin order is confirmed, but strong AFM spin fluctuations are still observed well below the magnetic ordering temperature. This reveals that Li_2CuO_2 is close to a quantum critical point. The presented method provides an excellent tool to characterize new one-dimensional cuprate materials and to search for novel magnetic ground states.

Topical Talk TT 7.5 Mon 18:00 H 0104

Fractionalization of electronic degrees of freedom in low-dimensional cuprates — •Justine Schlappa[1,2], Thorsten Schmitt[1], Kejin Zhou[1], Krzysztof Wohlfeld[3], Jeroen van den Brink[3], Maurits Haverkort[4], Martin Mourigal[5], and Henrik Rønnow[5] — [1]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI, Switzerland — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-12489 Berlin, Germany — [3]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [4]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [5]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Quantum effects become important, when the space symmetry is lowered. In the extreme case of one dimension the fundamental degrees of freedom of the electron can break up into separate quasi-particles, carrying either one of the spin, charge or orbital degrees of freedom. Here we report the study of elementary excitations in the quasi 1D cuprate Sr_2CuO_3, using high-resolution Resonant Inelastic X-ray Scattering. In the low-energy range the fractionalization of magnons into two-spinons and higher order excitations is observed, as previously reported from neutron scattering [1]. At higher energies we observe the deconfinement of spin and orbital degrees of freedom [2]. This phenomenon allows for the first time a direct observation of strongly dispersive orbital excitations (orbitons).

[1] A.C. Walters et al., Nature Physics 5, 867 (2009).
[2] J. Schlappa, T. Schmitt et al., submitted

TT 8: Superconductivity: Fe-based Superconductors - 122 Part 1

Time: Monday 15:00–18:30 Location: H 2053

TT 8.1 Mon 15:00 H 2053

Elastic anomalies in $Ba(Fe_{1-x}Co_x)_2As_2$ — •Christoph Meingast[1], Anna Böhmer[1,2], Frederic Hardy[1], Philipp Burger[1,2], Peter Adelmann[1], Doris Ernst[1], Rainer Fromknecht[1], Peter Schweiss[1], Rolf Heid[1], and Thomas Wolf[1] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Fakultät für Physik, 76128 Karlsruhe, Germany

The elastic properties of $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals are studied using a three-point-bending arrangement in a capacitance dilatometer. In this novel setup, a constant pressure is applied and the elastic response is determined as a function of temperature. In the undoped compound we find a very large softening of the elastic response at the structural/magnetic transitions near 140 K. The high resolution of this setup allows us to distinguish the behavior at both transitions. The large softening for undoped crystals weakens with doping and in the overdoped crystals only the very small softening as usually seen in superconductors at T_c is observed. We discuss our results in light of recent ultrasound measurements [1,2].

[1] R. M. Fernandes et al., Phys. Rev. Lett. 105, 157003 (2010).
[2] Y. Yoshizawa et al., arXiv: 1111.0366

TT 8.2 Mon 15:15 H 2053

Pair-breaking in overdoped $Ba(Fe_{1-x}Co_x)_2As_2$: Evidence for s± superconductivity — •Frédéric Hardy, Robert Eder, Thomas Wolf, Rolf Heid, Philipp Burger, Anna Böhmer, Peter Schweiss, and Christoph Meingast — Institut für Festkörperphysik KIT, Karlsruhe, Germany

Using specific-heat measurements, we study the effect of disorder induced by Co substitution on the thermodynamic properties of overdoped $Ba(Fe_{1-x}Co_x)_2As_2$ ($x > 0.06$) superconductors. We find that scattering of electrons by these non-magnetic impurities is rather strong (beyond Born limit) explaining the rapid suppression of T_c for $x = 0.12$. The variation of the specific-heat discontinuity, the thermodynamic critical field, and the gapless contributions, with Co content can be accurately reproduced only if the superconducting ground state exhibits s± symmetry. Comparisons with other systems including K and P doped single crystals are given.

TT 8.3 Mon 15:30 H 2053

Spectroscopic study of transition metal impurities in iron pnictides — •Roberto Kraus, Valentina Bisogni, Luminita Harnagea, Saicharan Aswartham, Sabine Wuhrmehl, Bernd Büchner, and Jochen Geck — IFW Dresden, PF 270116, D-01171 Dresden, Germany

In $Ba(Fe,TM)_2As_2$, superconductivity emerges upon replacing Fe with heavier TM=Co or Ni. The prevalent interpretation of this effect is

that the TM-impurities add electrons to the Fe-band and thereby induce superconductivity. However, this interpretation has been questioned recently based on theoretical grounds [1].

To clarify this we have performed valence band photoemission and Auger spectroscopy studies of single crystalline $Ca(Fe,Co)_2As_2$ and $Ba(Fe,TM)_2As_2$ with TM=Ni or Cu. The valence band photoemission data together with model calculations show that the Co and Ni impurity states largely overlap in energy with the Fe-bands, whereas the Cu impurity states do not. The LVV Auger lines measured at the L_3-absorption edge of the impurities unambiguously reveal a $3d^8$ final state for Ni and Cu.

This experimental result is incompatible with the naive assumption that Ni and Cu dope, respectively, 2 and 3 electrons into delocalized Fe-states. Rather our results reveal a much more complex situation and support the isovalent substitution of Fe by Ni and Cu.

[1] Wadati et al., PRL **105**, 157004 (2010)

TT 8.4 Mon 15:45 H 2053

Scanning tunneling spectroscopy in Co-doped $BaFe_2As_2$: What density functional theory can tell us. — •Klaus Koepernik[1], Steven Johnston[1], Jeroen van den Brink[1], Erik van Heumen[2], and Mark S. Golden[2] — [1]IFW Dresden, Germany — [2]van der Waals-Zeeman institute, University of Amsterdam, the Netherlands

We us density functional theory to simulate the scanning tunneling spectra and topographic images of Co-doped $BaFe_2As_2$. The matrix element effects are evaluated and the specific contributions of the different surface atoms to the spectra are considered. The results give a better understanding of the measured spectra and assess the resolution of STS measurements in these systems.

TT 8.5 Mon 16:00 H 2053

Universal microscopic description of the infrared conductivity of 122 iron arsenides — •Aliaksei Charnukha[1], Oleg V. Dolgov[1], Alexander A. Golubov[2], Yulia Matiks[1], Dun Lu Sun[1], Cheng Tian Lin[1], Bernhard Keimer[1], and Alexander V. Boris[1] — [1]Max-Planck-Institut für Festköorperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Faculty of Science and Technology and MESA+ Institute of Nanotechnology, NL-7500 AE Enschede, The Netherlands

We report the full complex dielectric function of high-purity $Ba_{0.68}K_{0.32}Fe_2As_2$ single crystals with T_c=38.5 K determined by wide-band spectroscopic ellipsometry at temperatures 10 K$\leq$T$\leq$300 K. We discuss the microscopic origin of superconductivity-induced infrared optical anomalies in the framework of a multiband Eliashberg theory with two distinct superconducting gap energies $2\Delta_A = 6k_BT_c$ and $2\Delta_B = 2.2k_BT_c$. The observed unusual suppression of the optical conductivity in the superconducting state at energies up to 14 k_BT_c can be ascribed to spin-fluctuation–assisted processes in the clean limit of the strong-coupling regime. We further demonstrate that the same model provides a good description of the infrared conductivity of electron-doped compounds in this class of superconductors.

TT 8.6 Mon 16:15 H 2053

Multigap superconductivity in $(Ba,K)Fe_2As_2$ probed by thermal expansion — •Anna Böhmer[1,2], Philipp Burger[1,2], Frédéric Hardy[1], Thomas Wolf[1], Peter Schweiss[1], Rainer Fromknecht[1], and Christoph Meingast[1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Postfach 3640, 76021 Karlsruhe — [2]Fakultät für Physik, Karlsruher Institut für Technologie, Postfach 6980, 76049 Karlsruhe

Hole doped $(Ba,K)Fe_2As_2$ is one of the most widely studied iron-based superconductors. Here, we report on an investigation of its thermal expansion using capacitive dilatometry. Overdoped samples, which do not undergo the magneto-structural transition, exhibit clear signatures of two-gap superconductivity in the thermal expansion coefficients. The data are analyzed with an extension of the two-gap alpha model, which is widely used to describe the specific heat of multi-band superconductors. By combining specific-heat and thermal-expansion data we are able to extract the uniaxial pressure dependence of T_c, of the gap magnitudes and of the electronic density of states. The influence of uniaxial pressure on the phase diagram is discussed.

TT 8.7 Mon 16:30 H 2053

A light scattering study of the superconducting gap in $Ba_{0.6}K_{0.4}Fe_2As_2$ — •Florian Kretzschmar[1], Bernhard Muschler[1], Rudi Hackl[1], Tom Devereaux[2,3], and Hai-Hu Wen[4] — [1]Walther Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — [3]Geballe Laboratory for Advanced Materials & Dept. of Applied Physics, Stanford University, CA 94305, USA — [4]Nanjing University, Nanjing, P.R. China

We present results of electronic Raman scattering experiments on optimally doped $Ba_{0.6}K_{0.4}Fe_2As_2$ in the superconducting state. In contrast to $Ba(Fe_{1-x}Co_x)_2As_2$ we find superconductivity features in all symmetries. The observed gaps depend strongly on the band index but are only weakly momentum-dependent on the individual bands. We find a small gap 2Δ in the range 10 meV on one hole-like band and two large and rather isotropic gaps of 23 meV on the other hole-like band and 25 meV on the electron-like bands, respectively. Below a symmetry independent threshold of approximately 25 cm^{-1} the Raman response is very small and nearly energy independent. Although the intensity is not exactly zero it is safe to conclude that there is a full gap on all bands having a magnitude of at least $1\,k_BT_c$. This work is supported by the DFG via the SPP 1458.

15 min. break.

TT 8.8 Mon 17:00 H 2053

Calorimetric evidence of multiband superconductivity in $A_{1-x}Na_xFe_2As_2$ (A = Ba and Ca) single crystals — •Mahmoud Abdel-Hafiez, Saicharan Aswartham, Dirk Bombor, Luminita Harnagea, Manoj Kumar, Ashim Pramanik, Volodymr Zabolotnny, Vladislav Kataev, Christian Hess, Sabine Wurmehl, Anja U. B. Wolter, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany

We report on the electronic properties and the superconducting gap characteristics of superconducting single crystals of $A_{1-x}Na_xFe_2As_2$ (A = Ba and Ca) studied by low temperature specific heat measurements. The zero-field specific heat data manifests a high electronic specific heat in the normal state, which is comparable to other hole-doped 122 compounds. We demonstrate that the measured zero field temperature dependence of the specific heat can be well described by two s-wave gaps. This is further confirmed by the scaling based on the s-wave and d-wave scenario of the low temperature data at various magnetic fields. Our results are qualitatively similar to other hole-doped 122 compounds, but nevertheless the magnitude of the gaps and their ratio are quite different.

TT 8.9 Mon 17:15 H 2053

Microscopic interplay of superconducting and magnetic order parameters in ferropnictides — •H. Maeter[1], T. Goltz[1], J. Spehling[1], H.-H. Klauss[1], M. Bendele[2], H. Luetkens[2], R. Khasanov[2], G. Pascua[2], Z. Shermadini[2], A. Amato[2], S. Aswartham[3], J. E. Hamann-Borrero[3], A. Kondrat[3], C. Hess[3], A. Wolter[3], S. Wurmehl[3], G. Behr[3], B. Büchner[3], E. Wiesenmayer[4], D. Johrendt[4], H. Potts[5], and B. Banusch[5] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden,Germany — [4]Department Chemie, Ludwig-Maximilians-Universität München, Germany — [5]Swiss Nanoscience Institute, Universität Basel, Switzerland

We present results of μSR experiments of $Ba_{1-x}Na_xFe_2As_2$ that show a large coupling of the superconducting and magnetic order parameters. This is unexpected in light of the phase separation in $Ba_{1-x}K_xFe_2As_2$. However, in a μSR study of $Ba_{1-x}K_xFe_2As_2$ we unambiguously showed microscopic coexistence, even though there are many reports of phase separation in this system [1]. In $FeSe_{1-x}$ the interplay of phase separation and microscopic coexistence is also evident, here pressure can induce a change from microscopic coexistence to a combination of both [2]. In light of the μSR results it seems likely that phase separation and microscopic coexistence depend on the microscopic properties much more than on disorder.

[1] Wiesenmayer et al., Phys. Rev. Lett. 107, 237001 (2011);
[2] Bendele et al., Phys. Rev. Lett. 104, 087003 (2010).

TT 8.10 Mon 17:30 H 2053

Influence of doping in KFe_2As_2 superconducting single crystals — •S. Aswartham[1], M. Roslova[1,2], I. V. Morozov[1,2], A. U.B Wolter[1], M. Kumar[1], C. Hess[1], S. Wurmehl[1], and B.

Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, D-01069 Dresden, Germany — [2]Department of Chemistry, Moscow State University, Moscow 119991, Russia

Single crystals of the new unconventional superconductor KFe_2As_2 were grown using two different fluxes, i.e KAs and FeAs flux. The superconducting transition temperature and the superconducting volume fraction were found to be same in all crystals independent of the flux. However, the normal state susceptibility is changed significantly. On the other hand we investigated, the influence of various types of doping in KFe_2As_2. Specifically, we investigate the substitution of K by Na (yielding $K_{1-x}Na_xFe_2As_2$) and the substitution of Fe by other transition metals like Co, Cr, Rh (yielding $K(Fe_{1-x}TM_x)_2As_2$). We will present a systematic study of the crystal growth, characterization and superconducting properties of these newly synthesized superconductors.

TT 8.11 Mon 17:45 H 2053

Enhancement of the upper critical field in codoped iron-arsenic high-temperature superconductors — •H. Rosner[1], M. Nicklas[1], W. Schnelle[1], A. Leithe-Jasper[1], J. Wosnitza[2], and F. Weickert[1,3] — [1]MPI CPfS Dresden — [2]HLD Dresden-Rossendorf — [3]LANL Los Alamos

We present the first study of codoped iron-arsenide superconductors of the 122 family $(Sr/Ba)_{1-x}K_xFe_{2-y}Co_yAs_2$ with the purpose to increase the upper critical field H_{c2} compared to single doped $Sr/BaFe_2As_2$ materials. H_{c2} was investigated by measuring the magnetoresistance in high pulsed magnetic fields up to 64 T. We find, that H_{c2} extrapolated to T = 0 is indeed enhanced significantly to 90 T for polycrystalline samples of $Ba_{0.55}K_{0.45}Fe_{1.95}Co_{0.05}As_2$ compared to 75 T for $Ba_{0.55}K_{0.45}Fe_2As_2$ and $BaFe_{1.8}Co_{0.2}As_2$ single crystals. Codoping thus is a promising way for the systematic optimization of iron-arsenic based superconductors for magnetic-field and high-current applications.

TT 8.12 Mon 18:00 H 2053

Electronic properties of $BaFe_2As_2$ and $CaFe_2As_2$ under hydrostatic and non-hydrostatic pressure conditions — •Milan Tomić, Roser Valentí, and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität, Frankfurt am Main, Germany

We have examined the effects of different external pressure conditions on the structural and electronic properties of the 122 family of iron pnictides by considering ab initio constant pressure structural relaxations. We find magneto-structural phase transitions in both $CaFe_2As_2$ and $BaFe_2As_2$ and observe a high sensitivity of the electronic structure and Fermi surface topology on the nature of the pressure conditions. In this talk, we will present these results, compare them with the effects of phosphorus doping and will discuss possible implications for superconductivity.

TT 8.13 Mon 18:15 H 2053

Dispersive High-Energy Spin Excitations in Iron Pnictide Superconductors Investigated with RIXS — •Thorsten Schmitt[1], Kejin Zhou[1], Y. B. Huang[1,2], C. Monney[1], V. N. Strocov[1], J. van den Brink[3], and H. Ding[2] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]IOP, CAS, Beijing, China — [3]IFW Dresden, Germany

The discovery of iron-based high temperature superconductivity has triggered tremendous research efforts in searching for novel high-T_c superconductors. Unlike cuprates, which have long-range ordered antiferromagnetic Mott insulators as parent compounds, the parent compounds of iron-based superconductors are spin-density wave metals with delocalized electronic structure and more itinerant magnetism.

Recent developments of the high-resolution resonant inelastic X-ray scattering (RIXS) technique [1] have enabled investigations of magnetic excitations in cuprates [2], which show excellent agreement with results from Inelastic Neutron Scattering. In this presentation we demonstrate that RIXS can be used to measure collective magnetic excitations in iron-based superconductors despite their much stronger itinerancy compared to cuprates. The persistence of high-energy spin excitations even in optimally doped pnictide superconductors in a wide range of temperatures strongly suggests a spin-mediated Cooper pairing mechanism as proposed in cuprate superconductors.

[1] G. Ghiringhelli et al., Rev. Sci. Inst. 77, 113108 (2006); V. N. Strocov et al., J. Synch. Rad. 17, 631 (2010).
[2] J. Schlappa et al., Phys. Rev. Lett. 103, 047401 (2009); L. Braicovich et al., Phys. Rev. Lett. 104, 077002 (2010).

TT 9: Transport: Topological Insulators 2 (jointly with HL and MA)

Time: Monday 15:00–16:30 Location: H 3005

TT 9.1 Mon 15:00 H 3005

Majorana end states in disordered topological superconducting wires — •Alessandro Romito, Piet Brouwer, Mathias Duckheim, and Felix von Oppen — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universit at Berlin, 14195 Berlin, Germany

Zeeman fields can drive semiconductor quantum wires with strong spin-orbit coupling and in proximity to s-wave superconductors into a topological phase. Such topological phases are characterized by the presence of Majorana Fermions which obey non-abelian statistics, and provide a possible platform for a topological quantum computer. So far Majorana Fermions have never been observed in experiments. However, semiconducting wires with strong spin-orbit coupling offer a promising path towards this goal. A key question, both for theory and experiment, is whether the topological phase is robust against the unavoidable presence of disorder.

Here, after brefly introducing the proposals for the realization and control of Majorana Fermions in quantum wires, I will mainly address their robustness against disorder showing that Majorana fermions persist in disordered wires up to a critical disorder strength which, remarkably, depends sensitively and non-monotonously on the Zeeman field applied to the wire. In finite length disordered wires the Majorana states combine into fermionic excitation at finite energy with large sample-to sample fluctuations. I will discuss the probability distribution of such low energy level and the consequences for the speed at which such topological quantum bits can be operated.

TT 9.2 Mon 15:15 H 3005

Competition between d-wave and topological p-wave superconductivity in the doped Kitaev-Heisenberg model — •Timo Hyart[1], Anthony Wright[1], Giniyat Khaliullin[2], and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The competition between Kitaev and Heisenberg interactions away from half filling is studied for the hole-doped Kitaev-Heisenberg t-J_K-J_H model on a honeycomb lattice. While the isotropic Heisenberg coupling supports a time-reversal violating d-wave singlet state, we find that the Kitaev interaction favors a time-reversal invariant p-wave superconducting phase, which obeys the rotational symmetries of the microscopic model, and is robust for $J_H < J_K/2$. Within the p-wave superconducting phase, a critical chemical potential $\mu_c \approx t$ separates a topologically trivial phase for $|\mu| < \mu_c$ from a topologically non-trivial Z_2 time-reversal invariant spin-triplet phase for $|\mu| > \mu_c$.

TT 9.3 Mon 15:30 H 3005

s + p - wave proximity-induced superconductivity in impure topological insulators — •Grigory Tkachov, Pauli Virtanen, Florian Foohs, Patrik Recher, and Ewelina Hankiewicz — Universität Würzburg, Germany

In contacts with conventional s-wave superconductors (Ss), topological insulators (TIs) are expected to show both s- and p-wave superconducting correlations due to the spin-momentum locking on the surface. We analyze how the impurity scattering, extended defects (e.g. interfaces) and an external magnetic field influence such mixed proximity-induced superconductivity in topological insulators. As an example, we calculate a surface magnetosupercurrent through an S/TI/S Josephson junction.

TT 9.4 Mon 15:45 H 3005

Topologically protected zero-energy surface states of noncentrosymmetric superconductors — •Philip M. R. Brydon[1], An-

dreas P. Schnyder[2], and Carsten Timm[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

It has recently been pointed out that nodal noncentrosymmetric superconductors are topologically non-trivial, with the nodal rings possessing a non-zero topological charge [1]. In these systems a bulk-boundary correspondence can be developed, which guarantees the existence of a flat band of singly degenerate zero-energy states within the projection of the nodal lines onto the surface Brillouin zone. Using the quasiclassical method [2,3], we present results for the surface bound state spectra, and provide a condition for the existence of the zero-energy states in terms of the sign of the gaps, which is complementary to the topological condition. The zero-energy surface states are shown to leave distinct signatures in the tunneling conductance.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504(R) (2011).
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B 84, 020501(R) (2011).
[3] A. P. Schnyder, P. M. R. Brydon, and C. Timm, arXiv:1111.1207 (unpublished).

TT 9.5 Mon 16:00 H 3005

Quantum phase transitions in the Kane-Mele-Hubbard model — Martin Hohenadler[1], Zi Yang Meng[2], •Thomas C. Lang[3], Stefan Wessel[3], Alejandro Muramatsu[4], and Fakher F. Assaad[1] — [1]Universität Würzburg, Würzburg, Germany — [2]Louisiana State University, Baton Rouge, USA — [3]RWTH Aachen, Aachen, Germany — [4]Universität Stuttgart, Stuttgart, Germany

We study the two-dimensional Kane-Mele-Hubbard model at half filling by means of quantum Monte Carlo simulations. We present a refined phase boundary for the quantum spin liquid. The topological insulator at finite Hubbard interaction strength is adiabatically connected to the groundstate of the Kane-Mele model. In the presence of spin-orbit coupling, magnetic order at large Hubbard U is restricted to the transverse direction. The transition from the topological band insulator to the antiferromagnetic Mott insulator is in the universality class of the three-dimensional XY model. The numerical data suggest that the spin liquid to topological insulator and spin liquid to Mott insulator transitions are both continuous.

TT 9.6 Mon 16:15 H 3005

Majorana fermions in strongly interacting helical liquids — •Eran Sela, Achim Rosch, and Alexander Altland — Koeln university, Germany

Majorana fermions were proposed to occur at edges and interfaces of gapped one-dimensional systems where phases with different topological character meet due to an interplay of spin-orbit coupling, proximity-induced superconductivity and external magnetic fields. Here we investigate the effect of strong particle interactions and show that a helical liquid offers a mechanism that protects the very existence of Majorana edge states: whereas moderate interactions close the proximity gap that supports the edge states, in helical liquids the gap reopens due to two-particle processes. However, gapless fermionic excitations occur at spatial proximity to the Majorana states at interfaces and may jeopardize their long-term Majorana coherence.

TT 10: Correlated Electrons: (General) Theory 1

Time: Monday 15:00–18:15 Location: H 3010

TT 10.1 Mon 15:00 H 3010

Enhanced Perturbative Continuous Unitary Transformation — •Holger Krull, Nils A. Drescher, and Götz S. Uhrig — TU Dortmund, Theoretical Physics I, 44221 Dortmund, Germany

We present an enhanced version of continuous unitary transformations (CUTs) to derive effective models perturbatively and non-perturbatively for quantum lattice models. The underlying idea is to expand the Hamiltonian and the generator of the flow equation in the expansion parameter. The operators are described in second quantization. For the method to be efficient, it is essential to keep track of the relevant contributions according to their order in the expansion parameter. This enhanced perturbative CUT (epCUT) allows us to determine effective Hamiltonians to high order. In contrast to perturbative CUT, the expansion around unperturbed Hamiltonians with non-equidistant spectrum is possible. In addition, we found that the set of differential flow equations of the epCUT can be integrated non-perturbatively leading to a robust extrapolation similar to self-consistent diagrammatic techniques. This directly evaluated epCUT (deepCUT) provides robust results even for relatively large expansion parameter as long as the relevant processes with a spatial range up to the correlation length are included. The epCUT and the deepCUT are illustrated for the $S = \frac{1}{2}$ antiferromagnetic Heisenberg ladder and for an extension with alternating rung couplings implying a non-equidistant unperturbed spectrum. The results for the ground state energy (order 17/16) and the dispersion (order 15/13) are presented.

TT 10.2 Mon 15:15 H 3010

Spectral properties of one-dimensional spin systems using deepCUT — •N. A. Drescher, H. Krull, T. Fischer, and G. S. Uhrig — TU Dortmund, Theoretical Physics I, 44221 Dortmund

Directly evaluated enhanced perturbative continuous unitary transformations (deepCUT) are a novel scheme to systematically derive effective low-energy models for many-particle Hamiltonians. Founded on high-order perturbative expansion techniques (epCUT), deepCUTs generate robust results beyond perturbation theory. We use them to decouple ground state and low-lying excitations of one dimensional spin systems. From the effective Hamiltonian, dispersion and bound states can be obtained. Applying the same unitary transformation to observables, we calculate spectral weights and the dynamical spin structure factor for the one and two quasi-particle channel at $T = 0$.

We illustrate the deepCUT method by an analysis of the antiferromagnetic S=$\frac{1}{2}$ Heisenberg ladder compound $(C_7(D,H)_{10}N)_2CuBr_4$. We compare our results for dispersion and spectral weight with inelastic neutron scattering data. Predictions for S=0,1 spectral densities and bound states relevant for various scattering experiments are presented.

TT 10.3 Mon 15:30 H 3010

DMFT study of correlated systems in d+p basis sets utilizing a continuous time algorithm — •Nicolaus Parragh, Giorgio Sangiovanni, Alessandro Toschi, Philipp Wissgott, Philipp Hansmann, and Karsten Held — Institut für Festkörperphysik, TU Wien

Ab-initio calculations for strongly correlated materials are nowadays very often performed within the LDA+DMFT scheme, a combination of local density approximation and dynamical mean field theory. Within this approach, a key point is which bands to keep when defining the low energy Hamiltonian for which DMFT self-consistency is performed. We show how the inclusion of p-bands (typically coming from Oxygen ligands on top of the transition metal d-orbitals) in the DMFT cycle affects the physics of the system. This has implications for current research in, e.g., iron and copper based superconductors. We use continuous-time Quantum Monte Carlo algorithm to solve the auxiliary impurity problem and focus on the role of SU(2)-symmetric interactions.

TT 10.4 Mon 15:45 H 3010

Electronic correlation at the two-particle level — •Thomas Schaefer[1], Georg Rohringer[1], Alessandro Toschi[1], Giorgio Sangiovanni[1], Olle Gunnarsson[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Electronic correlated systems can often be successfully described by dynamical mean field theory (DMFT). If DMFT is applied to finite-dimensional systems it is self-consistent at the one-particle level. Extensions of DMFT based upon the systems' two-particle properties have been developed such as the dynamical vertex approximation (DΓA) [1] or the dual fermion approach [2]. In addition, the understanding and the calculation of two-particle quantities are crucial within DMFT to compute momentum-dependent response functions that can be compared directly with experiments. As hitherto the investigation of local and non-local two-particle properties has been merely sporadic, we provide a systematic analysis of the reducible and irreducible two-particle vertex functions by applying DMFT and the

dynamical cluster approximation (DCA) to the two-dimensional Hubbard model.
[1] A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B 75, 045118 (2007).
[2] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 77, 033101 (2008).

TT 10.5 Mon 16:00 H 3010

Dynamics in the Ising field theory after a quantum quench — •Dirk Schuricht[1,2] and Fabian H. L. Essler[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen — [2]JARA-Fundamentals of Future Information Technology — [3]The Rudolf Peierls Centre for Theoretical Physics, University of Oxford

We study the real-time dynamics of the magnetization $\langle\sigma^z(t)\rangle$ in the Ising field theory after a quench in the fermion mass, which corresponds to a quench in the transverse field of the corresponding transverse-field Ising chain. The long-time behavior is obtained analytically by a resummation of the leading divergent terms in a form-factor expansion for $\langle\sigma^z(t)\rangle$. We determine the dominant exponential relaxation and the corresponding relaxation rate and show that the leading corrections behave as $\sim 1/(Mt)$ and $\sim \cos(2Mt-\pi/4)/(Mt)^{3/2}$.

TT 10.6 Mon 16:15 H 3010

Bosonization in arbitrary dimensions and its applications to Quantum Monte Carlo simulations — •Ervand Kandelaki and Konstantin Efetov — Theoretische Physik III, Ruhr-Universität-Bochum

The applicability of Quantum Monte Carlo simulations for fermionic models using the Auxiliary Field method is often limited if the measure is not strictly positive. We investigate to what extent the recently suggested bosonization scheme for fermionic systems in an arbitrary dimension allows for simulations with positive weights. Choosing a proper regularization of the dynamical equation for the bosonic field, we derive an expression for the action which is purely real. We relate the partition function obtained after bosonization to the common fermionic one and present some first numerical results.
[1] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981)
[2] K. B. Efetov, C. Pépin, and H. Meier, Phys. Rev. Lett. 103, 186403 (2009)
[3] K. B. Efetov, C. Pépin, and H. Meier, Phys. Rev. B 82, 235120 (2010)

15 min. break.

TT 10.7 Mon 16:45 H 3010

Continued Fractions and Bath-Parametrizations for Quantum Cluster Methods — •Monica Bugeanu and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich

The Lanczos method is an ideal solver for dynamical mean-field approaches. Calculations are performed for the ground-state and extensions to finite temperature are straightforward. Dynamical quantities are obtained directly on the real axis without need for analytic continuations. The main limitation, however, is that calculations can only be done for finite baths. The rapidly growing size of the many-body Hilbert space limits actual calculations to quite small bath-sizes. It is therefore crucial to be able to treat as large baths as possible and to choose the bath parameters in an optimal way. We show how this can be achieved using continued fraction representations of the Green function.

TT 10.8 Mon 17:00 H 3010

Orbital and magnetic order in the infinite-dimensional two-band Hubbard model — •Ernst von Oelsen, Götz Seibold, and Jörg Bünemann — Lehrstuhl Computational Physics, BTU Cottbus, Postfach 101344, 03013 Cottbus

Based on the time-dependent Gutzwiller approximation (GA), generalized to the case of multiple bands [1,2], we investigate the stability of magnetic and orbital order in the infinite dimensional two-band Hubbard model. Contrary to the Hartree-Fock plus random-phase approximation, the incorporation of the local multiplet-structure within our approach leads to a much larger sensitivity of ferromagnetism on the the ratio between Hund coupling and intra-orbital repulsion J/U. Besides, we find that the Brinkman-Rice localization transition, which in the paramagnetic GA appears at integer doping is always masked by an antiferromagnetic (for two particles per site) or an orbitally ordered (for one particle per site) ground state. In addition, at larger values of J/U a quantum Lifshitz point is found where ferro-, para- and incommensurate magnetic phases meet.
[1] E. von Oelsen, G. Seibold, and J. Bünemann, New J. Phys. **13**, 113031 (2011).
[2] E. v. Oelsen, G. Seibold, and J. Bünemann, Phys. Rev. Lett. **107**, 076402 (2011).

TT 10.9 Mon 17:15 H 3010

Momentum-dependent pseudogaps in the half-filled 2d Hubbard model — •Daniel Rost[1], Elena Gorelik[1], Fakher Assaad[2], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg-University, Mainz, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Germany

A peculiar feature of (underdoped) high-T_c superconductors is the occurrence of pseudogaps in the normal state, i.e. a suppression of the density of states at the Fermi energy. It has been unclear for a long time whether and in which parameter regimes this phenomenon is captured by the two-dimensional Hubbard model: spectra obtained from determinantal quantum Monte Carlo (DQMC) simulations suffer from large finite-size (as well as Trotter and statistical) errors; partial conclusions for the thermodynamic limit were only possible by complementing DQMC data with cluster extensions of the dynamical mean-field theory (DMFT) and with the dynamical vertex approximation.

We present a method for extrapolating DQMC Green functions to the limit of infinite cluster size $L \to \infty$ and vanishing Trotter discretization $\Delta\tau \to 0$. Thus, we obtain, via the maximum entropy method, the first unbiased spectra in the thermodynamic limit. Our results establish that a pseudogap opens in the $2d$ Hubbard model at weak coupling below a characteristic temperature $T_{\rm pg}$ which (for $U = 4t$) agrees with DMFT Néel temperature. It opens first at $\mathbf{k}a = (\pi, 0)$, i.e. shows d wave type anisotropy at $T \lesssim T_{\rm pg}$ even at half filling; this momentum dependence (an effect not captured by DMFT) decays towards larger interactions.

TT 10.10 Mon 17:30 H 3010

Pomeranchuk and pairing instabilities in two-dimensional Hubbard models — •Jörg Bünemann[1], Tobias Schickling[2], and Florian Gebhard[2] — [1]Institut für Physik, BTU Cottbus, D-03013 Cottbus, Germany — [2]Fachbereich Physik, Philipps Universität Marburg, D-35032 Marburg, Germany

We have developed a diagrammatic method which permits the analytical evaluation of Gutzwiller wave functions in finite dimensions [1]. Unlike numerical schemes for the evaluation of such wave functions, our approach does not suffer from significant finite-size limitations and it can be readily generalised for the study of multi-band models. In our presentation we will introduce the main ideas of our approach and show results on single-band Hubbard models in two dimensions. In particular, we shall discuss the correlation-induced deformation of Fermi surfaces and the stability of phases with broken symmetry ("Pomeranchuk instabilities" and superconducting order).
[1] J. Bünemann, T. Schickling, F. Gebhard, arXiv:1108.4284

TT 10.11 Mon 17:45 H 3010

Superconductivity and the Pseudogap in the 2d Hubbard model — •Emanuel Gull[1], Olivier Parcollet[2], and Andrew J. Millis[1] — [1]Columbia University, New York, NY — [2]Institut de Physique Théorique (IPhT), CEA, France

Using a numerically exact continuous-time quantum Monte Carlo impurity solver and the DCA cluster dynamical mean field method with cluster sizes up to 16, we have been able to access the superconducting phase of the two dimensional Hubbard model for parameters believed to be relevant to high temperature copper oxide superconductivity. We present results for the phase diagram, the gap to transition temperature ratio, and the interplay of the pseudogap and the superconducting gap. The gap results are obtained by direct inference from imaginary frequency data and analytically continued spectral functions.

TT 10.12 Mon 18:00 H 3010

Heavy fermion properties in the Kondo lattice model — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, Institute for Theoretical Solid State Physics, P.O. Box 270116, D-01171 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, D-01062 Dresden, Germany

The Kondo lattice model is believed to describe the low-energy physics

of heavy-fermion systems. It includes a band of conduction electrons, interacting via an exchange with a regular array of immobile spins $\mathbf{S}_i$. No exact results are known for this model in any spatial dimension. We have studied the model using the quite novel projective renormalization method (PRM). Using this analytical technique we obtain a solvable effective Hamiltonian $\tilde{\mathcal{H}}$ which consists of conduction electrons with renormalized dispersion $\tilde{\varepsilon}_{\mathbf{k}}$ and an RKKY interaction term which is generated naturally within the renormalization procedure. The present approach allows us to evaluate static and dynamical properties such as the specific heat, the density of states or the electrical resistivity. For low enough temperatures we find an additional dispersionless excitation around the Fermi surface due to the formation of a singlet state. Simultaneously, a large γ-coefficient develops in the specific heat which is usually traced back to the huge effective mass of heavy fermion quasiparticles.

TT 11: Transport: Quantum Coherence and Quantum Information Systems 2 (jointly with MA and HL)

Time: Monday 15:00–17:30 Location: BH 243

TT 11.1 Mon 15:00 BH 243

Control Pulse Engineering for Fast Controlled-Z Gates — •Daniel Egger, Seth Taylor Merkel, and Frank Wilhelm — Universität des Saarlandes, Saarbrücken, Germany

When manipulating quantum systems it is key to do so before decoherence destroys the fragile states. For quantum computing this sets a time within which the desired qubit manipulations can be done. To increase the number of computations, either the coherence times must be increased or the gate durations must be decreased with the help of Optimal Control Theory. In the following work we show how Gradient Pulse Shape Engineering [1] can be used to optimize the time taken to perform a controlled-Z gate in the framework of the RezQu architecture [2]: two qubits, sufficiently far apart, are coupled to a bus resonator. The only controls considered are the two qubit-bus detunings. All elements have three levels to account for leakage. Additionally the finite bandwidth of the electronics is taken into account though an impulse response function. We give a value of the critical time below which a high fidelity gate can no longer be realized and explore what affects the control pulses. For the case of phase qubits we find that a controlled-Z gate with an error of 10^{-4} can be realized in 27 ns. Furthermore, the found control pulses are ready to be tested experimentally.

[1] N. Khaneja, J. Magn. Reson. **172**, 296
[2] M. Mariantoni, Science **334**, 6052

TT 11.2 Mon 15:15 BH 243

Relaxation and decoherence dynamics in the spin-boson model — •Oleksiy Kashuba, Mikhail Pletyukhov, Dirk Schuricht, and Herbert Schoeller — Institut für Theorie der statistischen Physik, RWTH Aachen, D-52056 Aachen

We study the real-time dynamics of the ohmic spin-boson model using a nonequilibrium renormalisation group method [1] successfully applied to the anisotropic Kondo model [2] and the interacting resonant-level model [3]. We discuss the relaxation and decoherence channel w/o bias. In all regimes of the coupling α, we obtain power law time dependence from non-Markovian contributions but always accompanied by exponential decay. For $\alpha \sim 1/2$, we recover the well-known localization transition but obtain different power-law exponents for the time evolution in the biased case. Finally, for $\alpha \sim 1$, we discuss the time-evolution close to a quantum critical point.

[1] H. Schoeller, Eur. Phys. J. Spec. Top. 168, 179 (2009).
[2] M. Pletyukhov, D. Schuricht and H. Schoeller, Phys. Rev. Lett. 104, 106801 (2010).
[3] S. Andergassen, M. Pletyukhov, D. Schuricht, H. Schoeller, and L. Borda, Phys. Rev. B 83 205103 (2011).

TT 11.3 Mon 15:30 BH 243

Simple ways to avoid leakage in qubit systems — •Frank Wilhelm[1,2], Felix Motzoi[2], Seth Merkel[3], and Jay Gambetta[3] — [1]Theoretical Physics, Saarland University, Saarbrücken — [2]IQC and Department of Physics and Astronomy, University of Waterloo, Canada — [3]IBM Watson Research Laboratories, Yorktown Heights, NY, USA

No physical system is just a two-state qubit. Many qubit candidates are in fact weakly nonlinear oscillators with leakage transitions that lead outside the computational subspace that are spectrally close to the qubit transition. The simple DRAG pulse-shaping method allows to efficiently supress these leakage transitions. We will show that there is a whole family of DRAG pulses that also allow to enhance spectral selectivity through multiple channels, and that allow to selectively address qubits driven through a common control. These ideas are applied to superconducting phase qubits, Transmons, and circuit QED architectures.

[1] F. Motzoi, J.M. Gambetta, P. Rebentrost, and F.K. Wilhelm, Phys. Rev. Lett. 103, 110501 (2009)
[2] J.M. Gambetta, F. Motzoi, S.T. Merkel, and F.K. Wilhelm, Phys. Rev. A 2011

TT 11.4 Mon 15:45 BH 243

Non-equilibrium dynamics of the central spin model — •Alexandre Faribault and Dirk Schuricht — Institute for Theory of Statistical Physics RWTH Aachen Physikzentrum Sommerfeldstrasse 52074 Aachen Germany

A long standing proposal for a q-bit is to use the spin of a single electron trapped in a quantum dot. In such solid-state based systems, the dominant decoherence mechanism is the hyperfine coupling of the electron spin to the nuclear spins in the substrate. In this work, the Central spin model describing such a quantum system is studied numerically by exploiting its quantum integrability via the algebraic Bethe ansatz. In doing so, it becomes possible to efficiently compute exact eigenstates which we then use to study non-equilibrium dynamics in scenarios describing the relaxation and decoherence of prepared states.

TT 11.5 Mon 16:00 BH 243

Impurity entanglement via electron scattering in a magnetic field — Raoul Dillenschneider, •Alexandros Metavitsiadis, and Sebastian Eggert — Physics Department and Research Center OPTIMAS, Technical University of Kaiserslautern, Kaiserslautern, Germany

A possible mechanism to entangle two non-interacting magnetic moments is via successive electron scattering. Of particular interest is the case when the magnetic moments are considered as embedded impurities in a one dimensional lattice. The amount of entanglement can be modified by appropriately choosing the initial state of the system. Furthermore, the presence of a magnetic field may play a crucial role to the resulting entanglement. In this work, we present analytical as well as numerical results for the time dependence of the entanglement of magnetic moments, as manifested in the concurrence, especially stressing the role of external fields.

15 min. break.

TT 11.6 Mon 16:30 BH 243

Decoherence of a qubit in a non-Markovian environment formed through a spin cluster — •Wenling Qiao[1,2], Mohammad Ansari[2], and Frank Wilhelm-Mauch[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]University of Waterloo, Waterloo, Canada

The error rate in quantum computing based on solid-state devices is mostly limited by the qubit decoherence behavior. While Markovian environments are well understood, the main experimental and theoretical challanges lie in the field of correlated non-Markovian noises. We study the quantum dynamics of a qubit in a toy non-Markovian environment model, a large spin cluster coupled to a thermal bath. By using the Holstein-Primokoff transformation,Bogoliubov transformation on the spin Hamiltonian and representing the master equation in phase space, we calculated the correlation function for the spin operator coupled to the qubit. This permits insight into the decoherence of the qubit.

TT 11.7 Mon 16:45 BH 243

Quantum state transfer in boundary-controlled and fully engineered spin chains — Analia Zwick[1,2], Gonzalo A. Álvarez[1], •Joachim Stolze[1], and Omar Osenda[2] — [1]Institut für Physik, TU Dortmund, Germany — [2]Facultad de Matemática, Astronomía y Física and Instituto de Física Enrique Gaviola, Universidad Nacional de Córdoba, Argentina

Quantum state transfer in presence of noise is one of the main challenges for building quantum computers. We compare the quantum state transfer properties for two classes of qubit chains under the influence of static randomness. In fully engineered chains all nearest-neighbor couplings are tuned in such a way that a single-qubit state can be transferred perfectly between the ends of the chain, while in boundary-controlled chains only the two couplings between the transmitting and receiving qubits and the remainder of the chain can be optimized. We study how the noise in the couplings affects the state transfer fidelity depending on the noise model and strength as well as the chain type and length. We show that the desired level of fidelity and transfer time are important factors in designing a chain. In particular we demonstrate that transfer efficiency comparable or better than that of the most robust engineered systems can also be reached in boundary-controlled chains without the demanding engineering of a large number of couplings.

TT 11.8 Mon 17:00 BH 243

Pauli blockade for Kramers-qubit readout in carbon nanotubes — •gábor széchenyi and andrás pályi — Institute of Physics, Eötvös University, Hungary

Carbon nanotube double quantum dots are promising candidates for a solid-state platform of quantum-information processing. In the ground state of the nanotube the physical qubit is a Kramers doublet, which involves two states with antiparallel alignment of spin and valley. To evaluate the potential in Pauli-blockade-based Kramers-qubit readout, we theoretically investigate electron transport in a situation where Pauli or spin-valley blockade is lifted by the combined effect of axial and transverse magnetic-field and short range disorder. We can identify a parameter regime where four-level (spin and valley) carbon nanotube quantum dot is reduced to an effective two-level system. We derive analytical formulas of the current as a function of applied transverse and axial magnetic field, which we compare with our numerical results.

TT 11.9 Mon 17:15 BH 243

Entanglement, Fluctuations, and Quantum Critical Points — •Stephan Rachel[1], Nicolas Laflorencie[2], H. Francis Song[1], and Karyn Le Hur[3,1] — [1]Department of Physics, Yale University, New Haven, CT 06520, USA — [2]Laboratoire de Physique Theorique, Universite de Toulouse, UPS, (IRSAMC), F-31062 Toulouse, France — [3]Center for Theoretical Physics, Ecole Polytechnique, 91128 Palaiseau Cedex, France

We show that bipartite fluctuations F can be considered an entanglement measure. We further demonstrate that the concept of bipartite fluctuations F provides a very efficient tool to detect quantum phase transitions in strongly correlated systems. We investigate paradigmatic examples for both quantum spins and bosons in one and two dimensions. As compared to the von Neumann entanglement entropy, we observe that F allows to find quantum critical points with a much better accuracy in one dimension. We further demonstrate that F can be successfully applied to the detection of quantum criticality in higher dimensions with no prior knowledge of the universality class of the transition. Promising approaches to experimentally access fluctuations are discussed for quantum antiferromagnets and cold gases.

TT 12: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2

Time: Monday 15:00–16:30 Location: BH 334

TT 12.1 Mon 15:00 BH 334

Mesoscopic Stoner instability in metallic nanoparticles revealed by shot noise — •Björn Sothmann[1], Jürgen König[2], and Yuval Gefen[3] — [1]Département de Physique Théorique, Université de Genève — [2]Theoretische Physik, Universität Duisburg-Essen — [3]Dept. of Condensed Matter Physics, Weizmann Institute of Science

The interplay between discrete level spacing and exchange interactions of electron spins in metallic nanoparticles leads to the so called mesoscopic Stoner instability. The nanoparticle becomes partially polarized and its spin depends on the ratio of exchange coupling and level spacing.

We study sequential tunneling through a metallic nanoparticle close to the Stoner instability coupled to parallely magnetized electrodes. Transport channels associated with the excitations of the nanoparticle's total spin open up when increasing the bias voltage. This leads to a steplike increase of the current. The Fano factor, in contrast, shows oscillations between large super-Poissonian and sub-Poissonian values as a function of voltage. We explain the enhanced Fano factor in terms of generalized random-telegraph noise and propose the shot noise as a convenient and robust tool to probe the mesoscopic Stoner instability.
[1] B. Sothmann, J. König, Y. Gefen, arXiv:1110.2589v2.

TT 12.2 Mon 15:15 BH 334

Nanotransformation and current fluctuations in exciton-condensate junctions — •Henning Soller and Andreas Komnik — Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, D-69120 Heidelberg

We analyse the transport properties of a bilayer exciton condensate that is contacted by four metallic leads. Using a generic model for the exciton condensate we derive the exact full counting statistics, which allows for the calculation of the nonlinear current-voltage characteristics as well as noise and cross correlations. Despite some similarities to other contacted condensates such as superconductors several features specifically show the properties of the correlated electron-hole exciton states. In particular these can be exploited when contacting the exciton condensate to another mesoscopic system (in our case a quantum point contact) which allows for transforming current on the nanoscale.

TT 12.3 Mon 15:30 BH 334

Dynamic production of entanglement in spin blockade quantum dots — •Rafael Sánchez and Gloria Platero — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)

Double quantum dots connected in series to source and drain electronic reservoirs can be tuned to show current suppression due to Pauli exclusion principle [1]. This effect is known as spin blockade. Driving the system with time dependent magnetic fields allows the coherent manipulation of the two electron states. Single spin rotations removes Pauli correlations and restitutes the flow of current [2,3]. Analyzing the current spectrum as a function of the driving frequency, we find dark resonances where spin blockade is restored due to collective rotations of the two spins. Furthermore, for such frequencies the system evolves towards a maximally entangled stationary state [4]. There, Rabi oscillations of two positive parity Bell states are robust for weak coupling to the reservoirs at low enough temperatures. We investigate the influence of the magnetic field polarization.
[1] K. Ono, D.G. Austing, Y. Tokura, S. Tarucha, Science 297, 1313 (2002).
[2] F.H.L. Koppens, C. Buizert, K. J. Tielrooij, I. T. Vink, K. C. Nowack, T. Meunier, L. P. Kouwenhoven, L. M. K. Vandersypen, Nature 442, 766 (2006).
[3] R. Sánchez, C. López-Monís, G. Platero, Phys. Rev. B 77, 165312 (2008).
[4] R. Sánchez, G. Platero, in preparation

TT 12.4 Mon 15:45 BH 334

DMRG study of transport in quantum dots out of equilibrium — •Elena Canovi, Alexander Moreno, and Alejandro Muramatsu — Institut fuer Theoretische Physik III, Pfaffenwaldring 57, 70550 Stuttgart

We study electrical transport in quantum dots (QD) out of equilibrium by means of the Density Matrix Renormalization Group (DMRG). This method allows to go beyond linear response theory, i.e. to deal with a finite bias, and to handle large interactions. We concentrate on charge fluctuations in QDs and study the interacting resonant level model (IRLM) which describes spinless fermions. The quantum dots are connected to two fermionic reservoirs, modeled as tight-binding chains.

We first study the one-impurity case. We benchmark the correctness of our code against known results for the I-V characteristics, study particle-hole symmetry breaking interactions and the case of generic fillings. We then switch to the case of two impurities, for which we show some new results.

TT 12.5 Mon 16:00 BH 334

Zero-temperature non-linear quantum transport through quantum dots: real-time renormalization-group (RT-RG) calculation of dI/dV stability diagrams — •Roman Saptsov[1,2], Maarten Wegewijs[1,2,3], and Herbert Schoeller[2,3] — [1]Peter Gruenberg Institut, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]JARA- Fundamentals of Future Information Technology — [3]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

The recently developed RT-RG approach was applied to study the non-linear transport through a quantum dot described by the Anderson impurity model. The RT-RG equations were solved numerically including both 1- and 2- loop orders in the limit of zero temperature and non-linear transport voltages where most standard theoretical methods break down. We predict non-perturbative tunneling effects in the transport stability diagram which can be measured experimentally. Moreover, we found the exact functional form of the renormalized spectra of the dot at any loop order. In the non-interacting case we show that the RT-RG recovers the exact solution within our 2 loop approach. In the strong-interacting limit the method breaks down as expected only at very small voltages on the order of the Kondo temperature, which we illustrate by comparison with the Friedel sum rule.

TT 12.6 Mon 16:15 BH 334

Tunneling renormalization of carbon nanotubes cotunneling spectroscopy — •Gediminas Kirsanskas, Karsten Flensberg, and Jens Paaske — Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark

We examine the effects of cotunneling threshold renormalization due to the tunneling in carbon nanotube quantum dots in Coulomb blockade regime. It is shown that tunneling can induce gate dependant splitting of fourfold degenerate levels. This results in gate dependant g-factor. We also find that asymmetric tunneling couplings introduce the asymmetry between the positive and negative bias cotunneling thresholds.

TT 13: Transport: Poster Session

We recommend to hang up the posters already during the morning sessions.

Time: Monday 15:00–19:00 Location: Poster B

TT 13.1 Mon 15:00 Poster B

Lab::Measurement — Measurement control and automation with Perl — Florian Olbrich[1], David Kalok[1], Daniela Taubert[2], Daniel Schröer[2], and •Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department für Physik, LMU München, Geschwister-Scholl-Platz 1, 80539 München, Germany

For quickly setting up varying and evolving complex measurement tasks involving diverse hardware, graphical logic programming quickly reaches practical limits. We present *Lab::Measurement*, a collection of Perl modules designed to control GPIB and serial instruments. It provides an interface to instrumentation control backends as e.g. Linux-GPIB or National Instruments' NI-VISA library. Dedicated instrument driver classes relieve the user from taking care of internal details. Recording a measurement trace, say $I(V_g)$, becomes as easy as programming a single for-loop, and much more complex setups can quickly be implemented. At the same time, the modules provide (live) plotting and metadata handling. *Lab::Measurement* has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

TT 13.2 Mon 15:00 Poster B

Possibility of superconductivity due to electron-phonon interaction in graphene — •Matthias Einenkel and Konstantin Efetov — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany}

We discuss the possibility of superconductivity in graphene taking into account both electron-phonon and electron-electron Coulomb interactions. The analysis is carried out assuming that the Fermi energy is far away from the Dirac points, such that the density of the particles (electrons or holes) is high. We derive proper Eliashberg equations that allow us to estimate the critical superconducting temperature. The most favorable is pairing of electrons belonging to different valleys in the spectrum. Using values of electron-phonon coupling estimated in other publications we obtain the critical temperature as a function of the electron (hole) density. This temperature can reach the order of 10 K at the Fermi energy of order 1-2 eV. We show that the dependence of the intervalley pairing on the impurity concentration should be weak.

TT 13.3 Mon 15:00 Poster B

Quenching photoluminescence in semiconducting nanorods in contact with epitaxial graphene — •Christian Sorger[1], Daniel Waldmann[1], Johannes Jobst[1], Stefan Hertel[1], Adam Faust[2], Uri Banin[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Institute of Chemistry, The Hebrew University, Jerusalem 91904 Israel

It is well known that the photoluminescence of semiconducting particles can be quenched in close vicinity to a metallic surface. In our experiment we deposit CdSe-nanorods in close contact to epitaxially grown graphene [1] and detect the photoluminescence on large areas. Substantial quenching is observed.

We are targeting the dependence of fluorescence quenching on the charge density in the graphene layer, which is tuned by a bottom gate [2]. Vice versa, the influence of photoexcitation on transport properties is investigated.

[1] K. V. Emtsev et al. , Nature Materials **8**, 203 (2009).
[2] D. Waldmann et al. , Nature Materials **10**, 357 (2011).

TT 13.4 Mon 15:00 Poster B

Symmetries and the conductance of graphene nanoribbons with long-range disorder — Jürgen Wurm[1], •Michael Wimmer[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, The Netherlands

We study the conductance of graphene nanoribbons with long-range disorder. Due to the absence of intervalley scattering from the disorder potential, time-reversal symmetry (TRS) can be effectively broken even without a magnetic field, depending on the type of ribbon edge. Even though armchair edges generally mix valleys, we show that metallic armchair nanoribbons possess a hidden pseudovalley structure and effectively broken TRS. In contrast, semiconducting armchair nanoribbons inevitably mix valleys and restore TRS. As a result, in strong disorder metallic armchair ribbons exhibit a perfectly conducting channel, but semiconducting armchair ribbons ordinary localization. TRS is also effectively broken in zigzag nanoribbons in the absence of valley mixing. However, we show that intervalley scattering in zigzag ribbons is significantly enhanced and TRS is restored even for smooth disorder, if the Fermi energy is smaller than the potential amplitude. The symmetry properties of disordered nanoribbons are also reflected in their conductance in the diffusive regime. In particular, we find suppression of weak localization and an enhancement of conductance fluctuations in metallic armchair and zigzag ribbons without valley mixing. In contrast, semiconducting armchair and zigzag ribbons with valley mixing exhibit weak localization behavior.

TT 13.5 Mon 15:00 Poster B

Resonant scattering in graphene with a gate-defined chaotic quantum dot — •Martin Schneider and Piet W. Brouwer — Dahlem Center for Complex Quantum Systems and Institut für theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We investigate the conductance of an undoped graphene sheet with two metallic contacts and an electrostatically gated island (quantum dot) between the contacts. Our analysis is based on the Matrix Green

Function formalism, which was recently adapted to graphene [1]. We find pronounced differences between the case of a stadium-shaped dot (which has chaotic classical dynamics) and a disc-shaped dot (which has integrable classical dynamics) in the limit that the dot size is small in comparison to the distance between the contacts. In particular, for the stadium-shaped dot the two-terminal conductance shows Fano resonances as a function of the gate voltage, which cross-over to Breit-Wigner resonances only in the limit of completely separated resonances, whereas for a disc-shaped dot sharp Breit-Wigner resonances resulting from higher angular momentum remain present throughout. [1] M. Titov, P. M. Ostrovskyi, I. V. Gornyi, A. Schuessler, and A. D. Mirlin, Phys. Rev. Lett. **104**, 076802 (2010)

TT 13.6 Mon 15:00 Poster B

Limitations of pulse-gating schemes for extracting relaxation times in graphene quantum dots — •Sebastian Kazarski[1], Christian Volk[1,2], Christoph Neumann[1], Fabian Hassler[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Institute for Bio- and Nanosystems, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Institute for Quantum Information, RWTH Aachen, 52074 Aachen, Germany

Solid state quantum dots are interesting candidates for future spin-based quantum information technology. In particular carbon materials, such as graphene and nanotubes are interesting for hosting quantum dots since these materials exhibit weak spin-orbit coupling and weak hyperfine interaction promising long spin coherence times. Here, we present low-temperature pulse-gating transport experiments on a graphene quantum dot, which potentially allow us to estimate relaxation times. The experimental data are compared with a detailed numerical simulation of the pulse-gating experiment to extract relaxation times which arise in a graphene quantum dot considering excited (ES) to ground state (GS) transitions. The simulation is based on solving the involved rate equations, taking into account tunnel coupling rates $\Gamma_{L,R}$, the relaxation rate Γ_τ from ES to GS, and a number different pulse-gate configurations. The average current I through the ES and GS, and the averaged electron number per cycle $\langle n \rangle$ are calculated numerically. We can find reasonable agreement with the experiment and discuss the limits of the used technique.

TT 13.7 Mon 15:00 Poster B

Tuning the electronic structure and transport properties in carbon-based devices — •Hernan L. Calvo[1], Claudia G. Rocha[2,3], Horacio M. Pastawski[4], Stephan Roche[5], Gianaurelio Cuniberti[3], and Luis E.F. Foa Torres[4] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen, Germany — [2]Department of Physics, NanoScience Center, University of Jyväskylä, Jyväskylä 40014, Finland — [3]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden D-01062, Germany — [4]IFEG-CONICET, FaMAF, Universidad Nacional de Córdoba, Argentina — [5]CIN2 (ICN-CSIC), Universidad Autónoma de Barcelona, Campus UAB, 08193 Bellaterra (Barcelona), and ICREA, 08070 Barcelona, Spain

Thanks to their outstanding electrical, mechanical and thermal properties, research in carbon-based materials is one of the most rapidly advancing fronts ever. In this work, we study the effects a time-periodic potential induces on the electronic structure and transport properties in graphene and carbon nanotubes. By combining Floquet theory with Green's function formalism, we describe two different situations: (1) the generation of laser-induced band gaps in graphene and (2) the enhancement of the pumped current in carbon nanotubes. For the first case, we show how the band gaps can be tuned by using the laser polarization and describe a strong suppression in the conductance. For the second case, we observe an enhancement of the pumped current by up to two orders of magnitude when gating the system close to a van Hove singularity (vHs).

TT 13.8 Mon 15:00 Poster B

Metal-to-insulator transition and electron-hole puddle formation in disordered graphene nanoribbons — •Holger Fehske and Gerald Schubert — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17487 Greifswald

The experimentally observed metal-to-insulator transition in hydrogenated graphene is numerically confirmed for actual sized graphene samples and realistic impurity concentrations. The eigenstates of our tight-binding model with substitutional disorder corroborate the formation of electron-hole-puddles with characteristic length scales comparable to the ones found in experiments. The puddles cause charge inhomogeneities and tend to suppress Anderson localization. Even though, monitoring the charge carrier quantum dynamics and performing a finite-size scaling of the local density of states distribution, we find strong evidence for the existence of localized states in graphene nanoribbons with short-range but also correlated long-range disorder.

TT 13.9 Mon 15:00 Poster B

CVD growth of carbon nanotubes on ultra-flat hexagonal boron nitride — •Lidia Saptsova[1,2], Stephan Engels[1,2], K. Watanabe[3], T. Taniguchi[3], Carola Meyer[2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Single-walled carbon nanotubes (SWNTs) are promising candidates for hosting high-quality quantum dots (QDs). However, at the present time it is difficult to achieve ultra-clean SWNT QDs on substrates, since the substrate, in particular SiO_2 introduce a significant disorder potential. For graphene devices it was recently shown that placing graphene on hexagonal boron nitride (hBN) significantly improves the device performance. Since hBN is a wide-bandgap insulator, has the graphene-like planar layer structure and is free of dangling bonds and charge traps at the surface, it might be used as a perfect substrate for CNT devices. Here, we present the fabrication technology for making SWNT quantum dots on hBN. We use a Ferritin-based Fe catalyst CVD growth method for obtaining uniformly distributed SWNTs with diameters of about 1.5-2 nm. To study the effect of the substrate material on the disorder in nanotubes, SWNTs lying on both hBN and SiO_2 were chosen using scanning force microscopy. Finally, SWNT QDs on hBN and SiO_2 were obtained by contacting individual 300 nm nanotube sections by metal electrodes.

TT 13.10 Mon 15:00 Poster B

Low temperature transport in carbon nanotubes — •Birgit Kiessig[1,2], Cornelius Thiele[2,3], Ralph Krupke[3], Kai Grube[1], Roland Schäfer[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik — [2]Karlsruher Institut für Technologie, Physikalisches Institut — [3]Karlsruher Institut für Technologie, Institut für Nanotechnologie

We present measurements on gold contacted metallic carbon nanotubes (CNTs) performed in a ^{3}He/^{4}He dilution refrigerator between base temperature ($\sim$ 10 mK) and 5 K. In addition to the electrodes spaced 300-400 nm apart, side gates were implemented 50-150 nm from the CNTs.

IV curves show Coulomb blockade at low voltages which can be lifted by gating. For higher voltages conductance increases nonlinearly and assymmetrically. Transport modifications induced by gate voltage and magnetic field up to 8 T are characterized.

TT 13.11 Mon 15:00 Poster B

Quantum dots in ultra-clean, suspended single-wall carbon nanotubes — •Peter Stiller, Daniel Schmid, Sabine Kugler, Alois Dirnaichner, Christoph Strunk, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Single suspended carbon nanotubes, CVD-grown over pre-defined contacts without any further chemical or lithographic processing, can exhibit their unperturbed electronic level structure in transport spectroscopy. We present measurements on the quantum dot forming in such a nanotube in the few carrier limit, characterizing the electronic and mechanical properties and the interaction of both. The measurements show the transition from strong Coulomb blockade to the Kondo regime on the electron conduction side and from Coulomb blockade to Fabry-Perot interference on the hole conduction side. On the electronic side the few carrier spectrum is characterized in detail, as well as the build-up of Kondo correlations towards higher electron numbers.

TT 13.12 Mon 15:00 Poster B

Magnetoresistance measurements on carbon nanotubes with CoPd contacts — •Dominik Metten[1], Caitlin Morgan[1], Claus M. Schneider[1,2], and Carola Meyer[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut (PGI-6) and JARA Jülich Aachen Research Alliance, 52425 Jülich, Germany — [2]Fachbereich Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

Carbon nanotubes (CNTs) are expected to show a long spin relaxation length because they exhibit small hyperfine coupling and have small spin-orbit interactions. These properties, along with ballistic electron transport, lead to a high potential for applications in the field of spintronics.

We study spin injection in CNT-based devices using $Co_{50}Pd_{50}$ as contacts. Palladium is known to have low contact resistivity to CNTs and is easily spin-polarized by cobalt. Shape anisotropy is used to ensure in-plane magnetization and to prevent formation of multiple domains in the contacts.

Here we present a magnetic characterization of the contacts including SQUID- and MFM-measurements. First magnetoresistance (MR) measurements show an MR effect of 5% with clear switching behavior. Our devices can be tuned using a backgate. Gate dependent measurements reveal different regimes for the MR effect. Since a potential barrier forms at the interface between the contacts and the CNT, tunneling MR is the expected mechanism.

TT 13.13 Mon 15:00 Poster B

Multiterminal electron transport in a quantum dot lattice — •Christian Morfonios[1], Daniel Buchholz[2], and Peter Schmelcher[1] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany

The multiterminal transport of electrons through a lattice of coupled quantum dots is studied in terms of the array topology and geometry, the internal features of its nodes, and an applied magnetic flux. The scattering properties of individual dots are addressed through separation of interfering lead-coupled states, boundary guiding and magnetic deflection. By assembling the dots into a lattice of variable spacing, connectivity and terminal positioning, the possibility of mode-resolved control of scattering between input and output lead states is investigated.

TT 13.14 Mon 15:00 Poster B

Liouville space formulation for interacting quantum dots with superconducting leads — •Jacek Swiebodzinski[1], Dirk Schuricht[2], Jürgen König[1], and Herbert Schoeller[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen, Germany

Following recent advances in nanofabrication, quantum dots in contact with superconducting leads have increasingly moved into the focus of spintronic related research. A key issue is hereby the occurrence of both superconducting correlations and Coulomb interaction combined with a general non-equilibrium situation. In the following contribution we present a diagrammatic method suitable to describe quantum dots with arbitrarily large interactions coupled to normal and superconducting leads. In the latter case transport can be provided either by quasiparticle or Andreev tunneling giving rise to a rich variety of interesting physical phenomena. The method is based upon a perturbative expansion in the dot-reservoir coupling and formulated in Liouville space. As compared to the standard diagrammatic approach in Keldysh space, in the Liouville formulation the two branches of the Keldysh contour are taken together simplifying the diagrammatic language. Relaxation and dephasing rates can be easily read off from the poles of the Liouvillian. We apply the method to a normal lead - quantum dot - superconductor system discussing some of its properties.

TT 13.15 Mon 15:00 Poster B

Dynamics of a doubly Monitored Charge Qubit — •Christian Nietner, Gernot Schaller, Christina Pöltl, and Tobias Brandes — TU Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin

We investigate the electronic transport through two parallel double quantum dots coupled via a perpendicularly aligned charge qubit. In our model, the presence of the qubit leads to a modification of the intrinsic tunnel amplitudes of each double quantum dot. Specifically, the two charge configurations of the qubit are associated with a suppression of the electronic tunneling in the respective double quantum dot. We study the influence of the qubit on the electronic steady state currents through the system. To this end we use a Born-Markov-Secular quantum master equation for the system and apply a full counting statistics ansatz. The obtained currents show signatures of the qubit for all bias regimes. Conversely, the stationary qubit state may be tuned and even rendered pure by applying suitable voltages.

TT 13.16 Mon 15:00 Poster B

Multiply Connected Graph Model for Dephasing in Diffusive Quantum Dots — •Maximilian Treiber, Oleg Yevtushenko, and Jan von Delft — Ludwig Maximilians Universität, Arnold Sommerfeld Center und Center for Nano-Science, München

We propose a model, based on the theory of diffusion in graphs, to study quantum transport through a diffusive quantum dot. The graph consists of a central region composed of many quasi-1d wires describing the dot, and two identical left- and right- wires connected to leads describing contacts. We evaluate the conductance for this model and compare our results to random matrix theory (RMT). An advantage compared to RMT-models is that we can take into account interaction-induced dephasing at finite temperatures. We present results for the temperature dependence of the weak localization correction and discuss the possibility to observe the elusive 0D-regime of dephasing in quantum dots.

TT 13.17 Mon 15:00 Poster B

Thermoelectric performance of quantum pumps — •Federica Haupt[1], Stefan Juergens[1], Michael Moskalets[2], and Janine Splettstoesser[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52074 Aachen, Germany — [2]Department of Metal and Semiconductor Physics, Kharkiv Polytechnical Institute, 61002 Kharkiv, Ukraine

Prototypical examples of quantum pumps are systems formed by one or a few coupled quantum dots, whose tunneling barriers and/or energy levels are modulated in time by external gate voltages. These devices can be regarded in many respects as quantum engines, with the difference that while classical engines are typically systems working out of equilibrium between hot and cold sources, the phenomenon of quantum pumping becomes especially relevant around equilibrium conditions. This makes a non trivial task the generalization to quantum pumps of concepts such as efficiency, typically used to quantify the performance of classical engines. To address this problem, we investigate in detail charge and energy current in different models of interacting quantum pumps, as well as their thermoelectric properties when brought out of equilibrium. This allows us to identify suitable quantities that permit to characterize the performance of the pump both at and out of equilibrium.

TT 13.18 Mon 15:00 Poster B

Finite Frequency Noise Spectrum of the Anderson Impurity Model — •Christoph Orth[1,2] and Andreas Komnik[1] — [1]Institut für Theoretische Physik, Universität Heidelberg — [2]Department of Physics, University of Basel

Quantum noise is an inherent property for quantum information and nanoscale physics. We analyze the finite frequency current noise spectrum of a quantum dot described by a two-terminal Anderson impurity model at bias voltage V. We focus on the electron-electron interaction effects in the electron-hole symmetric case: (i) perturbatively up to the second order in the interaction strength, and (ii) using a random phase approximation for the two-particle vertex function (screened interaction) to go beyond perturbation theory. Our method is based on a non-equilibrium Keldysh Green's function technique and is exact in tunneling.

An exact analytical formula is found for the non-interacting case which shows a staircase like structure with steps whenever ω reaches a characteristic energy of the system. The electron-electron interaction leads to non-vanishing correlations of currents with opposite spin. For small U we observe that the spectrum develops a distinct threshold at $\omega < -V/2$ and peaks at $\omega \approx V/2$. We expect that our results capture the generic properties of the noise spectra, which is also supported by recent publications.

TT 13.19 Mon 15:00 Poster B

Transport measurements on single Bi nanowires at temperatures below 1 K — •Arnold Seiler[1], Christopher Reiche[1,2], Torben Peichl[1], Sven Müller[3], Maria E. Toimil-Molares[3], Christina Trautmann[3], and Georg Weiss[1,2] — [1]Physikalisches Institut, KIT Karlsruhe — [2]Centrum für funktionelle Nanostrukturen, KIT Karlsruhe — [3]GSI Darmstadt

Bismuth is an interesting semimetal for studies of electronic transport phenomena at low temperatures and reduced dimensions due to its large Fermi wavelength and long mean free path. Previous experiments with bundles of crystalline Bi wires embedded in a polycarbonate membrane show a decrease in resistance below 300 mK. Different

measurements of Bi nanowires suggest that this drop is caused by superconductivity. This may be induced by surface oxidation or surface contaminants. Our Bi wires are fabricated by electrodeposition using an ion-track etched membrane as a template. We use an all organic process to extract the nanowires from the membrane without oxidation of the surface and developed various methods to contact single Bi wires in a 4-point geometry. Thus, the transport properties of Bi nanowires were successfully measured down to temperatures below 50 mK. Obtained results indicate that, depending on the growth conditions, the wires have a tendency to become either superconducting or insulating.

TT 13.20 Mon 15:00 Poster B

Electric transport and tunnel measurements on pure copper nanowires — •Maksym Kompaniiets[1], Dirk Klingenberger[1], Fabrizio Porrati[1], Oleksandr Dobrovolskiy[1], Oleksandr Foyevtsov[1], Cornelia Neetzel[2], Markus Rauber[2], Maria Eugenia Toimil-Molares[3], Wolfgang Ensinger[2], Christina Trautmann[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe Universität, Frankfurt a. M. — [2]Fachbereich Materialwissenschaften, TU Darmstadt, Darmstadt — [3]3GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt

Cu and Cu/Fe nanowires of well-defined shape and composition are well-suited for studying the spin-dependent scattering resistance contribution of ferromagnets and Kondo systems. We present first four-probe ac-resistance and tunnel measurements on cross-type junctions of individual nanowires with diameters of about $250 - 300$ nm and length of about $30-60$ μm. The nanowires have been prepared by electrochemical deposition in etched heavy-ion-track polycarbonate membranes (templates). For contacting individual nanowires ion beam induced deposits of $W - Ca - Ga - O$ electrodes with the precursor gas $W(CO)_6$ in a dual-beam SEM/FIB were used. Electric transport measurements on pure Cu nanowires reveal a decreasing resistivity with decreasing temperature, as is expected for metallic nanowires. Furthermore, in tunneling spectroscopy measurements we found clear indications of proximity-effect induced superconductivity in the Cu nanowires below 5 K, i.e. the critical temperature of the $W-C-Ga-O$ composites electrodes.

TT 13.21 Mon 15:00 Poster B

Weak localization and magnetoresistance in two-chain ladder models — •Michael P. Schneider, Sam T. Carr, Igor V. Gornyi, and Alexander D. Mirlin — Institut für Theorie der kondensierten Materie, KIT, D-76128 Karlsruhe

We study the weak localization correction to the conductivity of a disordered two-chain ladder in the limit of strong dephasing, paying particular attention to magnetoresistance. We observe an anomalous behaviour of the magnetoresistance in a specific range of parameters, due to a competition between an interference effect and the dimensionality of the system, and predict the curious phenomenon of magnetic field enhanced localization.

TT 13.22 Mon 15:00 Poster B

Magnetotransport properties of nanoporouse gold films — •Jaqueline Weissbon, Andreas Gondorf, Martin Geller, and Axel Lorke — Faculty of Physics and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

Nanoporous gold layers are prepared by etching thin films of Au/Ag-alloys in HNO_3. The morphology of the nanoporous films is determined by scanning electron microscopy for different etching conditions. The films are patterned into Hall bar geometries and their magnetotransport properties are investigated as a function of temperature. In the magnetic field range $B = 0 - 12$ T, we find a linear Hall resistance $\rho_{xy}(B)$ and a quadratic longitudinal magnetoresistance $\Delta\rho_{xx}(B) \propto B^2$. In the temperature range between 20 K and 350 K, we find a roughly linearly increasing specific resistance. The results are compared with recent reports in the literature [1,2] and discussed within the Fuchs-Sonderheimer model of scattering in thin films.
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[2] R. C. Munoz, M. A. Suarez, S. Oyarzun, R. Henrique, A. Espinosa, G. Kremer, L. Moraga, S. Cancino and R. Morales, Physical Review B, 81, 165408 (2010)

TT 13.23 Mon 15:00 Poster B

Spin polarized transport through noncollinear single-electron spin-valve transistors — •Stephan Lindebaum and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CeNIDE, D-47048 Duisburg

We study the electronic transport through a noncollinear single-electron spin-valve transistor, i.e., a metallic island with a continuous electron density of states tunnel coupled to two ferromagnetic leads. The polarization directions of the ferromagnets enclose an arbitrary angle. In the considered system, charging and spin effects play an important role and influence the transport behavior of the transistor. Furthermore, the interplay of Coulomb interaction and tunnel coupling to spin-polarized leads yields a many-body exchange field, in which the accumulated island spin precesses.

We derive kinetic equations for the island charge and spin within a diagrammatic real-time transport formalism. In our theory we perform a perturbative analysis of the transport properties up to first order in the tunnel-coupling strength (sequential-tunneling limit), which is reasonable due to the weak island-lead coupling.

Our formalism enables to analyze both the linear and nonlinear transport regimes. The electric current through the transistor and the accumulated island spin are considered in detail. In particular, we find that the exchange field can give rise to a high sensitivity of the island's spin orientation on the gate voltage.
[1] S. Lindebaum and J. König, arXiv:1109.5800v1

TT 13.24 Mon 15:00 Poster B

Quantum transport through coupled quantum dots attached to a Large spin — •Klemens Mosshammer, Gerold Kiesslich, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

We investigate theoretically the magneto-transport through a system of two coupled single level quantum dots, connected to ferromagnetic leads, where the electron spin is coupled to an external (pseudo-)spin via an exchange interaction, introducing non-linear dynamics. The system is examined using a semi-classical technique in combination with a quantum master equation approach to describe the sequential tunneling trough the system. We find regimes where the average current through the quantum dot system displays self-sustained oscillations reflecting limit-cycles behaviour of the transport electrons.

TT 13.25 Mon 15:00 Poster B

Charge transport in molecule-graphene nanojunctions using complex absorbing potentials — •Susanne Leitherer, Ivan Pshenichnyuk, Pedro B. Coto, and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Charge transport in molecule-graphene nanojunctions is studied employing the Landauer formalism in combination with complex absorbing potentials (CAPs). Within this approach, the self-energies, which describe molecule-electrode coupling in an extended system, are obtained using absorbing potentials and finite graphene electrodes. The performance of different CAPs is discussed, including CAPs in polynomial form [1] as well as CAPs derived using the WKB approximation [2,3]. The method is applied to molecular junctions consisting of a pentacene molecule and a polyyne chain between graphene electrodes.
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TT 13.26 Mon 15:00 Poster B

Statistical model for the effects of phase and momentum randomization on electron transport — •Thomas Stegmann[1], Matías Zilly[1], Orsolya Ujsághy[2], and Dietrich E. Wolf[1] — [1]Department of Physics, University of Duisburg-Essen and CeNIDE, Duisburg, Germany — [2]Department of Theoretical Physics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Budapest, Hungary

Recently, we have introduced a statistical model for the effects of dephasing on the transport properties of large systems [1]. This model has been applied successfully on the conduction of DNA molecules [2] and the dephasing-induced conductivity in the 1D Anderson model [3]. Now, we present an extension of our model which allows to adjust the degree of phase and momentum randomization independently.

As a first result, we demonstrate that the resistance of an ordered tight-binding chain is independent of the chain length and the degree of phase randomization if the dephasing is momentum conserving. In contrast, the resistance increases if the dephasing is momentum ran-

domizing.
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[2] M. Zilly, O. Ujsághy and D. E. Wolf, Phys. Rev. B, **82**:125125 (2010)
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TT 13.27 Mon 15:00 Poster B

Decoherence-induced conductivity in the 1D Anderson model: Resistivity, generalized Lyapunov exponents and localization length — •Matías Zilly[1], Orsolya Ujsághy[2], Marko Woelki[3], Thomas Stegmann[1], and Dietrich E. Wolf[1] — [1]Fakultät für Physik und CeNiDE, Universität Duisburg-Essen, Duisburg, Germany — [2]Department of Theoretical Physics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Budapest, Hungary — [3]Theoretische Physik, Universität des Saarlands, Saarbrücken, Germany

A recently proposed statistical model for the effects of decoherence on electron transport [1] manifests a decoherence-driven transition from quantum-coherent localized to ohmic behavior when applied to the Anderson model. Here [2] we derive the resistivity in the ohmic case and study the critical decoherence density at which the transition takes place. This density is shown to be related to the second-order generalized Lyapunov exponent, which under the assumption of a Gaussian limiting distribution for the logarithm of the transmission $\ln T$ allows to determine the localization length.
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[2] M. Zilly, O. Ujsághy, M. Woelki, and D. E. Wolf. arXiv:1111.6014

TT 13.28 Mon 15:00 Poster B

Attenuated total reflection (ATR)-study of the reversible switching of immobilized ring-opening/ring-closure molecular switches — •Katharina Luka-Guth[1], Dmytro Sysoiev[2], Youngsang Kim[1], Johannes Boneberg[1], Paul Leiderer[1], Jannic Wolf[2], Thomas Huhn[2], Ulrich Groth[2], and Elke Scheer[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Fachbereich Chemie, Universität Konstanz

We study the conformational changes of the photochromic difurylperfluorocyclopentene molecules induced by optical switching by attenuated total reflection (ATR) measurements.

A single layer of molecules is chemisorbed on a 40-nm thin layer of gold. We measure the reflected intensity of near infrared-light that is coupled-in from the rear side of the molecular layer on gold on a glass substrate (Kretschmann geometry) and observe the reflection decrease due to the excitation of surface plasmons at the interface between gold and the determine the atmosphere. Upon irradiation with UV and red light, respectively, the molecules are switched between the open, low-conducting and the closed, highly conducting state. We detect the change of the ATR signal while switching for a series of molecules in lock-in technique and discuss their potential applications in molecular electronics devices.

TT 13.29 Mon 15:00 Poster B

Electrical characterization of single molecules in liquid environments — Matthias Wieser, •Torsten Sendler, Jochen Grebing, and Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf

We have developed the mechanical controllable break junction technique for the use in liquid environments in order to characterize the electrical properties of single molecules in their solvents. The metallic electrodes, which form the contacts for the molecular structures, are produced on an insulating substrate in order to reduce all spurious effects coming from parallel conduction through the liquid. We present first electrical characterization of such junctions in dry and in liquid environments. The solvents range from aqueous buffer, which will be used for measurements of DNA fragments, to toluene and THF, which are typical solvents for short, conjugated organic molecules.

TT 13.30 Mon 15:00 Poster B

Large shot noise levels in single-molecule junctions due to electronic-vibrational coupling — •Christian Schinabeck, Rainer Härtle, and Michael Thoss — Institut für Theoreti-sche Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

We investigate shot noise in transport through single-molecule junctions using a master equation approach that is based on a second order expansion in the molecule-lead coupling [1]. Recently, large shot noise levels have been reported for a variety of single-molecule junctions with different molecular species [2]. This indicates that electrons are tunneling through these contacts in avalanches rather than in statistically uncorrelated tunneling events. Such a transport behaviour was found by Koch et al. for a model comprising a single electronic state that is very strongly coupled to a single vibrational mode [3]. In this contribution, we show that a weak to moderate coupling of the electrons to a multitude of vibrational modes may also give rise to large shot noise levels, as observed in experiments [2].
[1] C. Flindt *et al.*, Physica E 29, 411-418 (2005).
[2] D. Secker *et al.*, Phys. Rev. Lett. 106, 136807 (2011).
[3] J. Koch *et al.*, Phys. Rev. B 74, 205438 (2006).

TT 13.31 Mon 15:00 Poster B

Time-dependent transport through fluctuating molecular wires — •Bogdan Popescu and Ulrich Kleinekathöfer — Jacobs University Bremen, Germany

In the present study, the electron transport through a quantum wire, modeled as a linear chain of tight-binding sites and coupled to external fermion leads, is investigated using several distinct formalisms: nonequilibrium Green's functions [1], the hierarchical equations of motion approach [2] and by a perturbation expansion [3]. The first two methods are known to be exact for noninteracting fermions. Several accuracy and performance tests involving all three methods have been carried out for different configurations (site energy differences, voltages, temperatures). The propagation schemes are suited to be applied to investigate time-dependent transport through molecular wires, e.g., DNA molecules, where the on-site energies and next-neighbour couplings are time-dependent due to solvent fluctuations. First tests in this direction will be demonstrated.
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TT 13.32 Mon 15:00 Poster B

Vibration induced memory effects in molecular nanojunctions — •Abdullah Yar, Andrea Donarini, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We investigate the bistability and memory effects for a single molecule weakly coupled to metallic leads subject to time-dependent voltage. The system is described by an Anderson-Holstein model and its dynamics is calculated via a master equation approach. Particular emphasis is given to the role played by the excited vibronic states in the bistability and hysteretic switching dynamics as a function of the voltage sweeping rates. We discuss how the hysteretic behavior depends on the asymmetry of the voltage drop through the junction as well as on the time scales of voltage sweeping and quantum switching rates between metastable states.

TT 13.33 Mon 15:00 Poster B

The role of the tip symmetry on the STM topography of π-conjugated molecules — •Benjamin Siegert, Sandra Sobczyk, Andrea Donarini, and Milena Grifoni — Institute of Theoretical Physics, University of Regensburg, Germany

Motivated by recent STM experiments, where either Cu tips or CO-functionalized tips have been adopted [1], we compare theoretically the influence of *s*-, *p*- and *d*-wave tip states on the current maps of π-conjugated molecules. Our theory is based on the density matrix formalism and it is sufficiently general to be applied to any STM device consisting of a π-conjugated molecule weakly coupled to the substrate and the tip. Here we concentrate on the study of the topography of benzene, pentacene and hydrogen phthalocyanine. Our formalism is able to mirror experimental results quite well showing that the shape of the recorded images is strongly related to the orbital structure of the tip.
[1] L. Gross, *et al.*, Phys. Rev. Lett. **107**, 086101 (2011)

TT 13.34 Mon 15:00 Poster B

Current fluctuations in capacitively coupled double quantum dots — •Robert Hussein and Sigmund Kohler — Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

Based on a recent work [1], we study a coherent quantum ratchet that is driven by tunnel oscillations. It is realised by two capacitively coupled double quantum dots — the driving circuit is biased but undetuned, while the ratchet circuit is detuned but unbiased. We investigate the full counting statistics (FCS) of both subsystems and compare the results to those of an effective master equation in which the driving circuit is eliminated. While higher order cumulants exhibit discrepancies, Fano factor, skewness and kurtosis are in good agreement.
[1] M. Stark and S. Kohler, EPL 91, 20007 (2010)

TT 13.35 Mon 15:00 Poster B

Induced thermal gradient and quantum shot noise cross-talk in neighboring nanodevices — •Johannes Buelte[1], Federica Haupt[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52074 Aachen, Germany

Motivated by recent experimental results showing strong modifications of the current through a carbon nanotube quantum dot (QD) due to the bias voltage applied to a close-by graphene constriction, we investigate theoretically the cross-talk between neighboring nanodevices. We first show that several of the observed features can be understood assuming that a temperature gradient across the QD develops as the bias applied to the graphene constriction is increased. Next, we consider a model where the biased graphene constriction is treated as non-equilibrium electromagnetic environment for the quantum dot, and use such a model to a) draw a clear connection between the voltage applied to the former and the effective temperature gradient across the QD; b) investigate the dependence of the current in the QD on the spectral properties of the electromagnetic environment itself.

TT 13.36 Mon 15:00 Poster B

Light emission of tunneling electrons interacting via a localized plasmon — •Fei Xu[1], Federica Haupt[2], Cecilia Holmqvist[1], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, Aachen, Germany

Photon emission in electron tunneling can be related to current noise, which is an important tool to investigate quantum many-body effects in electron transport in a non-equilibrium mesoscopic conductor. Recent experiments on photon emission from atomic-size tunnel junctions formed by an STM tip and a metallic surface showed a considerable intensity of photons emitted with a frequency larger than the applied bias voltage $\hbar\omega > eV$ [1,2]. This is a fingerprint of electronic correlations involving electromagnetic plasmonic modes involving both the surface and the tip apex. We address the problem of this over-bias photon emission in terms of non-equilibrium current fluctuations in a conductor interacting with an electromagnetic environment. The latter can mediate tunneling processes, resulting in two electrons teaming up to cross the junction and emitting a single photon with energy higher than eV [3]. We model the plasmon resonance as an electrical RLC circuit and find that non-Gaussian noise yields one-photon emission with over-bias energy.
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TT 13.37 Mon 15:00 Poster B

Effects of Synchronisation and Noise in Coupled Optomechanical Arrays — •Michael Schneider[1], Georg Heinrich[1], and Florian Marquardt[1,2] — [1]Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1/Bau 24, 91058 Erlangen, Germany

Optomechanical systems couple light stored inside an optical resonator to the motion of a mechanical mode. Recent experiments have demonstrated setups, such as photonic crystal structures, that in principle allow one to confine several optical and vibrational modes on a single chip. For an array of several coupled optomechanical cells interesting nonlinear behaviour, especially synchronisation, arises. Here we investigate these dynamics and the effects of external noise thereupon. In particular we show how synchronisation affects phase stability.

TT 13.38 Mon 15:00 Poster B

Microcantilevers for Torque Magnetometry — •Stefanos Chalkidis, Stephan Albert, Benedikt Rupprecht, Marc Wilde, and Dirk Grundler — James-Franck-Straße 1, 85747 Garching, Deutschland

Torque magnetometry has proven to be powerful to measure magnetic oscillations of two-dimensional electron systems (2DES) at low temperature. For conventional 2DES in, e.g., semiconductor heterostructures, corresponding cantilevers supported 2DES of 1 mm2. Graphene, the first truly 2D crystal, is an intriguing candidate for examination by torque magnetometry. Our calculations show that magnetic oscillations in exfoliated high-mobility graphene are roughly four orders of magnitude smaller than for the conventional 2DES due to small sample size. This necessitates the development of miniaturized cantilevers. We report our calculation and the progress in the preparation of such cantilevers by reactive-ion-etching from the device layer of a silicon-on-insulator wafer. We will discuss different sensor designs that we analyze either analytically or by finite element simulations. Financial support by the DFG via project no. WI3320/1-1 in the priority programme "Graphene" is gratefully acknowledged as well as experimental support by the Nanosystems Initiative Munich.

TT 13.39 Mon 15:00 Poster B

Dynamics and decoherence in the Gaudin model — •Daniel Stanek, Carsten Raas, and Götz S. Uhrig — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund

The Gaudin or central spin model describes a single qubit which interacts with a bath of non-interacting spins 1/2, e.g., nuclear spins in a quantum dot. The model is widely applied in the fields of nuclear magnetic resonance and quantum information processing.

Using time-dependent density matrix renormalization group (tDMRG), we calculate the time-evolution of the qubit which is initialized in a well-defined state out of equilibrium. A detailed analysis of the longitudinal as well as of the transverse relaxation of the qubit for various distributions of the couplings between bath and qubit is presented. In addition, we discuss different initial states of the bath and their influence on the decoherence of the qubit.

TT 13.40 Mon 15:00 Poster B

Decoherence of Josephson junction qubits due to surface spins — •Pablo Schad[1], Boris Narozhny[1], Alexander Shnirman[1,2], and Gerd Schön[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Spins on surfaces of superconductors are considered to be responsible for the 1/f flux noise in SQUIDs and Josephson qubits [1,2,3,4,5]. In recent experiments the spin contribution to the inductance of superconducting wires was measured [6]. This inductance describes the response to a current, which polarizes spins by creating magnetic fields on the surface. In particular, low frequency fluctuations of the complex inductance were observed with roughly a 1/f noise spectrum. We provide an analysis of inductance noise in analogy to the theory of "noise of noise" and analyze some microscopic models that could explain these experiments. Special attention is paid to RKKY interaction.
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TT 13.41 Mon 15:00 Poster B

Full Counting Statistics applied to dissipative Cooper Pair Pumps — •Philip Wollfarth[1], Ingo Kamleitner[1], and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

We investigate geometric charge pumping in superconducting Josephson devices [1,2] using the method of Full Counting Statistics [3]. In previous studies the expectation value of the current operator was calculated and a very delicate handling of the dissipative master equation [4] governing the dynamics of the system was required. E.g., the rotating wave (secular) approximation turned out to be non-charge-conserving [5]. We include the counting field (charge measuring device) into the master equation and investigate the influence of voltage fluctuation on the pumping process.
[1] M. Möttönen et al., Phys. Rev. B 73, 214523 (2006).
[2] J.P.Pekola et al., Phys. Rev. B 60, R9931 (1999).

[3] L.S. Levitov et al., J. Math. Phys. 37, 10 (1996).
[4] H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems.
[5] J. Salmilehto, P. Solinas, and M. Möttönen, arXiv:1110.5427 [quant-ph] (2011).

TT 13.42 Mon 15:00 Poster B

Quantum metamaterials with superconducting flux qubits — •Pascal Macha[1], Gregor Oelsner[1], Markus Jerger[2], Uwe Hübner[1], Susanne Butz[2], Evgeni Il'ichev[1], Alexey V. Ustinov[2], and Hans-Georg Meyer[1] — [1]Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology and DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany

In recent years superconducting qubits have opened up a new route to explore the physics of quantum metamaterials. Artificial materials, formed by many qubits, can potentially exhibit unusual and controllable refraction (transmission) coefficients in the microwave range. We have fabricated cavities and transmission lines containing 20 flux qubits and more. We experimentally investigate the transmission of electromagnetic waves through these new types of media. First experimental results will be presented and discussed.

TT 13.43 Mon 15:00 Poster B

The Back Action of Josephson Photomultipliers — •Luke C.G. Govia[1,2], Emily J. Pritchett[2], Seth T. Merkel[2], Deanna Pineau[3], and Frank K. Wilhelm[2] — [1]Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Ontario, Canada — [2]Theoretical Physics, Universität des Saarlandes, Saarbrücken, Germany — [3]Department of Physics and Astronomy, University of Victoria, British Columbia, Canada

We describe the Josephson photomultiplier, a photon counter applicable to circuit QED. We show that its backaction is described by the regular photon annihilation operator at short interaction times and approaches a variant of the photon subtraction operator at long times. Understanding this backaction opens the opportunity to use multiplexed photomultipliers for, e.g., state tomography with few preparations.

TT 13.44 Mon 15:00 Poster B

A strategy to measure the Lamb shift in a superconducting two-level system embedded in a thermal broadband reservoir — •Vera Gramich[1], Paolo Solinas[2,3], Mikko Möttönen[2,3], Jukka Pekola[3], and Joachim Ankerhold[1] — [1]Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Department of Applied Physics/COMP, Aalto University, P.O. Box 14100, FI-00076 Aalto, Finland — [3]Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 Aalto, Finland

Realistic quantum systems are never completely isolated. Even a single atom in zero-temperature vacuum is influenced by the zero-point fluctuations of the electromagnetic field which in turn induces a shift of its transition frequencies known as the Lamb shift. Cavity quantum electrodynamics (QED) provides a particularly convenient setup to observe this shift since the restricted geometries of the cavities allow the atoms to interact only with the fluctuations of single harmonic fields. In contrast to single-frequency environments, typical reservoirs for mesoscopic solid-state devices are characterized by broadband spectral distributions in thermal equilibrium. Within weak-coupling master equations even explicit expressions for the reservoir-induced frequency shifts can be derived, while associated experimental observations are still missing. To fill this gap, we discuss and analyze a theoretical proposal to retrieve the Lamb shift for a superconducting two-level system embedded in an ohmic environment. Moreover, we present a possible way to measure the Lamb shift in a circuit containing a Cooper pair sluice.

TT 13.45 Mon 15:00 Poster B

Compact superconducting coplanar microwave beam splitters — •Alexander Baust[1,2], Norbert Kalb[2], Max Haeberlein[1,2], Jan Goetz[1,2], Elisabeth Hoffmann[1,2], Edwin P. Menzel[1,2], Manuel J. Schwarz[1,2], Friedrich Wulschner[1,2], Ling Zhong[1,2], Thomas Losinger[2], Frank Deppe[1,2], Achim Marx[1,2], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TUM, Garching, Germany

The recent evolution of circuit quantum electrodynamics systems making use of standing-wave microwave modes towards setups for propagating quantum microwaves has triggered the need for low-loss superconducting microwave beam splitters. Such a device should have ports compatible with the coplanar geometry relevant for circuit QED and, at the same time, be compact allowing for scalability. This combination presents fundamental and technological challenges. In this work, we present the fabrication and characterization of various compact superconducting coplanar microwave beam splitters. In addition, we discuss efforts towards a tunable beam splitter.

This work is supported by the DFG via SFB631 and by the German Excellence Initiative via NIM.

TT 13.46 Mon 15:00 Poster B

Strong coupling of paramagnetic spins to a superconducting microwave resonator — •Moritz Greifenstein[1], Christoph Zollitsch[1], Johannes Lotze[1], Fredrik Hocke[1], Rudolf Gross[1,2], Sebastian T.B. Goennenwein[1], and Hans Huebl[1] — [1]Walther-Meissner-Institut (WMI), Garching, Germany — [2]Physik-Department, TU München, Garching, Germany

Under application of an external magnetic field, non-interacting electron spins behave as an ensemble of identical two-level-systems with tuneable transition frequency. When such an ensemble collectively interacts with a single mode of an electromagnetic resonator, the entire system can be described as two coupled quantum harmonic oscillators. The criterion for the observation of the so-called strong coupling regime is that the collective coupling strength g exceeds both the loss rate of the resonator κ and of the spin ensemble γ.

In our experiment we realize a coupled spin-photon-system by introducing the spin marker DPPH (2,2-diphenyl-1-picrylhydrazyl) into the mode volume of a superconducting coplanar microwave resonator and investigate the interaction at 2.5, 5.0 and 7.5 GHz. For tuning the resonance, we apply an in-plane magnetic field and observe interaction at around ± 90, ± 180 and ± 270 mT. While the coupling with the fundamental mode and the first harmonic mode of the resonator is identified as weak, the second harmonic shows $g = 21$ MHz, $\kappa = 6$ MHz and $\gamma = 5$ MHz, i.e. the strong coupling regime. We further investigate the dependence of g on temperature and on microwave input power. This work is financially supported by DFG via SFB 631.

TT 13.47 Mon 15:00 Poster B

Master Equation Description of Subsystem and Subspace Qubits — •Sebastian Mehl[1,2] and David P. DiVincenzo[1,2] — [1]Peter Grünberg Institute: Theoretical Nanoelectronics, Research Center Jülich, D-52428 Jülich — [2]Institute for Quantum Information, RWTH Aachen, D-52056 Aachen

It is possible to implement and control qubits in a higher dimensional Hilbert space. Especially for spin based solid state qubits this approach is widely used to improve phase coherence properties. Encoded qubits are currently experimentally analyzed in double and triple quantum dot setups [1, 2].

We present the idea to encode qubits in a subspace and a subsystem of a Hilbert space [3]. Starting from a simple model describing the dissipative evolution of the density matrix in the full Hilbert space we develop a master equation description for the subsystem and subspace approach. Particular attention is paid to the influence of the chosen approach on the memory kernel of the Master equation.

[1] R. Hansen et al., Rev. Mod. Phys. 79, 1217 (2007)
[2] E. A. Laird et al., Phys. Rev. B 82, 075403 (2010)
[3] J. Kempe et al., PRA, 63, 042307 (2001)

TT 13.48 Mon 15:00 Poster B

Perfect state transfer in XX chains induced by boundary magnetic fields — •Thorben Linneweber, Joachim Stolze, and Götz S. Uhrig — Institut für Physik, TU Dortmund, Germany

A recent numerical study of short chains found near-perfect quantum state transfer between the boundary sites of a spin-1/2 XX chain if a sufficiently strong magnetic field acts on these sites. We show that the phenomenon is based on a pair of states strongly localized at the boundaries of the system and provide a simple quantitative analytical explanation.

TT 13.49 Mon 15:00 Poster B

Enhancing the hyperfine spin decoherence time of holes in quantum dots by strain — •Franziska Maier and Daniel Loss — Department of Physics, University of Basel, 4056 Basel, Switzerland

In this work we theoretically examine the effect of strain on the single

spin decoherence time T_2 of a heavy hole confined to a cylindrical InAs semiconductor quantum dot. To this end, we include strain in the **k·p**-Hamiltonian describing the states in the lowest conduction bands (CB) and the heavy hole (HH), light hole (LH) and split-off (SO) bands of the dot. For non-zero strain we find a modification of the existing confinement-induced hybridization of the HH states [1] which strongly depends on explicit values of the strain tensor components. Hyperfine interaction between the hybridized HH states and the surrounding nuclear spin bath leads to a reduction of the hole spin decoherence time T_2. Our results reveal that T_2 cannot only be tuned by external parameters such as nuclear polarization or external magnetic fields as it has been previously shown, but also by choosing different strain configurations.
[1] J. Fischer and D. Loss, Phys. Rev. Lett. **105**, 266603 (2010)

TT 13.50 Mon 15:00 Poster B

A Superconducting Quantum Register with Multiplexed Readout — •Markus Jerger[1], Stefano Poletto[1], Pascal Macha[1,2], Uwe Hübner[2], Jürgen Lisenfeld[1], Alexander Lukashenko[1], Evgeni Il'ichev[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany

A resonant circuit coupled to a qubit experiences a shift of its resonance frequency that depends on the quantum state of the qubit. By coupling every qubit to an individual readout resonator, the state of a quantum register of many qubits can be read out through a single transmission line connected to all resonators. The readout of all qubits can be performed simultaneously using digital modulation and de-modulation techniques. We experimentally demonstrate the simultaneous multiplexed readout of up to seven qubits through a single line. We integrated this readout system into a circuit QED architecture consisting of qubits interacting via a quantum cavity bus. Our latest measurements aiming at the demonstration of quantum gates will be presented.

TT 13.51 Mon 15:00 Poster B

Topological insulators in cold-atom gases with non-Abelian gauge fields: the role of interactions — •Peter Philipp Orth[1], Daniel Cocks[2], Stephan Rachel[3], Michael Buchhold[2], Karyn Le Hur[4,3], and Walter Hofstetter[2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]Institut für Theoretische Physik, Goethe Universität, 60438 Frankfurt/Main, Germany — [3]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [4]Center for Theoretical Physics, Ecole Polytechnique, 91128 Palaiseau Cedex, France

With the recent technological advance of creating (non)-Abelian gauge fields for ultracold atoms in optical lattices, it becomes possible to study the interplay of topological phases and interactions in these systems. Specifically, we consider a spinful and time-reversal invariant version of the Hofstadter problem. In addition, we allow for a hopping term which does not preserve S_z spin symmetry and a staggered sublattice potential. Without interactions, the parameters can be tuned such that the system is a topological insulator. Using a combination of analytical techniques and the powerful real-space dynamical mean-field (R-DMFT) method, we discuss the effect of interactions and determine the interacting phase diagram.

TT 13.52 Mon 15:00 Poster B

Magnetic impurities on edges of topological insulators — •Florian Goth and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The realization of the Spin-Hall-Effect in quantum wells has led to a plethora of studies regarding the properties of the edge states of a 2D topological insulator. These edge states constitute a class of one-dimensional liquids, called the helical liquid, where an electron's spin direction is coupled to its direction of movement. In contrast to one dimensional conductors, magnetic impurities – below the Kondo temperature – cannot block transport and one expects the current to circumvent the impurity. To study this phenomenon, we consider the single impurity Anderson model embedded into an edge of a Kane-Mele ribbon and use numerically exact continuous time QMC methods to study the Kondo effect. We will present results on the temperature dependence of the double occupancy as well as on the local spin susceptibility. To track the edge state we equally compute the temperature dependence of the local spectral function.

TT 13.53 Mon 15:00 Poster B

Topological Superconductivity in the Kitaev-Heisenberg model and the effect of impurities — •Lukas Kimme, Timo Hyart, and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany

The Kitaev-Heisenberg (KH) model describes the transition between a spin liquid and an antiferromagnet, and it is expected to be realised in iridates on the honeycomb lattice [1]. Viewing the Kitaev spin model as a Mott insulator at half filling, we investigate the competing interactions away from that limit by applying a slave boson theory. Contrary to the Heisenberg interaction the Kitaev interaction prefers topologically interesting p-wave superconductivity, which in the doped regime is robust against a comparatively strong Heisenberg coupling [2]. In the context of d-wave superconductors, understanding the effect of an isolated impurituy has contributed valuable insights into the nature of the superconducting state. In addition to scattering quasi-particles, an impurity is expected to lead to a local disruption of the strongly correlated ground state, which breaks triplet correlations in the KH model. As this effect cannot be captured in a T-matrix approach for quasi-particles, we perform a fully self-consistent numerical study of the local density of states in the vicinity of an impurity, including the modification of local superconducting order by the impurity.
[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009).
[2] T. Hyart, A.R. Wright, G. Khaliullin and B. Rosenow, preprint arXiv:1109.6681 (2011).

TT 13.54 Mon 15:00 Poster B

Weyl superconductors — •Tobias Meng[1] and Leon Balents[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, 93106-4030, U.S.A.

We study the physics of the superconducting variant of Weyl semimetals, which may for instance be realized in multilayer structures comprising topological insulators and superconductors. We show how superconductivity splits each Weyl node into two. The resulting Bogoliubov Weyl nodes can be pairwise independently controlled, allowing to access a set of phases characterized by different numbers of bulk Bogoliubov Weyl nodes and chiral Majorana surface modes. We analyze the physics of vortices in such systems, which trap zero energy Majorana modes only under certain conditions. We finally comment on possible experimental probes, thereby also exploiting the similarities between Weyl superconductors and 2-dimensional $p + ip$ superconductors.

TT 14: Matter At Low Temperature: Multiferroics (jointly with MA, DF, DS, KR

Time: Monday 16:45–18:00 Location: H 3005

Invited Talk TT 14.1 Mon 16:45 H 3005

Multiferroicity in an organic charge-transfer salt: Electric-dipole-driven magnetism — •Peter Lunkenheimer[1], Jens Müller[2], Stephan Krohns[1], Florian Schrettle[1], Alois Loidl[1], and Michael Lang[2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Physics, Goethe-University Frankfurt, Germany

Multiferroics, showing simultaneous electrical and magnetic ordering, are remarkable materials from both an academic and technological point of view. A prominent mechanism is the spin-driven ferroelectricity, often found in materials with helical spin order. However, recently a different mechanism, namely purely electronic ferroelectricity, where charge order breaks inversion symmetry, has attracted considerable interest. In the present talk, I will treat examples for both types of multiferroics like perovskite manganites and magnetite, concentrating on their dielectric properties, which often are only poorly characterized. An especially interesting case is a two-dimensional or-

ganic charge-transfer salt, which shows ferroelectricity, accompanied by antiferromagnetic spin order and belongs to a new class of multiferroics [1]. In this material, the ferroelectric ordering leads to a breaking of spin frustration, which triggers simultaneous dipolar and spin order. Hence, here the spin order is driven by the ferroelectricity, in marked contrast to the spin-driven ferroelectricity in helical magnets.
[1] P. Lunkenheimer, J. Müller, S. Krohns, F. Schrettle, A. Loidl, B. Hartmann, R. Rommel, M. de Souza, C. Hotta, J.A. Schlueter, M. Lang, preprint (arXiv:1111.2752).

TT 14.2 Mon 17:15 H 3005

Critical dynamics in $LiCuVO_4$ — •Christoph Grams[1], Maximilian Schalenbach[1], Daniel Niermann[1], Sandra Niesen[1], Petra Becker[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Kristallographie, Universität zu Köln, Germany

Without an external magnetic field $LiCuVO_4$ has a phase transition into a cycloidal spin ordered phase below 2.3 K where it simultaneously is antiferromagnetic and ferroelectric. The transition temperature of this phase transition can be lowered with increasing magnetic field.

Ferroelectric phase transitions are of continuous fashion and are accompanied with a symmetry lowering that yields soft modes. Near the critical point the dynamics of the ionic polarization mechanisms are slowed down and therefore denoted as critical ("critical slowing down").

We observe the critical dynamics of the low temperature multiferroic phase transition of $LiCuVO_4$ with broadband dielectric spectroscopy. Therefore the compound's dielectric response to an external electric AC field of frequencies from 10 mHz to several GHz in the temperature range 20 mK to 300 K was measured in dependence of magnetic fields up to 14 T.

Work supported by the DFG through SFB 608.

TT 14.3 Mon 17:30 H 3005

Vortex domain walls in helical magnets — •Thomas Nattermann[1], Fuxian Li[2], and Valery L. Pokrovsky[2,3] — [1]Institut für Theoretische Physik, Universität zu Köln, D-50937 Köln, Germany — [2]Department of Physics, Texas A&M University, College Station, Texas 77843-4242 — [3]Landau Institute for Theoretical Physics, Chernogolovka, Moscow District, 142432, Russia

The theory of domain walls in both centrosymmetric and non-centrosymmetric helical magnets is presented. With the exception of discrete orientations domain walls consist of an array of parallel vortex lines, their width is only weakly depending anisotropy, in contrast to ferromagnets and antiferromagnets. In conical phases vortex walls carry Berry phase flux which gives rise to an anomalous Hall effect. In multi-ferroics vortices are electrically charged.

TT 14.4 Mon 17:45 H 3005

Infrared and THz spectroscopy in multiferroic $Eu_{1-x}Ho_xMnO_3$ — •Zhenyu Chen[1], Michael Schmidt[1], Franz Mayr[1], Zhe Wang[1], A.A. Mukhin[2], Joachim Deisenhofer[1], and Alois Loidl[1] — [1]Experimentalphysik V, EKM, University of Augsburg, 86135 Augsburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia

We investigated $Eu_{1-x}Ho_xMnO_3$ with the concentration varying from 0.1 to 0.5. On cooling, $Eu_{0.9}Ho_{0.1}MnO_3$ enters an incommensurate antiferromagnetic phase, which turns into an commensurate antiferromagnetic one at lower temperatures. Doping leads to ferroelectricity with polarization parallel to the a-axis, which flips to P//c by further doping. In order to detect the coupling between low energy phonons and electromagnons [1-4], we performed systematic polarization dependent IR and THz studies. The data will be compared to $TbMnO_3$ and the related system $Eu_{1-x}Y_xMnO_3$.
[1] A.Pimenov et al., Nature Phys., 2, 97(2006).
[2] A.Pimenov et al., Phys. Rev. B, 77, 014438(2008).
[3] N.Kida et al., Phys. Rev. B, 78, 104414(2008).
[4] R.Valdés Aguilar et al., Phys. Rev. Lett., 102, 047203(2009).

TT 15: Correlated Electrons: Quantum Impurities, Kondo Physics 1

Time: Monday 16:45–18:00 Location: BH 334

TT 15.1 Mon 16:45 BH 334

Two-electron transfer dynamics in a donor-acceptor system coupled to a dissipative bosonic bath — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We model a donor-acceptor (DA) system coupled to a dissipative bosonic bath which is motivated by electron charge transfer within a DNA base pair. Using the time-dependent numerical renormalization-group (TD-NRG) we study the time-dependent electron dynamics in the DA system where two excess charges are initially localised on the donor. We consider the influence of the coupling strength of the DA system to the bosonic bath on the thermalisation. Additionally we introduce a finite bias between the donor and acceptor level and investigate the crossover between the two different regimes where the charge transfer is dominated by sequential or pairwise electron hopping.

TT 15.2 Mon 17:00 BH 334

Hybrid TD-NRG and tDMRG method — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a non-equilibrium hybrid method which uses the numerical renormalization group (NRG) to generate an effective low energy Hamiltonian. This Hamiltonian is then solved with the density matrix renormalization group (DMRG) thereby reducing the major drawbacks of both methods: (i) discretization errors are minimized by not using a pure Wilson chain and (ii) long time scales can be simulated even for a very large bandwidth. The validity of this method is established by comparing the results to exact results for the resonant level model (RLM). We also apply this new NRG+DMRG hybrid method to the interacting RLM, which is not exactly solvable, and compare with analytic results in the limit $U \to \infty$.

TT 15.3 Mon 17:15 BH 334

NRG calculations of the magnetization of isotropic and anisotropic Kondo impurities — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Bielefeld, Germany

The deposition of magnetic molecules on suitable substrates renders the addressing and thus manipulation of individual molecules possible and might facilitate their use for information storage or quantum computing purposes. However, the magnetic properties of the molecules, which are crucial for the proposed applications, will in general be influenced by the interaction with the substrate. Our goal is to better understand the form and extent of this effect by studying simplified model systems.

To this end, we perform Numerical Renormalization Group (NRG) calculations for single-impurity Kondo models with additional uniaxial anisotropy and a local or bulk magnetic field. The impurity part of the model might thus serve as a minimal representation of a magnetic molecule. We focus on the impurity magnetization, which has been measured in a number of experiments using XMCD and STM, and study its dependence on temperature and applied field for different anisotropy parameters. In case of a "hard axis" anisotropy, the magnetic field can lead to effective groundstate degeneracies and can therefore induce Kondo screening effects.

TT 15.4 Mon 17:30 BH 334

Numerical Renormalization Group for the Partially Broken SU(3) Kondo Model: 2-Channel Kondo Fixed Point. — •Evaristus Fuh Chuo, Laszlo Borda, and Johann Kroha — Physikalisches Institut der Universität Bonn, Germany

We use the numerical renormalization group (NRG) to investigate the partially broken two-channel SU(3) Kondo model with conserved conduction electron spin, comprised of a quantum impurity with a unique ground state and an excited doublet of the SU(2) subgroup of SU(3). The model was proposed earlier by Arnold et al. [1] to describe rotational impurities in a metal, like hydrogen ions in the interstitial space of a lattice, in order to explain the conductance anomalies (zero-bias anomaly and conductance spikes) found by Ralph and Buhrman [2] in point contact spectroscopy on ultrasmall Cu point contacts. We find a downward renormalization of the excited state energy by the

Kondo correlations in the SU(2) doublet. In a wide range of parameter values this stabilizes the two-channel Kondo fixed point, in full agreement with the earlier perturbative RG results of Arnold et al. [1]. We map out the phase diagram of the model in the parameter space of excited-state level spacing and of the Kondo couplings within the excited state doublet and between the impurity ground and excited states, respectively. The robustness of the model with respect to dynamical screening as well as to coupling to higher impurity excitations is discussed.

[1] M. Arnold, T. Langenbruch, and J. Kroha, Phys. Rev. Lett. **99**, 186601 (2007).
[2] D. C. Ralph and R. A. Buhrman, Phys. Rev. Lett. **69**, 2118 (2007).

TT 15.5 Mon 17:45 BH 334

Finite-frequency noise of the anisotropic Kondo model at finite bias and magnetic field: a real-time renormalization group analysis — •Sarah Müller, Sabine Andergassen, Dirk Schuricht, Mikhail Pletyukhov, and Herbert Schoeller — Institut für Theorie der Statistischen Physik und JARA - Fundamentals of Future Information Nanotechnology, RWTH Aachen University

The non-equilibrium electron transport through mesoscopic systems dominated by spin fluctuations is affected by the relaxation and decoherence processes resulting from the coupling of the spin to its environment. The understanding of their origin and their impact on the transport properties is of fundamental importance. We here study the finite-frequency noise of a quantum dot in the Kondo regime in presence of a magnetic field by using the real-time renormalization group in frequency space [1]. Based on a systematic expansion in the reservoir-system coupling, we integrate out the reservoir degrees of freedom and provide an analytic solution of the resulting two-loop RG equations in the weak-coupling regime. In particular, the relaxation and decoherence rates characterizing the non-equilibrium transport of mesoscopic systems emerge during the RG flow. We extend the approach of Ref. [2] to derive analytic expressions for the finite-frequency noise in the stationary state. We discuss the results in relation to recent experiments [3].

[1] H. Schoeller, Eur. Phys. J. Special Topics 168, 179 (2009).
[2] D. Schuricht and H. Schoeller, Phys. Rev. B 80, 075120 (2009).
[3] J. Basset et al., arXiv:1110.1570.

TT 16: Correlated Electrons: Low-dimensional Systems - Models 2

Time: Tuesday 9:30–13:15 Location: H 0104

TT 16.1 Tue 9:30 H 0104

The flat-band ferromagnetic transition as a Pauli-correlated percolation transition — •Mykola Maksymenko[1], Andreas Honecker[2], Roderich Moessner[3], Johannes Richter[4], and Oleg Derzhko[1] — [1]ICMP, 79011 Lviv, Ukraine — [2]ITP Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]MPIPKS, 01187 Dresden, Germany — [4]Universität Magdeburg, Germany

It is known that flat bands yield a route to ferromagnetism in the Hubbard model, but the actual location and nature of the para-ferro transition remain unknown. We study the N-site Hubbard model on the 2D Tasaki lattice. For electron densities $n \leq \mathcal{N} = N/3$ many-electron ground states can be constructed from one-particle states localized in trapping cells. Occupation of neighboring traps may lead to an increase of energy due to on-site repulsion U. However, if electrons in neigboring traps are in a symmetric spin state, due to the Pauli principle on-site repulsion is not active, i.e. electrons can form a ferromagnetic cluster. This problem can be analyzed as a new Pauli-correlated site-percolation problem on the square lattice, where due to the Kramers degeneracy of independent ferromagnetic clusters different cluster coverings of electrons obtain different weights. We provide an exact solution for the corresponding 1D case and a numerical algorithm for the 2D case of the new percolation problem. In 2D the para-ferro transition takes place at concentration $p = n/\mathcal{N} = p_f = 0.66 \pm 0.01$ that is well above the threshold for the standard percolation $p_c \approx 0.59$. Moreover, there exists a region above p_f where ferromagnetism is unsaturated.

TT 16.2 Tue 9:45 H 0104

Accurate determination of the Gaussian transition in spin-1 chains with single-ion anisotropy — •Shijie Hu[1,2], Bruce Normand[1], Xiaoqun Wang[1], and Lu Yu[3] — [1]Department of Physics, Renmin University of China, Beijing 100872, China — [2]Institut fuer Theoretische Physik, Georg-August-Universitaet Goettingen, 37077 Goettingen, Germany — [3]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

The Gaussian transition in the spin-one Heisenberg chain with single-ion anisotropy is extremely difficult to treat, both analytically and numerically. We introduce an improved DMRG procedure with strict error control, which we use to access very large systems. By considering the bulk entropy, we determine the Gaussian transition point to 4-digit accuracy, $D_c/J = 0.96845(8)$, resolving a long-standing debate in quantum magnetism. With this value, we obtain high-precision data for the critical behavior of quantities including the ground-state energy, gap, and transverse string-order parameter, and for the critical exponent, $\nu = 1.472(2)$. Applying our improved technique at $J_z = 0.5$ highlights essential differences in critical behavior along the Gaussian transition line.

TT 16.3 Tue 10:00 H 0104

Spontaneous Quasiparticle Decay in Low-Dimensional Quantum Spin Systems — •Tim Fischer and Götz S. Uhrig — Theoretische Physik I, Technische Universität Dortmund, 44221 Dortmund

In sufficiently dimerized quantum antiferromagnets the elementary excitations are gapped spin $S = 1$ triplon quasiparticles. Although these triplons are protected by a gap at low energies they may decay spontaneously at higher energies where the one-triplon dispersion merges with the two-triplon continuum. The decay implies the breakdown of the quasiparticle picture. No quantitative description by a Lorentzian resonance is possible.

We characterize the decay for low-dimensional quantum antiferromagnets in detail. In particular, three qualitatively different scenarios are identified depending on the one-triplon dispersion and the two-triplon interaction.

Based on the theoretical concepts we analyse the inelastic neutron scattering (INS) results for IPA-$CuCl_3$ [1]. Starting from the microscopic model obtained by adapted continuous unitary transformations (CUTs) [2] we provide a quantitative description of the decay measured in IPA-$CuCl_3$ by INS.

[1] T. Masuda *et al.* (2006) PRL **96** 047210
[2] T. Fischer, S. Duffe and G. S. Uhrig (2011) EPL **96** 47001

TT 16.4 Tue 10:15 H 0104

Channel-decomposed renormalization group equations for the vertex in a superconductor — •Andreas Eberlein and Walter Metzner — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

We study ground state properties of the attractive Hubbard model at weak coupling with the aim of finding an efficient description of the effective Nambu two-particle vertex in a singlet superconductor. We decompose the vertex into a sum of interaction channels, each capturing a particular singular dependence on external momenta and frequencies. Using the functional renormalization group, we derive flow equations for the interaction channels on one-loop level. We compute the frequency dependence of the self-energy as well as the momentum and frequency dependence of the two-particle vertex. Our results for the impact of fluctuations on the superconducting gap are in good agreement with the literature. This indicates that the channel-decomposition scheme indeed captures the singular momentum and frequency dependence of the vertex.

TT 16.5 Tue 10:30 H 0104

Functional RG for the Anderson Impurity Model — •Michael Kinza[1], Jutta Ortloff[2], Manuel Schmidt[1], and Carsten Honerkamp[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland — [2]Insititut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

We present a functional Renormalization Group (fRG) approach to the Anderson Impurity model at finite temperatures. Starting with

the exact spectral function and interaction vertex of a small system ('core') containing a correlated site, we switch on the hybridization with a non-interacting bath in the RG-flow and calculate spectra of the correlated site. We discuss the emergence of the Kondo-scale in different truncation-levels of the RG-flow-equations and for different choices of the core. Therefore the effective mass and the linear conductance as function of temperature and magnetic field is calculated. Furthermore we discuss an extension of our approach that can describe Anderson-impurities in helical liquids.

TT 16.6 Tue 10:45 H 0104

A renormalization group approach to time dependent transport through correlated quantum dots — •Dante Marvin Kennes[1], Severin Georg Jakobs[1], Christoph Karrasch[2], and Volker Meden[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, 52056 Aachen, Germany — [2]Department of Physics, University of California, Berkeley, California 95720, USA

We introduce a real time version of the functional renormalization group which allows to study correlation effects on nonequilibrium transport through quantum dots. Our method is equally capable to address (i) the relaxation out of a nonequilibrium initial state into a steady state driven by a bias voltage and (ii) the dynamics governed by an explicitly time-dependent Hamiltonian. All time regimes from transient to asymptotic can be tackled; the only approximation is the consistent truncation of the flow equations at a given order. As an application we investigate the relaxation dynamics of the interacting resonant level model which describes a fermionic quantum dot dominated by charge fluctuations. Moreover, we study decoherence and relaxation phenomena within the ohmic spin-boson model by mapping the latter to the interacting resonant level model.

TT 16.7 Tue 11:00 H 0104

A New View of the Mott-Hubbard Transition: Renormalization of the Fermi-Surface Topology — •Luca Fausto Tocchio[1], Federico Becca[2], and Claudius Gros[1] — [1]Institute of Theoretical Physics, Goethe University, Frankfurt am Main, Germany — [2]International School for Advanced Studies (SISSA), Trieste, Italy

We present the renormalization of the (underlying) Fermi-surface topology in the Hubbard model on a square lattice with frustrating hopping, that is relevant for the physics of high-temperature superconductors. With the help of novel high precision variational tools, including Jastrow factors and backflow correlations, we show that the Fermi surface renormalizes to perfect nesting at the interaction-driven Mott-Hubbard transition and in the large interaction limit. Moreover, we present new results for the density-driven Mott-Hubbard transition, investigating the Fermi-surface renormalization flow as a function of doping, where the renormalization occurs only when the half-filled case is insulating. Finally, we show also that Fermi surface renormalization is associated to a strong crossover at finite doping for the critical U corresponding to the Mott-Hubbard transition.

15 min. break.

TT 16.8 Tue 11:30 H 0104

Charge Fractionalization on Quantum Hall Edges — •Mats Horsdal[1], Marianne Rypestøl[2], Hans Hansson[3], and Jon Magne Leinaas[2] — [1]Institute for Theoretical Physics, University of Leipzig, D-04009 Leipzig, Germany — [2]Department of Physics, University of Oslo, N-0316 Oslo, Norway — [3]Department of Physics, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden

I will discuss the propagation and fractionalization of localized charges on the edges of quantum Hall bars of variable widths, where interactions between the edges give rise to Luttinger liquid behavior with a non-trivial interaction parameter g. I will focus in particular on the separation of an initial charge pulse into a sharply defined front charge and a broader tail. The front pulse describes an adiabatically dressed electron which carries a non-integer charge, which is $\sqrt{g}$ times the electron charge. I will discuss how the presence of this fractional charge can, in principle, be detected through measurements of the noise in the current created by tunneling of electrons into the system. The results are illustrated by numerical simulations of a simplified model of the Hall bar.

TT 16.9 Tue 11:45 H 0104

Valence bond crystal and possible analog of a supersolid in a t_{2g} orbital model — •Fabien Trousselet[1], Arnaud Ralko[2], and Andrzej M. Oleś[1,3] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut Néel, Grenoble, France — [3]Marian Smoluchowski Institute of Physics (Jagiellonian University), Kraków, Poland

We investigate an orbital model for localized t_{2g} electrons on the triangular lattice, and interacting via exchange processes between nearest neighbors. The Hamiltonian interpolates between two limits where either superexchange or direct-exchange predominates; it is relevant to some titanate compounds (e.g. $NaTiO_2$), in a situation where spins are polarized by e.g. a large magnetic field.

Within this frame, we analyze the ground state properties of the model, by exact diagonalizations and the use of effective Hamiltonians. When superexchange interactions dominate, they favor orbital singlets on nearest neighbor bonds, which results in a dimerized phase. We characterize this phase, with help of an effective quantum dimer model, as a valence bond crystal with a large unit cell. In the opposite regime of dominant direct-exchange, we find another exotic phase, which can be seen as an orbital analog of a supersolid, where long-ranged orbital order coexists with dynamics induced by perturbing kinetic terms.

TT 16.10 Tue 12:00 H 0104

Phase diagram of the bilinear-biquadratic-bicubic spin 3/2 chain — •Stephan Rachel[1] and Andreas M. Läuchli[2] — [1]Department of Physics, Yale University, New Haven, CT 06520, USA — [2]Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

The most general spin 3/2 chain with SU(2) invariant nearest neighbor interactions is investigated. Using exact diagonalization and density matrix renormalization group the corresponding phase diagram is explored. It hosts a plethora of phases. Besides the critical and ferromagnetic phases containing the usual Heisenberg models, we find dimerized, partial ferromagnetic, and a period-4 phase with enhanced SU(4) symmetry. Furthermore, in the vicinity of the antiferromagnetic Heisenberg point we identify a period-6 phase.

TT 16.11 Tue 12:15 H 0104

Application of Valence Bond States to Nano-Sized Spin Clusters — •Maren Gysler, Nikolaos P. Konstantinidis, and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

The importance of understanding correlations in nano-sized spin clusters has risen in recent years with the availability of magnetic systems such as single-molecule magnets and spins attached to surfaces, which consist of a dozen or so antiferromagnetically coupled metal centers with potentially large spin lengths. Strong correlations between neighboring spins are difficult to single out when the familiar product basis or irreducible tensor operator techniques are used. The valence bond states can be used in an efficient way to study ground-state correlations of the clusters as strong short range quantum correlations can naturally be captured by them.

In this talk we will present a general method to use valence bond states as an alternative basis for the antiferromagnetic Heisenberg Hamiltonian of spin clusters with arbitrary exchange coupling strength, spins, and coupling topologies. The complications due to the overcompletness and non-orthogonality are circumvented by diagonalizing the Hamilton matrix in the spin coupled basis. Subsequently the spin coupled states are expressed in what we call the physical valence bond states. The developed method will be applied to special examples of spin clusters for illustration.

TT 16.12 Tue 12:30 H 0104

Entanglement of hard-core bosons in bipartite lattices — •Raoul Dillenschneider, Xue-Feng Zhang, and Sebastian Eggert — Physics Dept. and Res. Center OPTIMAS, Univ. of Kaiserslautern, 67663 Kaiserslautern, Germany.

The entanglement of hard-core bosons in square and honeycomb lattices with Coulomb interactions is estimated by means of quantum Monte Carlo simulations and spin-wave analysis. The particular U(1)-invariant form of the concurrence is used to establish a connection with observables such as density and superfluid density. For specific regimes the concurrence is expressed as a combination of boson density and superfluid density. Symmetry breaking is demonstrated characterizing entanglement patterns.

TT 16.13 Tue 12:45 H 0104

The effect of a local perturbation in a fermionic ladder — Sam Carr[1], •Boris Narozhny[1], and Alexander Nersesyan[2,3,4] — [1]Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]The Abdus Salam International Centre for Theoretical Physics, 34100, Trieste, Italy — [3]The Andronikashvili Institute of Physics, 0177, Tbilisi, Georgia — [4]Ilia State University, Institute of Theoretical Physics, 0162, Tbilisi, Georgia

We study the effect of a local external potential on a system of two parallel nanowires placed close to each other. For single channel, spin-polarized nanowires with repulsive interaction we find that transport properties of the system are highly sensitive to the transverse gradient of the perturbation: the asymmetric part completely reflects the electrons leading to vanishing conductance at zero temperature, while the flat potential remains transparent. We envisage a possible application of this unusual property in the sensitive measurement of local potential field gradients. We then further extend our results to the case of nanowires in the absence of the polarized field.

TT 16.14 Tue 13:00 H 0104

Constraints on measurement-based quantum computation in effective cluster states — Daniel Klagges and •Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The aim of this work is to study the physical properties of a one-way quantum computer in an effective low-energy cluster state. We calculate the optimal working conditions as a function of the temperature and of the system parameters. The central result of our work is that any effective cluster state implemented in a perturbative framework is fragile against special kinds of external perturbations. Qualitative aspects of our work are important for any implementation of effective low-energy models containing strong multi-site interactions.

TT 17: Superconductivity: Fe-based Superconductors - 122 Part 2 & Theory

Time: Tuesday 9:30–12:30 Location: H 2053

TT 17.1 Tue 9:30 H 2053

Intra-gap absorption in iron-pnictide $Ba(Fe_{1-x}Co_x)_2As_2$ films — •Sina Zapf[1], Boris Gorshunov[1,2,3], Dan Wu[1], Elena Zhukova[1,2,3], Vadim Nozdrin[2], Silvia Haindl[4], and Kazumasa Iida[4] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institute of General Physics, RAS, Russia — [3]Moscow Institute of Physics and Technology, Russia — [4]Institut für Metallische Werkstoffe, IFW Dresden, Germany

Optical measurements on $Ba(Fe_{1-x}Co_x)_2As_2$ thin films [1] indicated strong intra-gap absorption (dynamical conductivity) in the superconducting (SC) state. There, conductivity at lowest frequencies was extracted with rather large uncertainty caused by huge negative dielectric constants, which is a common problem in optical measurements of superconductors. Our aim now was to perform further, more detailed investigation on the THz response of $Ba(Fe_{1-x}Co_x)_2As_2$ films. We measured their complex transmissivity with a coherent-source Terahertz (THz) spectrometer over a wide frequency range and demonstrate a remarkable improvement in resolving the frequency and temperature dependence of the intra-gap optical conductivity. Additionally, in order to enhance the interaction of the radiation with the SC films, we have performed further measurements: Two identical films on dielectric LSAT substrates were positioned face-to-face separated by a spacer, leading to multiple Fabry-Pérot resonances. We present an analysis of such a five layer system that describes the increase in sensitivity to the dynamical conductivity and discuss the experimental challenges and improvements.

[1] B. Gorshunov et al., Phys. Rev. B 81, 060509 (2010)

TT 17.2 Tue 9:45 H 2053

Electronic phase diagram of Co-doped $BaFe_2As_2$ films prepared by PLD — •Fritz Kurth, Kazumasa Iida, Jens Hänisch, Steffen Oswald, Konstantin Nenkov, Jochen Werner, Ludwig Schultz, Bernhard Holzapfel, and Silvia Haindl — IFW Dresden, Helmholtzstrasse. 20, 01069 Dresden; Germany

$Ba(Fe_{1-x}Co_x)_2As_2$ thin films with different Co-concentrations, x, were prepared on Fe-buffered MgO(100) substrates using pulsed laser deposition under ultra high vacuum conditions. All films were grown epitaxially with high phase purity as confirmed by X-ray diffraction. The c-axis lattice parameter was observed to decrease with increasing x, as observed as well in bulk material. The superconducting transition temperature, T_c, shows the typical dome shaped dependence on x where the maximum T_c of over 26 K is found at a doping level of $x = 0.044$, which is different from the results observed on single crystals and bulk pellets. This difference might be due to a change in the Co or As stoichiometry in the films compared to the nominal target compositions. A detailed chemical analysis by Auger electron spectroscopy reveals Co diffusion into the Fe buffer. At high deposition temperatures a large gradient of the Co-content is observed from 18,2 % to 8,7 %. Finally, transport properties of the doping series will be presented in this talk. This work was supported by DFG under Project no. HA5934/3-1.

TT 17.3 Tue 10:00 H 2053

Signatures of non-Fermi liquid behavior in hole-doped and chemically pressurized $EuFe_2As_2$ single crystals — •Jeevan .s Hirale, Jannis Maiwald, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany

We report a detailed study of the effect of hole-doping and chemical pressure (isovalent doping) in single crystals of $K_xEu_{1-x}Fe_2As_2$ and $EuFe_2(As_{1-y}P_y)_2$, respectively, by measurements of the thermopower, $S(T)$, and electrical resistivity, $\rho(T)$. In this class of FeAs-based superconductivity (SC), it is found that SC appears close to a magnetic instability, suggesting a possible unconventional pairing mechanism. We have synthesized single crystals of both K and P doped samples by the self-flux method. Upon doping Eu with K >30%, T_{SDW} gets suppressed and SC appears with $T_{c,max} \approx 34$ K. Additionally, the Eu^{2+} ordering is suppressed to low temperatures, due to the dilution of magnetic moments. On the other hand, P doping the As site suppresses the SDW transition and results in a SC phase at y >16%. The electrical resistivity data suggest non-Fermi liquid behavior near $x = 0.5$ and $y = 0.2$. This is supported by the observation of a logarithmic divergence in the thermoelectric power coefficient S/T for both systems. We also observe distinct signatures in the thermopower evolution at $x_{cr} = 0.30$ and $y_{cr} = 0.22$, which may hint at Lifshitz transitions of the Fermi surface.

Work supported by DFG through priority program SPP 1458.

TT 17.4 Tue 10:15 H 2053

In-plane anisotropy of electrical resistivity and thermoelectric power in underdoped $EuFe_2(As_{1-x}P_x)_2$ single crystals — •Shuai Jiang[1,2], Hirale S. Jeevan[1], Jannis Maiwald[1], Martin Dressel[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]1. Physikalisches Institut, Universität Stuttgart, Germany

We have studied the in-plane anisotropy of detwinned isovalent substituted $EuFe_2(As_{1-x}P_x)_2$ single crystals using a uniaxial pressure clamp. In the studied regime $0 < x \leq 0.12$ the structural and magnetic phase transitions are clearly separated. We reveal that the structural transition breaks the C_4 rotational symmetry and induces nematic phase via the in-plane anisotropic measurements of resistivity and thermoelectric power. The observed anisotropy in both properties indicates the existence of nematic phase below the structural phase transition. A reconstruction of the Fermi surface below the magnetic transition is deduced by the thermopower anisotropy. Additionally, the resistivity anisotropy is larger than the orthorhombic distortion, indicating the difference of underlying electronic excitation near Fermi surface. The anisotropy below the Néel transition is caused by the intrinsic electronic structure, whereas the electronic nematicity plays an important role for the larger anisotropy above the Néel transition.

15 min. break.

TT 17.5 Tue 10:45 H 2053

Magnetic Resonance from the Interplay of Frustration and

Superconductivity — •Johannes Knolle[1], Ilya Eremin[2], Jorg Schmalian[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [3]Karlsruhe Institute of Technology, Institute for Theory of Condensed Matter, D-76131 Karlsruhe, Germany

Motivated by iron-based superconductors, we develop a self-consistent electronic theory for the itinerant spin excitations in the regime of coexistence of the antiferromagnetic stripe order with wave vector $Q_1 = (\pi, 0)$ and s± superconductivity. The onset of superconductivity leads to the appearance of a magnetic resonance near the wave vector $Q_2 = (0, \pi)$, where magnetic order is absent. This resonance is isotropic in spin space, unlike the excitations near Q_1, where the magnetic Goldstone mode resides. We discuss several features which can be observed experimentally. In particular, we find that the additional subtle effects of microscopic coexistence of AF and s± SC order, such as damping of the spin waves at Q_1 and the modified dispersing behavior of the spin resonance around Q_2, can be used by INS to distinguish the coexistence phenomenon from phase separation effects.

TT 17.6 Tue 11:00 H 2053

Spectral density in a nematic state of a three-orbital model for iron pnictides — •Maria Daghofer[1], Andrew Nicholson[2], and Adriana Moreo[2] — [1]IFW Dresden, Germany — [2]University of Tennessee and Oak Ridge National Laboratory, TN, USA

We study a nematic phase, i.e., broken rotational symmetry without long-range magnetic order, for a three-orbital model describing the dominant orbitals and bands around the Fermi surface of pnictide superconductors. Using cluster-perturbation theory, we calculate the spectral density $A(\mathbf{k}, \omega)$ for the case of very short-range magnetic order that chooses the ordering vector $(\pi, 0)$ over the equivalent $(0, \pi)$ and thus breaks the fourfold lattice symmetry. The resulting asymmetry between the xz band at $Y = (0, \pi)$ and the yz band $X = (\pi, 0)$ is in very good agreement with angle-resolved photo-emission spectroscopy: The yz bands at X moves to higher energies. We also discuss the impact of onsite Coulomb repulsion and orbital polarization.

TT 17.7 Tue 11:15 H 2053

Eight-band model for the iron arsenides studied by functional RG — •Julian Lichtenstein, Stefan Maier, and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University

We analyze the superconducting instabilities in eight-band models for the iron arsenides by a functional renormalization group approach. This approach allows us to include the arsenic p-states and their nonlocal interactions directly without having to use descriptions where these states are included via down-folding of the single-particle part and additional screening of the interactions. We compare the results with those found in five-band studies and discuss trends of the superconducting instability as function of various material parameters.

TT 17.8 Tue 11:30 H 2053

Small-q Phonon Mediated Unconventional Superconductivity in the Iron Pnictides — •Alex Aperis[1], Panagiotis Kotetes[1,2], Georgios Varelogiannis[1], and Peter M. Oppeneer[3] — [1]Department of Physics, National Technical University of Athens, GR-15780 Athens, Greece — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Department of Physics and Materials Science, Uppsala University, Box 530, S-751 21 Uppsala, Sweden

We report full momentum-dependent self-consistent calculations of the gap symmetry for the iron-based high-temperature superconductors using a realistic small-q phonon mediated pairing potential within a four-band model. When both electron and hole Fermi surface pockets are present, we obtain the nodeless $s_\pm$ state that was first encountered in a spin-fluctuations mechanism picture. Nodal gap structures such as $d_{x^2-y^2}$, $s_\pm + d_{x^2-y^2}$ and even a p-wave *triplet* state, are accessible upon doping within our phononic mechanism [1]. Our results *resolve* the conflict between phase sensitive experiments reporting a gap changing sign attributed previously only to a non-phononic mechanism and isotope effect measurements proving the involvement of phonons in the pairing. Application of our theory to specific members of the pnictide family will also be briefly discussed.
[1] A. Aperis *et al.*, Phys. Rev. B **83**, 092505 (2011).

TT 17.9 Tue 11:45 H 2053

Competing antiferromagnetic states in the pnictides — •Philip M. R. Brydon, Jacob Schmiedt, and Carsten Timm — Technische Universität Dresden, Dresden, Germany

Motivated by the complicated nesting properties of the Fermi surface [1], we present a study of the magnetic order in the pnictides focusing upon the competition of the observed stripe order with other commensurate and incommensurate states. Starting from a phenomenological microscopic model, we derive the mean-field Ginzburg-Landau free energy, and systematically construct the magnetic phase diagram as a function of the doping and key band structure parameters [2]. We show that the number, location, and relative size of the hole pockets crucially controls the magnetic state, which we explain in terms of the competition between different nesting instabilities. We discuss the implications for electronic-only models of the magnetic order.
[1] J. Schmiedt, P. M. R. Brydon, and C. Timm, arXiv:1108.5296 (unpublished).
[2] P. M. R. Brydon, J. Schmiedt, and C. Timm, arXiv:1109.2071 (accepted for publication in Phys. Rev. B).

Invited Talk TT 17.10 Tue 12:00 H 2053

Magnetism and Superconductivity: A new era of convergence in condensed matter physics — •Piers Coleman — Center for Materials Theory, Rutgers University, Piscataway, New Jersey

Three years after the discovery of superfluid He-3 was discovered, Physicists first observed heavy fermion superconductivity, yet the open mind-set required to embrace these results as a discovery, rather than a materials artifact was lacking. It took the efforts of a brave and determined set of heavy electron pioneers, to overcome this resistance and change the mind-set.

Today, we are increasingly conscious of the convergence of magnetism and superconductivity in condensed matter physics, of the central role of spin as a driver for heavy electron metals and superconductors - not just as the glue of pairing - but as the basic fabric of these materials. Many of us suspect that the nexus of these phenomena lies at the quantum critical point that appears to present in heavy electron, cuprate and iron-based superconductors.

I'll talk about how our ideas about spins and their role in correlated electron physics are changing. I want to talk about the severe challenges the physicists face in trying to describe the incompressible spin component of these materials. I'll discuss the all-important links between f- and d-electron materials and some of the new kinds of order we are encountering, including a hidden and topological order.

TT 18: Correlated Electrons: Quantum Impurities, Kondo Physics 2

Time: Tuesday 9:30–12:45 Location: H 3005

TT 18.1 Tue 9:30 H 3005

Dynamical Mean-Field Theory of Indirect Magnetic Exchange — •Irakli Titvinidze, Andrej Schwabe, Niklas Rother, and Michael Potthoff — I. Institut für Theoretische Physik Universität Hamburg Jungiusstraße 9 20355 Hamburg Germany

Two magnetic impurities on a metallic substrate surface experience the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction. This indirect non-local magnetic exchange competes with the local Kondo effect. While the latter is described in principle exactly within single-site dynamical mean-field theory, the effects of the RKKY coupling are taken into account approximately only. Here, this is demonstrated by comparing the DMFT results with numerically exact data obtained by the density-matrix renormalization group for a one-dimensional model with two Anderson impurities. With the two-site DMFT, we also benchmark a simplified DMFT variant. Varying the inter-impurity distance d and the local exchange coupling $J \sim -V^2/U$, different parameter regimes with dominating Kondo physics or with dominating RKKY interaction are studied. The reliability of DMFT for magnetic nanostructures on metallic surfaces is shown to crucially depend on the respective parameter regime as well as on geometrical and finite-size

effects. The prospects of DMFT (and two-site DMFT) as a reliable approach to study nanomagnetism of more complex RKKY-interacting systems are discussed.

TT 18.2 Tue 9:45 H 3005

DFT++ Method for Vacuum States — •Michael Karolak, Tim O. Wehling, and Alexander I. Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

The theoretical description of scanning probe experiments, like scanning sunneling microscopy (STM), still poses a challenge. Since these methods probe electronic states in the vacuum a few angstrom above the actual sample a theory focussing exclusively on electronic states of the bulk must be necessarily incomplete.

To bridge this gap we have extended our DFT++ methodology [1] to incorporate vacuum states. We are thus able to investigate the effects of strong electronic correlations on states in the vacuum above the sample. In this way we can provide a true *ab initio* description of an STM experiment including electronic correlations. As an application we investigate the recently reported Two-Site Kondo Effect in $CoCu_nCo$ clusters on Cu(111) [2].

[1] M. Karolak *et al.*, J. Phys.: Condens. Matter **23**, 085601 (2011).
[2] N. Néel *et al.*, Phys. Rev. Lett. **107**, 106804 (2011).

TT 18.3 Tue 10:00 H 3005

Distributional exact diagonalization formalism for quantum impurity models — •Mats Granath and Hugo Strand — Department of Physics, University of Gothenburg, Gothenburg, Sweden

We develop a method for calculating the self energy of a general quantum impurity problem using a distribution of finite size Anderson models. When used in the context of dynamical mean field theory it provides an extension of the exact diagonalization formalism which gives a continuous real frequency self energy without the need for analytic continuation from imaginary frequencies.

TT 18.4 Tue 10:15 H 3005

Complex charge ordering in CeRuSn — •Ralf Feyerherm[1], Esther Dudzik[1], Sergio Valencia[1], John A. Mydosh[2,3], Wilfried Hermes[4], and Rainer Pöttgen[4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin — [2]MPI-CPFS, 01187 Dresden — [3]Kamerlingh Onnes Laboratory, Leiden University, 2300RA Leiden, The Netherlands — [4]Institut für Anorganische und Analytische Chemie, Universität Münster, 48149 Münster

At room temperature (RT), CeRuSn exhibits coexistence of trivalent Ce^{3+} and intermediate valent $Ce^{(4-\delta)+}$ in a metallic environment. Charge ordering produces a doubling of the unit cell along the *c*-axis with respect to the basic CeCoAl type structure. Below RT, a phase transition with broad hysteresis has been observed in various bulk properties. The present x-ray diffraction results show that at low temperatures the doubling of the CeCoAl type structure is replaced by an ill-defined modulated ground state in which at least three modulation periods compete. The dominant mode is close to a tripling of the basic cell. XANES data suggest that the average Ce valence remains constant. We propose a qualitative structure model with modified stacking sequences of Ce^{3+} and $Ce^{(4-\delta)+}$ layers in the various modulated phases. Surprisingly, far below 100 K the modulated state is sensitive to synchrotron x-ray irradiation. With a photon flux $\approx 10^{12}$ s^{-1}, the modulated ground state is destroyed on a timescale of minutes and the doubling of the CeCoAl cell observed at room temperature is recovered. The final state is metastable at 10 K. Heating the sample above 60 K again leads to a recovery of the modulated state.

TT 18.5 Tue 10:30 H 3005

Non-equilibrium transport through a multichannel Kondo dot at finite magnetic field — •Christoph B. M. Hörig and Dirk Schuricht — RWTH Aachen, Germany

Motivated by a recent work [1] on non-equilibrium transport through a multichannel Kondo model, we study a spin-1/2 quantum dot in a finite magnetic field using the real-time renormalization group (RG) method [2].

The quantum dot is coupled to K independent reservoirs via spin exchange interaction, which leads to the overscreened Kondo effect. Based on a systematic expansion in the exchange coupling we integrate out the reservoir degrees of freedom and solve the resulting two-loop RG equations in the weak-coupling regime $K >> 1$. We derive the scaling functions of the coupling constants towards the K-channel fix point and investigate the influence of decoherence during this flow.

Furthermore, we determine the effect of channel-dependent bias voltages on the magnetization and the differential conductance via inelastic cotunneling processes, and discuss our results in the context of previous experiments [3].

[1] A. Mitra and A. Rosch, Phys. Rev. Lett. 106, 106402 (2011).
[2] H. Schoeller and F. Reininghaus, Phys. Rev. B 80, 045117 (2009).
[3] R. M. Potok et al., Nature 446, 167 (2007).

TT 18.6 Tue 10:45 H 3005

Non-Fermi liquid physics in two-channel Kondo models — •Andrew Mitchell — Institut für Theoretische Physik, Universität zu Köln, Germany

The two-channel Kondo (2CK) model possesses a non-Fermi liquid (NFL) quantum critical point, arising when two conduction channels compete to Kondo-screen a single spin-$\frac{1}{2}$ impurity. The two-impurity Kondo (2IK) model also has a NFL critical point. We establish an exact connection between the models, showing that the 2IK critical fixed point is identical to that of a 2CK model with potential scattering. Furthermore, we demonstrate that the same critical physics arises in chains of impurities, and the spin-S generalization of the 2IK model. But conductance lineshapes measurable in experiment encode the full RG flow. We study the onset of NFL physics, showing that distinctive signatures arise as a function of device asymmetry; and the ultimate recovery of standard Fermi liquid behavior resulting from symmetry-breaking perturbations.

[1] Mitchell, Sela, Logan, `arXiv:1111.6503v1` (2011)
[2] Mitchell, Logan, Krishnamurthy, Phys. Rev. B **84**, 035119 (2011)
[3] Sela, Mitchell, Fritz, Phys. Rev. Lett. **106**, 147202 (2011)

15 min. break.

TT 18.7 Tue 11:15 H 3005

Nonequilibrium Kondo model: the RG flow from weak to strong coupling — •Mikhail Pletyukhov and Herbert Schoeller — Institut für Theorie der statistischen Physik, RWTH Aachen, Physikzentrum, D - 52074 Aachen

A renormalization group flow of the nonequilibrium Kondo model from high energies (weak coupling) to low energies (strong coupling) is discussed. A new flowing scheme (E-flow) within the Real Time Renormalization Group (RTRG) approach which uses the Laplace variable E as a flow parameter is introduced. The accuracy of this scheme in equilibrium is checked via the comparison against the benchmark NRG calculation of the linear conductance at finite temperatures. In nonequilibrium, the new results for the voltage dependence of the differential conductance are presented.

Another remarkable feature of the E-flow scheme is that it provides an access to the full time dynamics of a system, once the corresponding flow equations have been integrated. An application of the E-flow scheme to the study of time evolution of the Kondo model in the strong coupling regime is discussed.

TT 18.8 Tue 11:30 H 3005

Non-abelian symmetries and the numerical renormalization group — •Markus Hanl, Andreas Weichselbaum, and Jan von Delft — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Munich, Germany

We present a numerical study of the magneto-conductance $G(B,T)$ of the fully symmetric three-channel Anderson-like model, which has been suggested recently as the microscopic model for Fe-impurities in gold or silver [1]. For this, we use the numerical renormalization group method (NRG) which allows us to calculate the magneto-conductance $G(B,T)$ for the relevant parameter space of both, the magnetic field B as well as the temperature T. We use an implementation of the NRG which allows to explicitly exploit any set of non-abelian symmetries. In the given case, this includes the SU(3) channel symmetry. This increases the efficiency by orders of magnitude compared to plain abelian NRG, which thus renders the simulation feasible. We show that our results are well converged, and, though the calculations are numerically very involving, the remaining error is small and controllable.

[1] T. Costi et al., Phys. Rev. Lett. **102**, 056802 (2009)

TT 18.9 Tue 11:45 H 3005

Kondo correlations in a disordered medium — •Michael Becker, Andrew Mitchell, and Ralf Bulla — Institut für theoretische Physik, Universität zu Köln

The Kondo effect is a classic paradigm, describing the formation of a many-body spin-singlet state between a local magnetic impurity and delocalized conduction electrons at low temperatures. However, in disordered systems, localization physics plays a key role. Here we consider the subtle interplay between Kondo physics and Anderson localization in disordered 1D and quasi 2D and 3D systems which contain a single correlated impurity site. Equations of motion and exact diagonalization are used to calculate hybridization functions for the non-interacting system, which constitute the input for NRG calculations in the interacting case. Real-space quantities are then extracted for the full system, and provide information on the Kondo screening length and localization length, whose relative magnitudes dictate the underlying physics.

TT 18.10 Tue 12:00 H 3005

Discarded weight and entanglement spectra in the numerical renormalization group — •Andreas Weichselbaum — Ludwig Maximilians University, Munich

A quantitative criterion to prove and analyze convergence within the numerical renormalization group (NRG) is introduced. By tracing out a few further NRG shells, the resulting reduced density matrices carry relevant information on numerical accuracy as well as entanglement. Their spectra can be analyzed twofold. The smallest eigenvalues provide a sensitive estimate of how much weight is discarded in the low-energy description of later iterations. As such, the discarded weight indicates in a site-specific manner whether sufficiently many states have been kept within a single NRG run. The largest eigenvalues of the reduced density matrices, on the other hand, lend themselves to a straightforward analysis in terms of entanglement spectra, which can be combined into entanglement flow diagrams. The latter show strong similarities with the well-known standard energy flow diagram of the NRG, supporting the prevalent usage of entanglement spectra to characterize different physical regimes [1].
[1] Phys. Rev B **84**, 125130 (2011)

TT 18.11 Tue 12:15 H 3005

Universal out-of-equilibrium transport in Kondo-correlated quantum dots: a renormalized superperturbation theory on the Keldysh contour — •Stefan Kirchner[1,2], Enrique Munoz[3], and Carlos Bolech[4] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute for Chemical Physics of Solids — [3]Pontificia Universidad Catolica de Valparaiso, Chile — [4]University of Cincinnati, US

The non-linear conductance of semiconductor heterostructures and single molecule devices exhibiting Kondo physics has recently attracted attention[1,2]. We address the observed sample-dependence across various systems by considering additional electronic contributions present in the effective low-energy model underlying these experiments. To this end we develop a novel version of the superperturbation theory [3] in terms of dual fermions on the Keldysh contour. We analyze the role of particle hole asymmetry on the transport coefficients. Our approach systematically extends the work of Yamada and Yosida and others to the particle-hole asymmetric Anderson model and reproduce the exactly solvable resonant level model and the special case considered in [4]. It correctly describes the strong coupling physics and is free of internal inconsistencies that would lead to a breakdown of current conservation.
[1] M. Grobis et al., Phys. Rev. Lett. 100, 246601 (2008).
[2] G. D. Scott et al., Phys. Rev. B 79, 165413 (2009).
[3] H. Hafermann et al., EPL 85, 27007 (2009).
[4] K. Yamada, Prog. Theo. Phys. 62, 354 (1979).

TT 18.12 Tue 12:30 H 3005

Indirect magnetic exchange and Kondo screening in one-dimensional metals with few magnetic impurities — •Andrej Schwabe and Michael Potthoff — University Hamburg, Hamburg, Germany

The Kondo effect of one impurity coupled to a metallic substrate by an exchange interaction J is known as an impressive many-body effect which is regarded as well understood. Adding another impurity may cause two separate Kondo effects, but can also introduce a new inter impurity RKKY coupling. The competition between both interactions gives rise to different parameter regimes: In the large J or large distance limit both impurities are separately screened while in the weak J or small distance limit they form a non-local spin which itself can be screened by the substrate.
We apply our variational matrix-product states code (VMPS) which is based on the implementation of the corrected one-site algorithm and exploits $U(1)$ symmetries. Calculations are presented for three impurities coupled to a nano chain within an Anderson model. We discuss its manifold properties by referring to results for the single and two impurity model. We focus explicitly on a substrate of finite size and discuss the consequences of finite-size gaps and symmetry.
The transition from the diluted case with few impurities to the dense lattice with one impurity on every substrate site, leads to further, even richer physics, including the exhaustion problem and magnetic long-range order. General trends considering the transition to dense chains are given.

TT 19: Correlated Electrons: (General) Theory 2

Time: Tuesday 9:30–13:00 Location: H 3010

TT 19.1 Tue 9:30 H 3010

Multiplet ligand-field theory using Wannier orbitals — •M. W. Haverkort[1], M. Zwierzycki[2], and O. K. Andersen[1] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Molecular Physics, Poznań, Poland

We demonstrate how *ab initio* cluster calculations including the full Coulomb vertex can be done in the basis of the localized, generalized Wannier orbitals which describe the low-energy density functional (LDA) band structure of the infinite crystal, *e.g.* the transition metal $3d$ and oxygen $2p$ orbitals. The spatial extend of our $3d$ Wannier orbitals (orthonormalized Nth order muffin-tin orbitals) is close to that found for atomic Hartree-Fock orbitals. We define Ligand orbitals as those linear combinations of the O $2p$ Wannier orbitals which couple to the $3d$ orbitals for the chosen cluster. The use of ligand orbitals allows for a minimal Hilbert space in multiplet ligand-field theory calculations, thus reducing the computational costs substantially. The result is a fast and simple *ab initio* theory, which can provide useful information about local properties of correlated insulators. We compare results for NiO, MnO and $SrTiO_3$ with x-ray absorption, inelastic x-ray scattering, and photoemission experiments. The multiplet ligand field theory parameters found by our *ab initio* method agree within ∼10% to known experimental values.

TT 19.2 Tue 9:45 H 3010

Quantification of correlations in quantum many-particle systems — •Krzysztof Byczuk[1], Jan Kunes[2], Walter Hofstetter[3], and Dieter Vollhardt[4] — [1]Physics Faculty, Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, 00-681 Warszawa, Poland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 53 Praha 6, Czech Republic — [3]Institut for Theoretische Physics, Goethe-Universitat, 60438 Frankfurt/Main, Germany — [4]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We introduce a well-defined and unbiased measure of the strength of correlations in quantum many-particle systems which is based on the relative von Neumann entropy computed from the density operator of correlated and uncorrelated states [1]. The usefulness of this general concept is demonstrated by quantifying correlations of interacting electrons in the Hubbard model and in a series of transition metal oxides using dynamical mean-field theory.
[1] K. Byczuk, J. Kunes, W. Hofstetter, and D. Vollhardt; arXiv:1110.3214

TT 19.3 Tue 10:00 H 3010

What do $LaCoO_3$ and ^{4}He- ^{3}He mixtures have in common? — •Jan Kuneš and Vlastimil Křápek — Institute of Physics, AS CR, Cukrovarnicka 10, Praha 6, Czech Republic

The perovskite $LaCoO_3$ has been studied for almost half a century for its peculiar magnetic and transport properties. It is generally accepted

that quasi-degeneracy of a magnetic and non-magnetic multiplets is the key feature of this material, however, the understanding how it affects its physics is far from complete. We have used a two-band Hubbard model as a minimum description of a material with competing atomic states. Using the dynamical mean-field theory we have studied the temperature dependencies of the magnetic susceptibility and the one-particle spectra. At intermediate temperatures we have observed formation of a two-sublattice order, which can be understood by mapping the Hubbard model on the classical Blume-Emery-Griffiths model.

TT 19.4 Tue 10:15 H 3010

Dynamical screening effects in correlated materials — •Silke Biermann — CPHT Ecole Polytechnique, Palaiseau, France

Materials with strong Coulomb correlations are challenges for electronic structure calculations. During the last years new methods for their description have been developed. The combination of dynamical mean field (DMFT) techniques with density functional theory within the local density approximation (LDA) allows for the calculation of electronic properties of materials from first principles, taking into account the effect of arbitrarily strong Coulomb interactions. We will describe recent developments to include dynamical screening effects into such calculations [1,2]. Based on an ab initio determination of the frequency-dependent local Coulomb interactions within the constrained random phase approximation [3,4] we discuss satellite features and spectral weight transfers associated to plasmon and electron-hole excitations.

[1] M. Casula, A. Rubtsov, S. Biermann, submitted, arXiv:1107.3123
[2] Ph. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. Millis, S. Biermann, submitted, arXiv:1107.3128
[3] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein Phys. Rev. B 70, 195104 (2004).
[4] L. Vaugier, H. Jiang, S. Biermann, in preparation.

TT 19.5 Tue 10:30 H 3010

Generalized Coulomb interaction parameters for every point group symmetry — •Anna Toth[1,2], Andrey Kutepov[2], Gabriel Kotliar[2], Philipp Hansmann[3,1], Nico Parragh[1], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austria — [2]Department of Physics, Rutgers University, Piscataway, New Jersey, USA — [3]Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, Cedex, France

We show how to construct the independent two-electron interactions in arbitrary crystal field and for arbitrary spin-orbit coupling strength. We establish the correspondence between these interactions and the Hubbard term and Hund's rule coupling. Our scheme, which takes the point group fully into account, gives additional parameters beyond the standard Slater integrals (which describe the spherical symmetric case), or the Kanamori scheme. As an application, we determine the strength of these couplings in $BaFe_2As_2$ based on the self-consistent GW method, and give a comprehensive comparison between the different schemes.

TT 19.6 Tue 10:45 H 3010

Phase diagram of honeycomb bilayer from functional RG — •Stefan Uebelacker, Michael Scherer, and Carsten Honerkamp — Institut für Theoretische Festkörperphysik C, RWTH Aachen University, Aachen, Germany

The phase diagram for interacting electrons on the honeycomb bilayer with Bernal stacking is explored by means of the functional renormalization group. For half-filling and including a range of repulsive onsite, nearest-neighbor and next-to-nearest neighbor interaction terms we analyze the emergent instabilities and find antiferromagnetic, (modulated) charge-density-wave and quantum spin Hall order. The presented phase diagram covers the region of the bilayer graphene parameters suggested by ab initio calculations which overlaps with the phase boundary between the antiferromagnetic state and the quantum spin Hall state. We comment on the effect of small dopings and third nearest neighbor interaction.

TT 19.7 Tue 11:00 H 3010

Phase transitions of the three-state (anti-)ferromagnetic Potts model in transverse field — •Marc Daniel Schulz[1,4], Sébastien Dusuel[2], Roman Orùs[3], Julien Vidal[4], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany — [4]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

The investigation of phase transitions in two-dimensional quantum lattice systems is a challenging task. Here, we study the three-state Potts model on a two-dimensional square lattice in transverse field for antiferromagnetic and ferromagnetic coupling. To this end, we combine the methods of perturbative continuous unitary transformations (pCUT) and variational techniques using infinite projected entangled pair states(iPEPS). For the ferromagnetic coupling, we confirm the already known first-order nature of the phase transition, whereas for the anti-ferromagnetic coupling we provide strong evidence for a novel second-order phase transition compatible with the 3dXY universality class.

15 min. break.

Invited Talk TT 19.8 Tue 11:30 H 3010

Interactions and disorder in topological quantum matter — •Simon Trebst — Universität zu Köln

The emergence of topological order is one of the most intriguing phenomena in quantum many-body physics and one of possibly far reaching relevance – topological quantum matter is increasingly appreciated as possible medium for quantum computation purposes. In this talk, I will discuss the stability of topological quantum matter when considering the effects of interactions and disorder on the collective quantum state formed by a set of topological excitations, so-called anyons. In particular, I will discuss the formation of a thermal metal of Majorana fermions in a two-dimensional system of interacting non-Abelian anyons in the presence of moderate disorder. This bulk metallic phase occurs for various proposed systems supporting Majorana fermion zero modes when disorder induces the random pinning of a finite density of vortices. This includes all two-dimensional topological superconductors in so-called symmetry class D. A distinct experimental signature of the thermal metal phase is the presence of bulk heat transport down to zero temperature. I will finish by discussing implications for topological quantum computing proposals.

TT 19.9 Tue 12:00 H 3010

Robustness of a perturbed topological phase — Michael Kamfor[1], Sebastien Dusuel[2], Roman Orus[3], Julien Vidal[4], and •Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany — [2]Lycée Saint-Louis, 75006 Paris, France — [3]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — [4]LPTMC, Université Pierre et Marie Curie, 75252 Paris Cedex 05, France

We investigate the stability of the topological phase of the toric code model in the presence of a uniform magnetic field by means of variational and high-order series expansion approaches. We find that when this perturbation is strong enough, the system undergoes a topological phase transition whose first- or second-order nature depends on the field orientation. Our work represents the first high-order series expansion for the anyonic quasi-particles of a topological phase. As a consequence, we get access to the critical properties of the perturbed toric code.

TT 19.10 Tue 12:15 H 3010

Supersymmetry in Rydberg-dressed lattice fermions — •Hendrik Weimer[1], Liza Huijse[1], Alexey Gorshkov[2], Guido Pupillo[3], Peter Zoller[4], Mikhail Lukin[1], and Eugene Demler[1] — [1]Physics Department, Harvard University, Cambridge, MA, USA — [2]IQI, Caltech, Pasadena, CA, USA — [3]University of Strasbourg, Strasbourg, France — [4]University of Innsbruck and IQOQI, Innsbruck, Austria

Supersymmetry is a powerful tool that allows the characterization of strongly correlated many-body systems, in particular in the case of supersymmetric extensions of the fermionic Hubbard model [1]. At the same time, these models can exhibit rich and exotic physics on their own, such as flat bands or exponentially large ground state degeneracy. We show that such lattice models can be realized with Rydberg-dressed fermions in optical lattices. Strong interactions within the ground state manifold of the atoms can be realized by admixing a weak contribution of a highly excited Rydberg state [2]. By tuning the experimental parameters away from the supersymmetric point, it is possible to assess the validity of a supersymmetric approach to strongly correlated

electrons in a systematic way.
[1] P. Fendley, K. Schoutens, J. de Boer, PRL **90**, 120402 (2003).
[2] J. Honer, H. Weimer, T. Pfau, H. P. Büchler, PRL **105**, 160404 (2010).

TT 19.11 Tue 12:30 H 3010

Application of wave function based electron correlation methods to van der Waals bound crystals — •Carsten Müller[1] and Denis Usvyat[2] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin Takustr. 3, Berlin, 14195, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Regensburg Universitätsstr. 31, Regensburg, 93040, Germany

The treatment of van der Waals bound systems, such as molecular crystals is a remains challenging in theoretical solid state chemistry. In these systems, electron correlation is crucial and HF or standard DFT functionals often fail to produce reliable cohesive energies. On the other hand, common implementations of wave function based post-HF methods, such as MP2 or Coupled Cluster theory, suffer from an unfortunate scaling with system size, and are difficult to adopt to periodic systems.

In our investigations we have combined the Method of Increments, which is one type of local correlation method, with embedded cluster calculations to investigate physisorption Ar fcc and the CO_2 crystal at the LMP2 and LCCSD(T) levels. First, periodic LMP2 calculations were performed to obtain appropriate parameters for the size of the excitation domains and to assess the convergence of the incremental expansion. Then different schemes for the embedding of the finite clusters were assessed for their influence on the convergence behavior of the incremental expansion. And finally calculations at the LCCSD(T) level and with larger basis sets were used to obtain the cohesive energy of Ar fcc and CO_2 with benchmarking quality.

TT 19.12 Tue 12:45 H 3010

Temperature evolution of phonon spectra of elemental iron near the α-γ phase transition — •I. Leonov[1], A. I. Poteryaev[2,3], V. I. Anisimov[2], and D. Vollhardt[1] — [1]TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]Institute of Quantum Materials Science, Yekaterinburg, Russia

We present results of a theoretical investigation of the electronic and lattice dynamical properties of elemental iron at finite temperatures obtained within dynamical mean-field theory implemented with the frozen-phonon method [1]. This approach allows us to compute correlation induced lattice transformations and their temperature evolution. We find that electronic correlations are important to explain the lattice stability of iron at the bcc-fcc phase transition. We notice a weak anomaly in the transverse T_1 acoustic mode in the Γ-N direction of the bcc phase. This behavior can be ascribed to a dynamical precursor effect of the bcc-to-fcc phase transition and is found to occur above the Curie temperature. Upon further heating, the bcc phase becomes dynamically unstable due to the T_1 mode near the N point. By contrast, the fcc lattice is found to be dynamically stable in a broad temperature range, including temperatures above and below the bcc-fcc phase transition temperature. Our results for the structural phase stability and lattice dynamical properties of iron are in good agreement with experiment.
[1] I. Leonov *et al.*, Phys. Rev. Lett. **106**, 106405 (2011); I. Leonov *et al.*, arXiv:1110.0439 (2011).

TT 20: Transport: Quantum Coherence and Quantum Information Systems 3 (jointly with MA and HL)

Time: Tuesday 9:30–12:15 Location: BH 243

Invited Talk TT 20.1 Tue 9:30 BH 243

Making and manipulating Majorana fermions for topological quantum computation — •Felix von Oppen — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Unviversitaet Berlin, 14195 Berlin

Known theoretically for decades, Majorana fermions have never been observed as fundamental particles. But there is growing excitement among condensed matter physicists that Majorana fermions could be observed as quasiparticles in the solid state. This excitement is fueled by their remarkable properties: They are their own antiparticle and obey an exotic (and yet unobserved) form of quantum statistics called non-Abelian statistics. These properties make Majorana fermions the simplest candidate for realizing topological quantum information processing which could go a long way towards alleviating the problem of decoherence in conventional quantum computation.

Among the systems predicted to support Majorana fermions are exotic fractional quantum Hall states as well as hybrid structures of topological insulators, semimentals, or semiconductors with conventional superconductors. Realizations based on semiconductor quantum wires in proximity to conventional superconductors are perhaps particularly promising since they allow for relatively detailed scenarios of how to manipulate the Majorana fermions. In this talk, I will discuss this proposal to realize Majorana fermions.

TT 20.2 Tue 10:00 BH 243

Engineering and manipulating Majorana bound states in 1D quantum wires — •Panagiotis Kotetes[1], Alexander Shnirman[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

Recently, the interest in topological quantum computing has grown due to the appearance of promising platforms for realizing the long sought Majorana bound states. Among the proposals that appear suitable for engineering the Majorana bound states, the most prominent involves a 1D semiconducting quantum wire in proximity to a bulk s-wave superconductor, where in addition a Zeeman magnetic field is applied. In this work, we investigate the possibility of performing qubit operations via the adiabatic variation of certain internal parameters without using any external gates or network of wires. The crucial feature of our model is the combination and interplay of phases for the magnetic field and the superconducting order parameter. In an appropriate junction setup, we explore the possible phase configurations that could lead to a Majorana bound state exchange.

TT 20.3 Tue 10:15 BH 243

Coulomb-assisted braiding of Majorana fermions in a Josephson junction array — •Fabian Hassler[1], Bernard Van Heck[2], Anton Akhmerov[2], Michele Burrello[2], and Carlo Beenakker[2] — [1]Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We show how to exchange (braid) Majorana fermions in a network of superconducting nanowires by control over Coulomb interactions rather than tunneling. Even though Majorana fermions are charge-neutral quasiparticles (equal to their own antiparticle), they have an effective long-range interaction through the even-odd electron number dependence of the superconducting ground state. The flux through a split Josephson junction controls this interaction via the ratio of Josephson and charging energies, with exponential sensitivity. By switching the interaction on and off in neighboring segments of a Josephson junction array, the non-Abelian braiding statistics can be realized without the need to control tunnel couplings by gate electrodes. This is a solution to the problem how to operate on topological qubits when gate voltages are screened by the superconductor.

TT 20.4 Tue 10:30 BH 243

Quantum information transfer between topological and spin qubit systems — •Martin Leijnse and Karsten Flensberg — Nano-Science Center and Niels Bohr Institute, University of Copenhagen, Denmark

In this talk I will introduce a method to coherently transfer quantum information, and to create entanglement, between topological qubits and conventional spin qubits. The transfer method uses gated control to transfer an electron (spin qubit) between a quantum dot and edge Majorana modes in adjacent topological superconductors. Because of the spin polarization of the Majorana modes, the electron transfer translates spin superposition states into superposition states of the

Majorana system, and vice versa. Furthermore, I will discuss how a topological superconductor can be used to facilitate long-distance quantum information transfer and entanglement between spatially separated spin qubits [1,2].
[1] M. Leijnse, K. Flensberg, PRB **84**, 140501(R) (2011)
[1] M. Leijnse, K. Flensberg, PRL **107**, 210502 (2011)

15 min. break.

Invited Talk TT 20.5 Tue 11:00 BH 243

Distinguishing quantum and classical transport through nanostructures — •Clive Emary[1], Neill Lambert[2], Franco Nori[2,3], and Yueh-Nan Chen[4] — [1]TU Berlin, Germany — [2]RIKEN, Japan — [3]University of Michigan, USA — [4]National Cheng-Kung University, Tainan, Taiwan

I will discuss the question of how to distinguish quantum from classical transport through nanostructures using fundamental quantum-mechanical inequalities. I will briefly discuss how Bell's inequalities can be employed to investigate entanglement in the solid-state, before focusing on a less well-known inequality, the Leggett-Garg inequality. This latter probes the 'macroscopic realism' of a system, i.e. whether or not the system has a well-defined state independent of the observer. I will describe how the Leggett-Garg inequality can be realised in transport context, and how it can be violated by quantum coherent transport.

TT 20.6 Tue 11:30 BH 243

Spin-orbit-induced strong coupling of a single spin to a nanomechanical resonator — •Andras Palyi[1,2], Philipp R. Struck[1], Mark Rudner[3], Karsten Flensberg[3,4], and Guido Burkard[1] — [1]University of Konstanz, Germany — [2]Eotvos University, Budapest, Hungary — [3]Harvard University, Cambridge, Massachusetts, United States — [4]Niels Bohr Institute, Copenhagen, Denmark

We theoretically investigate the coupling of electron spin to vibrational motion due to curvature-induced spin-orbit coupling in suspended carbon nanotube quantum dots. Our estimates indicate that, with current capabilities, a quantum dot with an odd number of electrons can serve as a realization of the Jaynes-Cummings model of quantum electrodynamics in the strong-coupling regime. A quantized flexural mode of the suspended tube plays the role of the optical mode and we identify two distinct two-level subspaces, at small and large magnetic field, which can be used as qubits in this setup. The strong intrinsic spin-mechanical coupling allows for detection, as well as manipulation of the spin qubit, and may yield enhanced performance of nanotubes in sensing applications [1].
[1] arXiv:1110.4893)

TT 20.7 Tue 11:45 BH 243

Emission spectrum of a driven nonlinear resonator — •Stephan André[1,2], Lingzhen Guo[1,3], Michael Marthaler[1,2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Department of Physics, Beijing Normal University, Beijing 100875, China

Motivated by recent "circuit QED" experiments [1,2] we investigate the properties of coherently driven nonlinear resonators. By using Josephson junctions in superconducting circuits, strong nonlinearities can be engineered, which lead to the appearance of pronounced quantum effects with a low number of photons in the resonator.

Based on a master equation approach we determine the emission spectrum and observe for typical circuit QED parameters, in addition to the primary side-peaks, second-order peaks which are not predicted by a linearized theory. These peaks result from transitions between next-to-nearest levels in the rotating frame and from fluctuations of the oscillation amplitude. We show that an effective Planck constant provides a measure for the importance of the quantum effects.
[1] I. Siddiqi *et al.*, Phys. Rev. B **73**, 054510 (2006).
[2] F.R. Ong *et al.*, Phys. Rev. Lett. **106**, 167002 (2011).

TT 20.8 Tue 12:00 BH 243

Noise-induced transition in an electronic Mach-Zehnder interferometer — •Andreas Helzel[1], Leonid Litvin[1], Werner Wegscheider[2], and Christoph Strunk[1] — [1]Institute of exp. and applied physics, University of Regensburg, Germany — [2]Solid State Physics Laboratory, ETH Zurich, 8093 Zurich, Switzerland

The visibility of Aharonov-Bohm interference of an electronic Mach-Zehnder interferometer (MZI) shows a lobe structure when changing the applied DC bias. Multiple side lobes are present at filling factors from 1.5 to 2. By varying the transmission of a quantum point contact set in series at a distance D before the MZI (QPC0) we can suppress the multiple side lobes to a single side lobe. This occurs at a transmission probability of $T_{QPC0} = 0.5$. Above this transmission the lobe structure is robust and does not change qualitatively. For $T_{QPC0} < 0.5$ the multiple side lobes disappear and the central lobe width increases drastically with decreasing transmission. We see these properties both in the visibility and in the AB-phase. This behavior coincides with a recently proposed noise-induced phase transition [1].
[1] Ivan P. Levkivskyi, Eugene V. Sukhorukov, Phys. Rev. Lett. **103**, 036801 (2009)

TT 21: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3

Time: Tuesday 9:30–13:00 Location: BH 334

TT 21.1 Tue 9:30 BH 334

Quantum spin relaxation by a nonequilibrium current — •Daniel Becker[1,2], Stephan Weiss[2], Michael Thorwart[2], and Daniela Pfannkuche[2] — [1]Department Physik, Universität Basel, 4056 Basel, Schweiz — [2]I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg

For a Coulomb-interacting single-level quantum dot in contact with two metallic leads and a spin-1/2 magnetic impurity, which is exchange-coupled to the electron spin, the interplay between the correlated charge- and (interaction-induced) real-time impurity dynamics is studied. To this end, the numerically exact, non-perturbative scheme of iterative summation of path integrals (ISPI)[1,2] is employed in a regime, where all appearing energy scales are of the same order of magnitude. A systematical investigation of the mutual dependencies between charge current and impurity relaxation dynamics is provided. By comparison to a perturbative theory both for (a) the case of either vanishing Coulomb- or electron-impurity interaction and (b) non-vanishing interactions, it is clearly shown that correlation effects due to the on-dot interactions considerably affect the system behavior. In particular, our approach reveals how a quantum spin relaxes to its stationary state under the influence of a nonequilibrium current.
[1] S. Weiss et al., Phys. Rev. B 77, 195316 (2008)
[2] D. Becker et al., J. Phys.: Conf. Ser. 245 012021 (2010)

TT 21.2 Tue 9:45 BH 334

Current from hot spots — •Rafael Sánchez[1] and Markus Büttiker[2] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) — [2]Département de Physique Théorique, Université de Genève

In electrical circuits hot spots occur naturally at places where energy is dissipated. Here we propose a controlled experiment which can demonstrate the appearance of directed current as a consequence of a hot spot. We investigate transport generated in Coulomb coupled electrical conductors from excess fluctuations at the coupling capacitance. If one of the conductors supports a bias voltage, out of equilibrium charge fluctuations remove detailed balance in the unbiased system manifested in a drag current. Non linear fluctuation relations can nevertheless be obtained [1].

Coulomb coupled conductors permit separate directions of the heat and current flux [2]. In our model, one of the conductors is connected via only one lead to a hot reservoir. The other conductor connects to two leads. We investigate the minimal conditions needed to generate directed current flow for a system of two quantum dot conductors in which both energy and charge states are quantized. In quantum dots energy to current conversion can be optimal with one electron transferred for every heat quantum given up by the hot reservoir. We show that at the point of maximum power extraction the efficiency approaches one half of the Carnot efficiency.

[1] R. Sánchez, R. López, D. Sánchez, and M. Büttiker, Phys. Rev. Lett. 104, 076801 (2010)
[2] R. Sánchez, and M. Büttiker, Phys. Rev. B 83, 085428 (2011)

TT 21.3 Tue 10:00 BH 334

Nonequilibrium transport through quantum dots with Dzyaloshinsky-Moriya-Kondo interaction — •Mikhail Pletyukhov and Dirk Schuricht — Institut für Theorie der statistischen Physik, RWTH Aachen, Physikzentrum, D - 52074 Aachen

We study nonequilibrium transport through a single-orbital Anderson model in a magnetic field with spin-dependent hopping amplitudes. In the cotunneling regime, it is described by an effective spin-1/2 dot with a Dzyaloshinsky-Moriya-Kondo (DMK) interaction between the spin on the dot and the electron spins in the leads. Using a real-time renormalization group technique we show that at low temperatures (i) the DMK interaction is strongly renormalized, (ii) the renormalized magnetic field acquires a linear voltage dependence, and (iii) the differential conductance exhibits a voltage asymmetry which is strongly enhanced by logarithmic corrections. We propose transport measurements in which these signatures can be observed.

TT 21.4 Tue 10:15 BH 334

Zero bias anomalies in electron transport across quantum dots — •Johannes Kern and Milena Grifoni — Universität Regensburg, D-93040 Regensburg, Germany

We describe the electron transport across a quantum dot which is coupled to two contacts at different chemical potentials using a diagrammatic approach. By summing up a subclass of diagrams of all orders in the tunneling Hamiltonian, we are able to describe a low temperature regime where the differential conductance develops a maximum at zero bias. We exemplify our theory for the case of the single impurity Anderson model and compare our results with experimental findings.

TT 21.5 Tue 10:30 BH 334

Nanocaloritronic performance analysis of an interacting quantum dot thermoelectric system — •Bhaskaran Muralidharan and Milena Grifoni — nstitut I - Theoretische Physik Universität Regensburg D-93040 Regensburg

By subjecting a weakly coupled quantum dot system to an applied voltage and temperature gradient, we present notable subtleties involved in its thermoelectric energy conversion efficiency. First, is the well known, but non-intuitive aspect in the non-interacting case, of achieving a reversible operation with Carnot efficiency. Second, is the rather surprising result in the presence of Coulomb interactions that similar operating conditions lead to zero efficiency [1]. It is then shown that even in this case, operating efficiencies close to the Carnot value may be attained, but, under non-equilibrium conditions [1]. Consequently, the inadequacies of traditionally employed performance metric zT in capturing the aforementioned non-equilibrium conditions are pointed out.
[1] B. Muralidharan and M. Grifoni, cond-mat/1110.4357 (2011).

TT 21.6 Tue 10:45 BH 334

Time scales in the dynamics of an interacting quantum dot — •Janine Splettstoesser[1], Debora Contreras-Pulido[1], Michele Governale[2], Jürgen König[3], and Markus Büttiker[4] — [1]Theorie für Statistische Physik, RWTH Aachen University — [2]School of Physical and Chemical Sciences, Victoria University, Wellington, New Zealand — [3]Theoretische Physik, Universität Duisburg-Essen — [4]Physique Théorique, Université de Genève, Switzerland

The subject of this presentation is the relaxation behavior of an interacting quantum dot, brought out of equilibrium by a fast switch, e.g. of the gate potential [1,2]. We study a single-level quantum dot with strong Coulomb interaction, weakly coupled to a single lead, taking the role of a mesoscopic capacitor. The transient response to the fast change of an external parameter is computed by means of a real-time diagrammatic expansion in the tunnel-coupling strength. We find that the exponential relaxation of the dot state is governed by three different time scales: Charge and spin relaxation depend on the final state of the dot and they differ from each other due to Coulomb repulsion. A further, gate-independent relaxation rate is related to electron-hole correlations and can be extracted, e.g., from deviations from the equilibrium charge. We study different setups and driving schemes to address the three independent decay rates separately.
[1] J. Splettstoesser, M. Governale, J. König, and M. Büttiker, Phys. Rev. B **81**, 165318 (2010).
[2] L.-D. Contreras-Pulido, J. Splettstoesser, M. Governale, J. König, and M. Büttiker, arxiv:1111.4135.

TT 21.7 Tue 11:00 BH 334

Cotunneling conductance of nonabelian excitations in fractional quantum Hall edge systems — •Robert Zielke[1], Bernd Braunecker[2], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Departamento de Física Teórica de la Materia Condensada, Facultad de Ciencias, Universidad Autónoma de Madrid, Spain

We consider theoretically a fractional quantum Hall (FQH) system at filling fraction 5/2, containing a dot or antidot in the bulk. We look for specific signatures of the Moore-Read state, which is the most prominent candidate state for the 5/2-FQH system and supports nonabelian excitations. Two different setups are considered: (a) cotunneling of electrons between two different FQH samples via a dot and (b) cotunneling of fractional charges between the edge states of one single FQH sample via an antidot. Both setups lead to characteristic tunneling currents with line shapes significantly different from the one of a Fermi liquid.

15 min. break.

TT 21.8 Tue 11:30 BH 334

Scanning probe microscopy imaging of metallic nanocontacts prepared by electromigration — •Dominik Stöffler[1], Shawn Fostner[2], Hilbert v. Löhneysen[1,3], Peter Grütter[2], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Department of Physics, McGill University, Montreal, Canada — [3]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

Controlled electromigration of thin metallic films represents a promising technique for fabricating nanometer-sized gaps for possible applications in molecular electronics. We show scanning force microscopy measurements of metallic nanocontacts that are formed during controlled electromigration cycles. The nanowires used for the thinning process are fabricated by shadow evaporation. During the first few electromigration cycles an overall slit in the nanocontact is formed, with a few grains still maintaining metallic contact. At a later stage the remaining grains disintegrate and their remnants accumulate in regions away from the slit. Resistance measurements during the electromigration cycle suggest that first the whole wire is heated. During the subsequent thinning process the current apparently passes through several smaller contacts and less power is needed for electromigration. We also discuss the influence of the environment (ambient, ultra-high vacuum) on the electromigration process.

TT 21.9 Tue 11:45 BH 334

Readout of carbon nanotube vibrations based on spin-phonon coupling — •Christoph Ohm[4], Christoph Stampfer[2,3], Janine Splettstoesser[1], and Maarten R. Wegewijs[1,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Institut für Quanteninformation, RWTH Aachen University, Germany

We theoretically study a carbon nanotube (CNT) double quantum dot consisting of a suspended and a non-suspended part. We propose a scheme for spin-based detection of the CNT bending motion in which the vibrational frequency is converted to a lower, more accessible frequency range. We make use of the spin-orbit coupling in CNTs. In the presence of vibrations, this yields a weak effective spin-phonon coupling. Classical vibrations of the CNTs are shown to induce a time dependent field acting on the electrons confined to the suspended dot, thereby generating spin flips. Within a rotating-wave approximation we find that the weakness of the spin-phonon coupling results in an effective down-mixing of the high vibrational frequency to a much lower spin-flip frequency. The latter can be controlled by the strength of an external magnetic field. We propose to read out the vibration-induced spin flips by measuring the leakage current through the double dot tuned to the spin-blockade regime as a function of the magnetic field. From a master equation we predict that the leakage current shows a pronounced peak allowing to read out the vibrational frequency.

TT 21.10 Tue 12:00 BH 334

Coulomb blockade of non-local electron transport in metallic

conductors — •Dmitry Golubev and Andrei Zaikin — Institut für Nanotechnologie, Karlsruhe Institut für Technologie, Karlsruhe

We consider a metallic wire coupled to two metallic electrodes via two junctions placed nearby. A bias voltage applied to one of such junctions alters the electron distribution function in the wire in the vicinity of another junction thus modifying both its noise and the Coulomb blockade correction to its conductance. We evaluate such interaction corrections to both local and non-local conductances demonstrating non-trivial Coulomb anomalies in the system under consideration. Experiments on non-local electron transport with Coulomb effects can be conveniently used to test inelastic electron relaxation in metallic conductors at low temperatures.

TT 21.11 Tue 12:15 BH 334

Cooperative Emission in Transport Setting through a Quantum Dot — •Martin J. A. Schuetz, Eric M. Kessler, Geza Giedke, and Juan Ignacio Cirac — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

We theoretically show that intriguing features of coherent many-body physics can be observed in electron transport through a quantum dot (QD). In particular, we show that electron transport in the Pauli-blockade regime is coherently enhanced by hyperfine interaction (HF) with the nuclear spin ensemble in the QD. For an initially polarized nuclear system this leads to a strong current peak in close analogy with superradiant emission of photons from atomic ensembles. This effect could be observed with realistic experimental parameters and would provide clear evidence of coherent HF dynamics of nuclear spin ensembles in QDs.

TT 21.12 Tue 12:30 BH 334

Spin-active scattering in ferromagnet-quantum dot-superconductor junctions — •Henning Soller — Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, D-69120 Heidelberg

Based on the Hamiltonian formalism we study spin-active scattering in a ferromagnet-quantum dot-superconductor junction. Compared to simple tunnel contacts quantum dot junctions exhibit a strongly energy-dependent transmission that is further affected by the presence of the ferromagnetic correlations and on-site Coulomb interaction on the dot. We derive an effective model for a quantum dot in an even charge state. We find a qualitatively new subgap conductance feature related to spin-active scattering and compare our findings to recent experimental results.

TT 21.13 Tue 12:45 BH 334

Keldysh field integral theory for the Kondo effect in interacting nanoscopic systems — •Sergey Smirnov and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We derive a nonequilibrium Keldysh field theory valid for a system with finite electron-electron interactions much stronger than the coupling of the system to contacts. Finite electron-electron interactions are treated involving as many slave-boson degrees of freedom as one needs for a concrete many-body system. For clarity the theory is presented for the Kondo regime of the single impurity Anderson model. The effective Keldysh action takes into account weak slave-bosonic oscillations excited by the electronic tunneling between the nanoscopic system and contacts. This allows us to derive an analytical expression for the tunneling density of states at temperatures close to and above the Kondo temperature [1,2]. The differential conductance is then obtained as a function of an external voltage. We also obtain the temperature dependence of the linear conductance and compare it with the one obtained in numerical renormalization group calculations. We find that our Keldysh field integral theory predicts a universal temperature dependence of the linear conductance and that the scaling of this dependence is given by the standard Kondo temperature.
[1] S. Smirnov and M. Grifoni, Phys. Rev. B 84, 125303 (2011).
[2] S. Smirnov and M. Grifoni, arXiv:1109.1540.

TT 22: Correlated Electrons: Low-dimensional Systems - Materials 1

Time: Wednesday 9:30–13:00 Location: H 0104

TT 22.1 Wed 9:30 H 0104

Magnetic properties of ultra-thin layer of LCMO in oxides heterostructures — •Soltan Soltan[1,2], Joachim Albrecht[3], Eberhard Goering[4], Georg Christiani[1], Gennady Logvenov[1], and Hanns-Ulrich Habermeier[1] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Physics Department, Faculty of Science, Helwan University,11792-Cairo, Egypt — [3]Hochschule Aalen, Beethovenstr. 1, 73430 Aalen, Germany — [4]Max-Planck-Institut fue Intelligent System, Heisenbergstr. 3, D-70569 Stuttgart, Germany

We investigate the variety of high quality magnetic heterostructures of different nonmagnetic oxides (YBCO and LNO) with magnetic LCMO layers grown by PLD on single crystal substrate $SrTiO_3$ with <100> and <110> orientations. We have used the X-ray diffraction to characterize the quality of these heterostructures including crystal structure and interface roughness. We have measured magnetization of these heterostructures at different temperatures and magnetic fields by using SQUID magnetometer. It has been found that a single LCMO layer with thickness of 2-3 unit cells shows ferromagnetism with a Curie temperature close to the bulk value. We present detailed discussion of the magnetic properties of the ultrathin LCMO layers in these heterostructures.

TT 22.2 Wed 9:45 H 0104

Negative compressibility at $LaAlO_3/SrTiO_3$ interfaces explored with scanning force microscopy — •Veronika Tinkl[1], Martin Breitschaft[1], Christoph Richter[1,2], German Hammerl[1], Thilo Kopp[1], and Jochen Mannhart[1,2] — [1]Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, Augsburg — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

The interface between the band insulators $LaAlO_3$ and $SrTiO_3$ is currently one of the most actively investigated structures in the field of oxide interfaces. If the $LaAlO_3$-film thickness exceeds three unit cells on a TiO_2-terminated $SrTiO_3$ substrate a conducting layer is formed at the interface. This conducting layer can be driven insulating by electric fields. In this presentation we will demonstrate that the interface exhibits negative compressibility as the carrier density is reduced.

We investigated interfaces consisting of four unit cells $LaAlO_3$ with a low temperature ultra-high vacuum scanning probe microscope. Contact potential difference measurements were performed at various carrier densities of the interface electron system. The difference in the work functions of interface and tip depends on the applied electric field. We will show that the chemical potential at the interface increases with decreasing carrier density. This effect is caused by electron-electron interactions and corresponds to a negative compressibility. The negative compressibility gives rise to applications by, for example, making use of the resulting large enhancement of the capacitance.
[1] Lu Li *et al.*, Science **332**, 825 (2011).

TT 22.3 Wed 10:00 H 0104

Magnetism and superconductivity at LAO/STO-interfaces: the role of Ti 3d interface electrons — •Natalia Pavlenko[1], Thilo Kopp[1], Evgeny Tsymbal[2], George Sawatzky[3], and Jochen Mahhnart[4] — [1]EKM and Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Department of Physics and Astronomy, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588-0299, USA — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada V6T1Z1 — [4]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Ferromagnetism and superconductivity are in most cases adverse. However, recent experiments reveal that they coexist at interfaces of $LaAlO_3$ and $SrTiO_3$. We analyze the ferromagnetic state within density functional theory and provide evidence that it is also generated by Ti 3*d* interface electrons, as is the two-dimensional electron liquid at the interface which gives rise to superconductivity. We demonstrate that oxygen vacancies in the TiO_2 interface layer enhance the tendency for ferromagetism considerably. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic

behavior in the superconducting state.

TT 22.4 Wed 10:15 H 0104

Electrostatic doping of a Mott insulator in an oxide heterostructure: the case of $LaVO_3/SrTiO_3$ — •Andreas Müller[1], Hans Boschker[2], Florian Pfaff[1], Martin Kamp[2], Gertjan Koster[2], Guus Rijnders[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Insititut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany — [2]Faculty of Science and Technology and MESA$^+$ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The discovery of a quasi-two-dimensional electron system at the interface between the two band insulators $LaAlO_3$ and $SrTiO_3$ has triggered intense investigations of oxide heterostructures with other material combinations. The hope is that by combining a polar overlayer with a non-polar substrate electronic reconstruction will lead to highly mobile interface charge carriers with special properties. The formation of a conducting interface layer in epitaxial $LaVO_3/SrTiO_3$, where $LaVO_3$ is a Mott insulator, is studied by transport measurements and hard x-ray photoelectron spectroscopy. We identify an insulator-to-metal transition above a critical $LaVO_3$ thickness with transport properties similar to those recently reported for $LaAlO_3/SrTiO_3$ interfaces. Interestingly, our photoemission measurements give evidence that electronic charge is transferred exclusively to the $LaVO_3$-side of the interface caused by an electronic reconstruction within the film itself. This opens the opportunity to study a band-filling controlled Mott transition induced by a purely electrostatic mechanism.

TT 22.5 Wed 10:30 H 0104

Confinement induced metal-to-insulator transition in strained $LaNiO_3/LaAlO_3$ superlattices — •Arianda Blanca-Romero and Rossitza Pentcheva — Ludwig Maximilians University, Munich, Germany.

Using density functional theory calculations including a Hubbard U term we explore the effect of strain and confinement on the electronic ground state of superlattices containing the band insulator $LaAlO_3$ and the correlated metal $LaNiO_3$. Besides a suppression of holes at the apical oxygen, a central feature is the asymmetric response to strain in single unit cell superlattices: For tensile strain a band gap opens due to charge disproportionation at the Ni sites with two distinct magnetic moments of $1.45\mu_B$ and $0.71\mu_B$. Under compressive stain, charge disproportionation is nearly quenched and the band gap collapses due to overlap of $d_{3z^2-r^2}$ bands through a semimetallic state. This asymmetry in the electronic behavior is associated with the difference in octahedral distortions and rotations under tensile and compressive strain. The ligand hole density and the metallic state are quickly restored with increasing thickness of the $(LaAlO_3)_n/(LaNiO_3)_n$ superlattice from $n = 1$ to $n = 3$.
Funding by DFG within SFB/TR80 is gratefully acknowledged.

TT 22.6 Wed 10:45 H 0104

Soft-X-Ray ARPES: From Three-Dimensional Materials to Multilayer Heterostructures — •Vladimir N. Strocov[1], Masaki Kobayashi[1,2], Ming Shi[1], Thorsten Schmitt[1], and Luc Patthey[1] — [1]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland — [2]Department of Applied Chemistry, University of Tokyo, Tokyo 113-8656, Japan

Soft-X-ray ARPES benefits from free-electron final states, simplified matrix elements and increasing photoelectron escape depth. The latter, apart from allowing bulk sensitivity and access to deep layers in heterostructures, improves intrinsic resolution in surface-perpendicular momentum k_z crucial for three-dimensional (3D) systems.

The ADRESS beamline (J. Synchrotron Rad. **17** (2010) 631) delivers soft X-rays with photon energies from hv = 300 to 1600 eV. The flux tops up 10^{13} photons/s/0.01%BW which allows breakthrough of the notorious valence band cross-section problem. The acquisition time is typically only a few minutes with energy resolution of 110 meV, increasing to a few tens of with 60 meV.

Apart from technical details, we give an overview of recent soft-X-ray ARPES results, including 3D Fermi surface (FS) of VSe_2, with its warping giving rise to 3D charge density waves, alternating FS shapes in 3D pnictides, topological surface state in 3D valence band of $PbBi_4Te_7$, FS of buried layers in $LaAlO_3/LaNiO_3$ and $LaAlO_3/SrTiO_3$ hererostructures, etc. These results demonstrate an immense potential of soft-X-ray ARPES for electronic structure of 3D materials and multilayer heterostructures.

TT 22.7 Wed 11:00 H 0104

Geometric frustration and competing phases of the Sn/Si(111) surface system — •Gang Li[1], Philipp Höpfner[2], Jörg Schäfer[2], Ralph Claessen[2], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

One third of a monolayer of Sn adatoms on the (111) surface of Si presents a quasi-two dimensional realization of a Mott-Hubbard system on an effective triangluar lattice, displaying an intricate interplay between lattice reconstructions, inherent (magnetical) frustration and emerging and competing low-T phases. We study the Sn/Si(111)-$(\sqrt{3} \times \sqrt{3})$ adatom system with material specific many-body calculations and with angle-resolved photoelectron spectroscopy (ARPES). In a first step, we investigate the electronic correlation effects by combining the ab-initio density-functional approach with sophisticated many-body methods, i.e. DMFT, DCA, Dual Fermion and Variational Cluster methods. A metal-insulator transition with first (second) order at finite (zero) temperature is predicted, and the system is proven to be short-range correlated. The interplay of the electron-electron interaction and geometrical frustration favors a row-wise antiferromagnetic (RW-AFM) order. Comparing to ARPES, we find a good overall agreement between theory and experiment for the spectral function and its temperature dependence. In particular, the additional 3×3 symmetry observed in ARPES is explained as a spectral-weight redistribution corresponding to the RW-AFM.

15 min. break.

TT 22.8 Wed 11:30 H 0104

Charge density wave formation in $ErTe_3$ — •Hans-Martin Eiter[1], Michela Lavagnini[1], Rudi Hackl[1], E. A. Nowadnick[2,3], A. F. Kemper[2,3], Thomas P. Devereaux[2,3], J.-H. Chu[2,3], J. G. Analytis[2,3], Ian R. Fisher[2,3], and Leonardo Degiorgi[4] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — [3]Geballe Laboratory for Advanced Materials & Dept. of Applied Physics, Stanford University, CA 94305, USA — [4]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland

Rare-earth tritellurides are model systems to study low dimensional interacting electron gases. $ErTe_3$ undergoes two charge density wave (CDW) phase transitions at 265 K and 155 K at ambient pressure. External pressure can suppress both CDW transitions completely. Using Raman scattering, it is possible to detect the signature of both CDW energy gaps as well as the corresponding collective amplitude mode excitations. This allows us to map out the high pressure phase diagram. We also provide calculations on the basis of the electronic band structure which allow us to understand the selection rules as well as the spectra in a semi-quantitatively fashion.
This work is supported by the DFG under Grant No. Ha2071/5.

TT 22.9 Wed 11:45 H 0104

Pressure-induced superconducting phase in rare-earth tritellurides ($R\mathrm{Te}_3$, R = Gd, Tb, Dy) — •Diego A. Zocco[1], James J. Hamlin[1], M. Brian Maple[1], Jiun-Haw Chu[2], and Ian R. Fisher[2] — [1]Department of Physics, University of California, San Diego — [2]Department of Applied Physics, Geballe Laboratory for Advanced Materials, Stanford University

It has recently been reported that the low-dimensional rare-earth tritellurides $R\mathrm{Te}_3$ (R = La-Nd, Sm, Gd-Tm) enter an unidirectional, incommensurate charge-density-wave (CDW) state when cooled below a temperature $T_{CDW1} \sim$ 450 - 250 K, which decreases with increasing rare earth atomic number, due to the effect of chemical pressure. For the heavier R (*i.e.*, Dy-Tm), a second CDW appears at $T_{CDW2} < T_{CDW1}$, orthogonal to the first one. We have recently found that the application of external pressure induces a superconducting (SC) state in $GdTe_3$, $TbTe_3$ and $DyTe_3$ at low temperatures, coexisting or competing with the two CDWs and the local moment rare-earth magnetism. In this talk, we present the results of experiments we have performed on these materials at high pressure and low temperature, to help develop an understanding of the origin of the superconducting state.

TT 22.10 Wed 12:00 H 0104

High-pressure studies of electronic order and lattice dynamics in 1T-TaS_2 — •Tobias Ritschel[1], Jan Trinckauf[1], Jorge Enrique Hamann Borrero[1], Gaston Garbarino[2], Alexei Bossak[2], Helmuth Berger[3], Martin von Zimmermann[4], Bernd Büchner[1], and Jochen Geck[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Germany — [2]ESRF, Grenoble, France — [3]Ecole polytechnique Federale de Lausanne, Switzerland — [4]HASYLAB, Hamburg, Germany

The layered compound 1T-TaS_2 shows a very complex pressure-temperature phase diagram, including a commensurate (C), a nearly commensurate (NC) and an incommensurate (IC) charge density wave (CDW) phase. In addition, the material exhibits a pressure-induced superconducting phase with $T_c \approx 5\,K$.

We studied the static CDW-order performed by means of elastic X-ray diffraction as a function of temperature and external pressure. The intensity of the CDW-superlattice reflections within each phase was found to decrease with pressure, while the peak width and the position in reciprocal space was found to remain constant.

Furthermore, we investigated the pressure dependency of the lattice dynamics in the NC and IC phase at room temperature, using inelastic X-ray scattering. The Phonon dispersion around the IC wave vector is strongly pressure dependent and a Kohn anomaly was observed well above the NC to IC phase transition temperature. We will present the experimental data along with model calculations and discuss the results in relation to the pressure-induced superconductivity.

TT 22.11 Wed 12:15 H 0104

Phonon Instability in the CDW Systems 2H-$NbSe_2$ and $TiSe_2$ — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[2], Raymond Osborn[2], Goran Karapetrov[2], Takeshi Egami[3], Ayman Said[4], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, P. O. Box. 3640, D-76021 Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [5]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

Further investigations on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems 2H-$NbSe_2$ and $TiSe_2$ have been performed both theoretically in Density Functional Theory (DFT) based on ab-initio phonon calculations as well as experimentally by means of high resolution Inelastic X-ray Scattering (IXS). For both materials, the theoretical predictions for the phonon softening coincide with the experimentally observed CDW instability behaviour. For 2H-$NbSe_2$ the wave vector dependence of the electron-phonon coupling drives the CDW formation and determines its periodicity [1]. For $TiSe_2$, electron-phonon-coupling is strong enough to stabilize the structural phase transition at finite temperatures [2].

[1] F. Weber et al., Phys. Rev. Lett. 107, 107403 (2011).
[2] F. Weber et al., Phys. Rev. Lett. 107, 266401 (2011).

TT 22.12 Wed 12:30 H 0104

Realignment of the charge density wave in $TiSe_2$ by variation of the conduction band population — •Matthias M. May[1,2], Christoph Janowitz[1], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin — [2]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin

Recent experimental [1] and theoretical [2] studies of the charge density wave phase of $TiSe_2$ have pronounced the strong excitonic contributions to this phase transition. The effect of increasing the conduction band population by water adsorption [1] was studied with ARPES. Our results suggest a change of the energetically most favourable direction of the electronic superstructure in k-space above a certain population threshold: The 2x2 in plane part of the 2x2x2 superstructure is observable by ARPES for low H_2O-coverage, whereas the perpendicular x2 signature appears only for higher coverage, after the 2x2 has been reduced.

[1] May et al., *Phys. Rev. Lett.* **107**, 176405 (2011)
[2] van Wezel et al., *Phys. Rev. B* **81**, 165109 (2010)

TT 22.13 Wed 12:45 H 0104

Effect of Charge Order on the Plasmon Dispersion in Transition-Metal Dichalcogenides investigated by Electron Energy-Loss Spectroscopy — •Andreas König[1], Jasper van Wezel[2], Roman Schuster[1], Martin Knupfer[1], Helmuth Berger[3], Jeroen van den Brink[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P. O. Box 270116, D-01171 Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — [3]Institut de Physique de la Matière Condensée, EPFL, CH-1015 Lausanne, Switzerland

2H-$TaSe_2$ is one of the various polytypes of the transition-metal dichalchogenides (TMDC) that show a phase transition to a charge-density wave (CDW) and to a superconducting state. It is already proven for 2H-$TaSe_2$ [1] and a few other TMDCs that they show a negative dispersion of the bulk plasmon energy in the normal state and an even larger bandwidth of this negative dispersion in the CDW state, which is altogether not a behavior of a common metal.

We discuss the connection of the susceptibility to a CDW phase and of the negative plasmon dispersion by applying Electron Energy-Loss Spectroscopy (EELS) measurements in transmission on thin films of 2H-$TaSe_2$ as well as a semiclassical Ginzburg-Landau model [2]. The connection is further emphasized by intercalation experiments with potassium that show a suppression of the CDW as well as a change of slope of the plasmon dispersion.

[1] Schuster et al., Phys. Rev. B **79**, 045134 (2009)
[2] van Wezel et al., Phys. Rev. Lett. **107**, 176404 (2011)

TT 23: Superconductivity: Fe-based Superconductors - Fe(Se/Te)

Time: Wednesday 9:30–11:15 Location: H 2053

TT 23.1 Wed 9:30 H 2053

Separation of iron spin states in chalcogenide superconductors — Vladimir Gnezdilov[1], •Peter Lemmens[2], Yurii Pashkevich[3], Alexander Gusev[3], Tatiana Shevtsova[3], Karina Lamonova[3], Dirk Wulferding[2], Ekaterina Pomjakushina[4], and Kazimierz Conder[4] — [1]ILTPE NAS, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]DonFTI, Donetsk, Ukraine — [4]PSI, Villigen, Switzerland

We present a Raman study of superconducting single crystals $M_{1-x}Fe_{2-y}Se_2$ (M = Rb, Cs). Our data together with ab-initio spin-polarized band structure and phonon calculations show the presence of two phases: an insulating vacancy ordered $Rb_2Fe_4Se_5$ phase and a metallic phase with iron in a low spin state. At high frequencies we observe electronic d-d interband transitions, indicating the insulating state. Our results show that iron is in close proximity to a spin state instability. Work supported by DFG and Rus-Ukr.

TT 23.2 Wed 9:45 H 2053

Phase separation in superconducting and antiferromagnetic $Rb_{0.8}Fe_{1.6}Se_{2.0}$ probed by Mössbauer spectroscopy — •Vadim Ksenofontov[1], Gerhard Wortmann[2], Sergey A. Medvedev[1,3], Vladimir Tsurkan[4,5], Joachim Deisenhofer[4], Alois Loidl[4], and Claudia Felser[1] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — [2]Department Physik, Universität Paderborn, D-33095 Paderborn, Germany — [3]Max-Planck Institute for Chemistry, D-55128 Mainz, Germany — [4]Experimental Physics V, University of Augsburg, D-86159 Augsburg, Germany — [5]Institute of Applied Physics, Academy of Sciences, MD-2028, Chisinau, Republic of Moldova

^{57}Fe Mössbauer studies of superconducting $Rb_{0.8}Fe_{1.6}Se_{2.0}$ with T_c = 32.4 K were performed on single-crystalline and polycrystalline samples in the temperature range 4.2 K to 295 K. They reveal the presence of 88% magnetic and 12% non-magnetic Fe^{2+} species with the same polarization dependence of their hyperfine spectra. The magnetic species are attributed to the 16i sites of the $\sqrt{5} \times \sqrt{5} \times 1$ superstructure and the non-magnetic Fe species to a nano-sized phase observed in recent structural studies of superconducting $K_xFe_{2-y}Se_2$ systems. The ^{57}Fe spectrum of a single-crystalline sample in an external field of 50 kOe

applied parallel to the crystallographic c-axis confirms the antiferromagnetic order between the fourfold ferromagnetic Fe(16i) supermoments and the absence of a magnetic moment at the Fe sites in the minority phase. Our study provides convincing evidence about the nano-scale phase separation in $Rb_{0.8}Fe_{1.6}Se_{2.0}$.

TT 23.3 Wed 10:00 H 2053

Itinerant magnetic excitation in $Rb_{0.8}Fe_{1.6}Se_2$ — •G. Friemel[1], J.T. Park[1], Y. Li[1], V. Tsurkan[2], J. Deisenhofer[2], H.-A. Krug von Nidda[2], A. Loidl[2], A. Invanov[3], B. Keimer[1], and D. S. Inosov[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg Univ., 86135 Augsburg, Germany — [3]Institut Laue-Langevin, 6 rue Jules Horowitz, F-38042 Grenoble Cedex 9, France

The recently discovered superconductors $A_xFe_{2-y}Se_2$ (A=K, Rb, Cs) concurrently exhibit strong magnetism (T_N =534 K) and superconductivity (SC) with T_c = 32 K. Recent reports relate the magnetic ordering to an insulating phase with a $\sqrt{5} \times \sqrt{5}$ iron vacancy superstructure. Superconductivity, however, seems to originate from a separate phase, which possesses large electron pockets at the M point and no hole pocket at the Γ point, according to ARPES. We present investigations of the magnetic response of this phase by inelastic neutron scattering experiments. We found resonant enhancement of magnetic excitations near $Q = (\pi, 0.5\pi)$ and E = 14 meV and mapped out its Q-dependence in the $(HK0)$-plane and out of the plane. Our results agree well with published RPA-calculations of the normal state and SC state [1], which peak at the nesting vectors of the Fermi surface seen by ARPES and which suggest a sign changing d-wave SC order parameter for this new family of superconductors.
[1] Maier et al., Phys. Rev. B, 83, 100515, (2011).

TT 23.4 Wed 10:15 H 2053

Magneto-structural investigations on $Fe_{1+x}(Te_{1-y}Se_y)$ single crystals — •Mathias Doerr[1], Wolfram Lorenz[1], Dona Cherian[2], Sahana Rössler[3], Steffen Wirth[3], Philipp Materne[1], and Michael Loewenhaupt[1] — [1]Technische Universität Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany — [2]Dept. of Physics, Indian Inst. of Science, Bangalore-560012, India. — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany

The class of $Fe_{1+x}(Te_{1-y}Se_y)$ compounds is the counterpart of Fe-pnictides, special effects as magnetic order or superconductivity are found. A special topic is the interplay of magnetic and lattice properties which is crucial for a number of correlation phenomena. Thermal expansion and isothermal magnetostriction was measured on $Fe_{1+x}Te$ (x = 0, 0.06, 0.13) and compared to other experiments and model concepts. As one fact, it is shown that magnetic order exists independently of lattice distortions, already at higher temperatures than the latter ones. Moreover, strong thermal hysteresis effects occur. This behaviour differs from that of the Fe-pnictides and therefore, microscopic mechanisms (as for example magnetic fluctuations) should stay a matter of particular interest.

TT 23.5 Wed 10:30 H 2053

Superconductivity of $Fe_{1.07}Se_{0.5}Te_{0.5}$ studied by Spectroscopic-Imaging Scanning Tunneling Microscopy — •Udai Raj Singh[1], Seth White[1], Stefan Schmaus[1], Joachim Deisenhofer[2], Vladimir Tsurkan[2], Alois Loidl[2], and Peter Wahl[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Lehrstuhl für Experimentalphysik V, Universität Augsburg, Augsburg, Germany

The unconventional superconductivity in the recently discovered iron-based superconductors has become an active field of research [1]. We study the electronic structure of $Fe_{1.07}Se_{0.5}Te_{0.5}$ ($T_c \sim 15$ K) by spectroscopic-imaging scanning tunneling microscopy (SI-STM). SI-STM has been shown to be an important tool to investigate the electronic inhomogeneities and electronic structure in high temperature superconductors [2]. The iron chalcogenide superconductor $Fe_{1.07}Se_{0.5}Te_{0.5}$ provides a well defined cleavage plane, making it an ideal candidate for STM investigation. We find the superconducting gap consistent with earlier studies [3]. We show in our study the temperature dependence of the superconducting gap. We observe significant nanoscale inhomogeneity of the superconducting gap.
[1] Y. Kamihara, et al., J. Am. Chem. Soc. 128, 10012 (2006) and Y. Kamihara, et al., J. Am. Chem. Soc. 130, 3296 (2008).
[2] J. E. Hoffman, et al., Science 297, 1148 (2002); K. McElroy, et al., Nature 422, 592 (2003).
[3] T. Hanaguri, et al., Science 328, 474 (2010).

TT 23.6 Wed 10:45 H 2053

Lattice dynamics of FeTe: a combined DFT and inelastic neutron scattering study — •Rolf Heid, Klaus-Peter Bohnen, Sven Krannich, Lothar Pintschovius, and Frank Weber — Karlsruher Institut für Technologie, Institut für Festkörperphysik

For all pnictide families DFT calculations of lattice dynamical properties predict a high sensitivity on structural and magnetic degrees of freedom. Comparison with experiment thus can provide valuable information about the appropriate theoretical model. For the 1111 and 122 families, however, DFT significantly overestimates the size of the ordered magnetic moment which potentially hampers such a comparison. In contrast, the Fe chalcogenide family represents a much better test case, as both theory and experiment agree on the existence of large ordered moments.
Here we present results of a combined DFT and inelastic neutron scattering study of the phonon dispersion of FeTe. Large parts of the dispersion curves were mapped out at low temperature and compared with DFT results for nonmagnetic and antiferromagnetic phases using various lattice structures. A satisfactory description of the data is obtained only when the Fe-Te distance of the magnetic calculation is used. The spin-polarization itself, however, is found to be of minor importance.

TT 23.7 Wed 11:00 H 2053

Paramagnons in FeSe close to Magnetic Phase Transition — •Leonid Sandratskii, Frank Essenberger, Pawel Buczek, Arthur Ernst, and Eberhard Gross — Max-Planck-Institut für Mikrostrukturphysik, Halle

The magnetic excitations in FeSe are studied from first principles applying linear response density functional theory. The position of the selenide layer is varied to model the transition between paramagnetic and antiferromagnetic phases. In the paramagnetic phase, close to the point of magnetic instability we find a branch of long lived collective spin excitations, paramagnons. The phase transition to the AFM phase changes the character of the spin excitations drastically.

TT 24: Nanomechanics

Time: Wednesday 9:30–12:45 Location: H 3005

TT 24.1 Wed 9:30 H 3005

Dynamics of strongly coupled nanomechanical resonators — •Benjamin A. Gmeiner, Onur Basarir, Jörg P. Kotthaus, and Eva M. Weig — Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität (LMU), Geschwister-Scholl-Platz 1, D-80539 München, Germany

In this work we study the modal interactions between two strongly coupled nanoelectromechanical (NEMS) resonators. To this end, we have fabricated a system of two doubly-clamped silicon nitride (SiN) string resonators coupled via a shared mechanical support using a series of standard clean room techniques. Each string resonator is equipped with a set of integrated electrodes allowing for an independent frequency tuning and mechanical excitation using dielectric gradient forces [1]. A shot noise-limited Fabry-Perot interferometer operating at 1550 nm has been used for the detection of the nanomechanical motion. We have characterized a set of devices with fundamental resonance frequencies around 8 MHz and quality factors of $Q > 2 \cdot 10^4$ at room temperature in high vacuum. By tuning the resonance frequencies and driving each resonator across its resonance we have observed avoided mechanical mode crossings in the high frequency spectrum, characteristic for a strongly coupled system. These experiments are the important steps in understanding strongly coupled mechanical sys-

tems and might be utilized for enhanced sensor configurations based on collective and non-linear phenomena.
[1] Q. P. Unterreithmeier, E. M. Weig, and J. P. Kotthaus, Nature (London) 458, 1001 (2009)

TT 24.2 Wed 9:45 H 3005

Optomechanically Induced Transparency and Slow Microwaves in Circuit Nano-electromechanics — •Xiaoqing Zhou[1,2], Fredrik Hocke[3], Albert Schliesser[1,2], Achim Marx[3], Hans Hübl[3], Rudolf Gross[3,4], and Tobias J. Kippenberg[1,2] — [1]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Walther-Meißner-Institut, Garching, Germany — [4]Technische Universität München, Garching, Germany

Using a low-mass (≈ 15 pg), high-Q ($> 100\,000$) nanomechanical oscillator coupled to a Nb superconducting quarter wave cavity, we realize a circuit nano-electromechanical system coupling microwaves to mechanical motion oscillating at 1.45 MHz. By exciting the system on the lower motional sideband with a strong drive tone, a transparency window for a probe field is created originating from the effect of optomechanically induced transparency (OMIT) [1]. This phenomenon, analogous to electromagnetically induced transparency in Atomic Physics, arises from the interference of different excitation pathways for an intracavity probe field. We utilize the transparency window to demonstrate slow microwave propagation. A tunable delay up to 4 ms is demonstrated experimentally for a microwave pulse on resonance with the cavity. Furthermore, we systematically investigate the temporal dynamics of this transparency window when the drive tone is modulated, and the effect of the oscillator's Duffing nonlinearity on the OMIT window.
[1] S.Weis *et al.*, Science **330**, 1520 (2010)

TT 24.3 Wed 10:00 H 3005

Optomechanically Induced Absorption and Parametric Effects in a Circuit Nano-Electromechanial System Driven on Blue Sideband — •Fredrik Hocke[1], Xiaoqing Zhou[3,4], Albert Schliesser[3,4], Achim Marx[1], Rudolf Gross[1,2], Tobias Kippenberg[3,4], and Hans Huebl[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany — [4]Ecole Polytechnique Fédérale de Lausanne, Switzerland

In the field of optomechanics, a light field trapped in an optical resonator is dynamically coupled to a mechanical mode, enabling cooling and amplification of mechanical motion. This concept of light matter interaction can be transferred to the microwave (MW) regime combining superconducting MW circuits with nanometer-sized mechanical beams. With such a system we demonstrate optomechanically induced absorption: In the presence of a blue-detuned pump field, constructive interference of two excitation pathways leads to a mechanically enhanced coupling of a probe field into the MW cavity. There, probe photons are dissipated to the environment, leading to reduced transmission of the probe tone. Our experimental findings quantitatively agree with model predictions, including narrowing of the absorption window with increased pump power. We also discuss parametric effects when varying the pump power and driving the mechanical system via an additional AC-field at the mechanical resonance of $f_m = 1.45$ MHz. This work is supported by the Excellence Cluster "Nanosystems Initiative Munich (NIM)" .

TT 24.4 Wed 10:15 H 3005

Microwave cavity-enhanced transduction for plug and play nanomechanics at room temperature — •Thomas Faust, Peter Krenn, Stephan Manus, Jörg P. Kotthaus, and Eva M. Weig — Fakultät für Physik and Center for NanoScience, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany

The readout and manipulation of nanomechanical systems can be significantly enhanced by coupling them to an optical or electrical cavity. The latter has the advantage of allowing to read out a large array of resonators with only one cavity without any positioning involved. Up to now experiments employing the coupling to microwave cavities are performed at cryogenic temperatures to benefit from capacitively coupled superconducting cavities and resonators.

We present an approach based on a conventional $\lambda/4$ microstrip cavity at room temperature. It is dielectrically coupled to a doubly-clamped high stress silicon nitride beam with an extremely high mechanical quality factor of 290,000 at a mechanical resonance frequency of 6.6 MHz. Displacement detection is performed by monitoring the mechanically induced sidebands in the microwave cavity transmission signal. The sensitivity is sufficient to resolve the Brownian motion. Furthermore, the obtained coupling is strong enough to observe back-action effects of the microwave field on the mechanical resonator. We realise both cooling of the fundamental mode to 150 K as well as entering the regime of cavity-pumped self-oscillation. Thereby, an adjustement-free, all-integrated and self-driven resonator interfaced by just two microwave connectors is realised.

TT 24.5 Wed 10:30 H 3005

Development of a Mechanical Single Electron Shuttle — •Darren Southworth and Eva Weig — Ludwig-Maximilians-Universität, Fakultät für Physik, München

We present progress in the development of a mechanical single electron shuttle. The shuttle is composed of a gold island on a silicon nitride beam situated in a gap between source and drain electrodes. Oscillation of the beam brings the island into contact with the electrodes, and in the presence of a DC bias, charging of the island results in electron transport. The island is equipped with a gate electrode and the motion of the beam can be driven dielectrically. The current design has potential to function as a mechanical single electron transistor at 4K.

TT 24.6 Wed 10:45 H 3005

Single-wall carbon nanotubes as nano-electromechanical resonators — Daniel Schmid, Peter Stiller, Sabine Kugler, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Nano-electromechanical systems realized with carbon nanotubes display outstanding both electronical and mechanical properties. We present measurements on strong coupling between single electron tunneling and mechanical motion of a carbon nanotube quantum dot. The ultra-clean, freely suspended carbon nanotube in the few carrier limit is coupled to superconducting leads. Transport measurements show the transition from strong Coulomb blockade to the Kondo regime on the electron conduction side and from Coulomb blockade to Fabry-Perot interference on the hole conduction side. Connected to these different coupling strengths, we examine the behavior of the resonance frequency of the mechanical motion, detected via dc-current measurements.

15 min. break.

TT 24.7 Wed 11:15 H 3005

Cooling in the single-photon regime of optomechanics — •Andreas Nunnenkamp[1], Kjetil Borkje[2], and Steven Girvin[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Departments of Physics and Applied Physics, Yale University, New Haven, Connecticut 06520, USA

Optomechanics experiments are rapidly approaching the regime where the radiation pressure of a single photon displaces the mechanical oscillator by more than its zero-point uncertainty. We show that in this limit the power spectrum has multiple sidebands and that the cavity response has several resonances in the resolved-sideband limit [1]. We then discuss how red-sideband cooling is modified in this nonlinear regime. Using Fermi's Golden rule we calculate the transition rates induced by the optical drive. In the resolved-sideband limit we find multiple cooling resonances for strong single-photon coupling. They lead to non-thermal steady states and are accompanied by multiple mechanical sidebands in the optical output spectrum. Our study provides the tools to detect and take advantage of this novel regime of optomechanics.
[1] Phys. Rev. Lett. **107**, 063602 (2011).

TT 24.8 Wed 11:30 H 3005

Optomechanical circuits for nanomechanical continuous variable quantum state processing — •Michael P. Schmidt[1], Max Ludwig[1], and Florian Marquardt[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1/Bau 24, D-91058 Erlangen, Germany

Optomechanical crystals are novel on-chip realizations of an optomechanical system. Recently, Painter et. al. prepared the vibrational mode of such a structure in its quantum ground state by means of

optical sideband cooling, opening the door to the investigation of its quantum dynamics. We propose and analyze an architecture, in which linear quantum operations can be performed selectively on the vibrational modes: By suitable modulation of the driving laser intensity, it is possible to generate entanglement, squeezing and state transfer between modes.

TT 24.9 Wed 11:45 H 3005

Photon Statistics in Ultrastrong Coupling Optomechanics — •Andreas Kronwald[1], Max Ludwig[1], and Florian Marquardt[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1/Bau 24, D-91058 Erlangen, Germany

A standard optomechanical system consists of a laser-driven photonic mode coupled to a mechanical degree of freedom. In the ultrastrong coupling regime, where a single photon is able to strongly affect the mechanical mode, a wide range of nontrivial phenomena is expected. In this work, we focus on the full counting statistics of the photonic mode using a quantum jump trajectory method. Thereby, we observe photon antibunching as well as photon avalanches, which are induced by the ultrastrong light-mechanics coupling.

TT 24.10 Wed 12:00 H 3005

Enhanced photon and phonon detection in ultrastrong-coupling optomechanics — •Max Ludwig[1], Amir H. Safavi-Naeini[2], Oskar Painter[2], and Florian Marquardt[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen, Deutschland — [2]Thomas J. Watson, Sr., Laboratory of Applied Physics, California Institute of Technology, Pasadena, CA 91125, USA

The regime of ultrastrong coupling in optomechanics is reached when the optomechanical coupling rate becomes comparable to the cavity linewidth. In this regime we consider a setup comprising two cavity modes and a single mechanical mode. For mechanical frequencies nearly resonant to the optical level splitting the photon-phonon and the photon-photon interaction is boosted enabling QND phonon and photon detection.

TT 24.11 Wed 12:15 H 3005

Adiabaticity in semiclassical nanoelectromechanical systems — •Anja Metelmann and Tobias Brandes — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We compare the semiclassical description of NEMS within and beyond the adiabatic approximation. We consider a NEMS model which contains a single phonon (oscillator) mode linearly coupled to an electronic few-level system in contact with external particle reservoirs (leads). Using Feynman-Vernon influence functional theory, we derive a Langevin equation for the oscillator trajectory that is non-perturbative in the system-leads coupling. A stationary electronic current through the system generates nontrivial dynamical behavior of the oscillator, even in the adiabatic regime. The 'backaction' of the oscillator onto the current is studied as well [1].
For the case of two coupled electronic levels, we discuss the differences between the adiabatic and the non-adiabatic regime of the oscillator dynamics.
[1] A. Metelmann and T. Brandes, Phys. Rev. B **84**, 155455 (2011).

TT 24.12 Wed 12:30 H 3005

Detecting Majorana Bound States by Nanomechanics — •Stefan Walter[1], Thomas L. Schmidt[2], Kjetil Børkje[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Yale University, 217 Prospect Street, New Haven, Connecticut 06520, USA

We propose a nanomechanical detection scheme for Majorana bound states, which have been predicted to exist at the edges of a one-dimensional topological superconductor, implemented, for instance, using a semiconducting wire placed on top of an *s*-wave superconductor. Existing detection schemes focus, for instance, on tunnel setups, interferometer setups and the Josephson effect. However, it is fair to say that true qualitative experimental signatures of Majorana fermions that persist in realistic systems are rather difficult to predict.

Our detection scheme, makes use of an oscillating electrode, which can be realized using a doubly clamped metallic beam, tunnel coupled to one edge of the topological superconductor. We find that a measurement of the nonlinear differential conductance provides the necessary information to uniquely identify Majorana bound states.

TT 25: Correlated Electrons: Quantum-Critical Phenomena 1

Time: Wednesday 9:30–12:45 Location: H 3010

TT 25.1 Wed 9:30 H 3010

Deconfined quantum criticality and logarithmic violations of scaling — •Flavio Nogueira[1] and Asle Sudbo[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway

Recently logarithmic corrections to scaling were observed numerically in the so called $J-Q$ model. These violations of standard scaling were seen in numerical measurements of the spin-stiffness at zero temperature and uniform susceptibility at finite temperature. This result led to speculations that the deconfined quantum criticality scenario has to be revised in order to explain this new feature. We use the CP^{N-1} representation to derive the leading contribution to the spin stiffness at large N near the quantum critical point and show that it exhibits a logarithmic correction to scaling. This result shows that such logarithmic violations of scaling are in fact predicted by deconfined quantum criticality. Furthermore, the $U(1)$ gauge symmetry plays a crucial role here, since models without such local gauge symmetry do not exhibit logarithmic violations of scaling in 2+1 dimensions.

TT 25.2 Wed 9:45 H 3010

Usadel equation approach to fluctuation conductivity in disordered superconductors — Konstantin Tikhonov[1,2], •Georg Schwiete[3], and Alexander Finkelstein[1,4] — [1]Texas A&M University, College Station, Texas, USA — [2]Landau Institute for Theoretical Physics, Moskow, Russia — [3]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany — [4]The Weizmann Institute of Science, Rehovot, Israel

We study fluctuation corrections to the longitudinal and transverse conductivities in disordered superconducting films. The calculation covers a broad range of perpendicular magnetic fields and temperatures, including the vicinity of the magnetic field-tuned quantum critical point. Our calculation scheme is based on the Usadel equation, which we adjust to account for the fluctuating order parameter field.

TT 25.3 Wed 10:00 H 3010

Quantum dynamical crossover from coherent to incoherent dynamics in a Sub-Ohmic independent Boson model — •Peter Nalbach and Michael Thorwart — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

The sub-Ohmic spin-boson model shows with increasing coupling to a Sub-Ohmic bath a crossover from coherent to incoherent dynamics at zero (and at low) temperatures. The same system shows a quantum phase transition. However, in general both effects happen for different coupling strength. In order to study the connection between the dynamic crossover and the quantum phase transition we investigate an asymmetric Sub-Ohmic spin boson model and focus on the limit of vanishing tunneling. This results in a Sub-Ohmic independent Boson model which is exactly solvable. For this, we calculate the time evolution of the correlation function of the tunneling operators at zero temperature which allows to study the coherence properties even in absence of a direct tunnel coupling. Thus, we can determine the crossover coupling strength analytically. Most importantly, we compare it with numerical findings in the symmetric Sub-Ohmic spin boson model.

TT 25.4 Wed 10:15 H 3010

Quantum criticality with multiple dynamics — •Tobias Meng, Markus Garst, and Achim Rosch — Institut für Theoretische

Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Close to a quantum critical point, physical properties obey scaling laws characterizing the nature of the quantum critical point and allowing to conveniently interpret experiments. Conventional quantum critical scaling however depends on the hypothesis that only a single time scale diverges at the critical point, $\tau \sim \xi^z$, where the correlation length ξ becomes infinite. We analyze systems with multiple degrees of freedom that have two distinct characteristic time scales. While in some cases, the different dynamics influence each other only mildly, the interplay of multiple dynamics can also generate new critical exponents and give rise to unusual scaling laws.

TT 25.5 Wed 10:30 H 3010

Quantum criticality of the sub-ohmic spin-boson model — •Stefan Kirchner[1,2], Kevin Ingersent[3], and Qimiao Si[4] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute for Chemical Physics of Solids — [3]Department of Physics, University of Florida — [4]Department of Physics & Astronomy, Rice University

The sub-ohmic spin-boson model has a quantum critical point separating a delocalized phase in which the impurity degree of freedom is quenched and a boson-dominated localized phase that retains a two-fold local-moment degree of freedom. Whether this quantum phase transition is described by a ϕ^4-theory has recently received considerable attention. Here, we present an analysis of both the leading and subleading terms in the temperature dependence of the inverse static local spin susceptibility calculated using a numerical renormalization-group method. This provides evidence that the quantum critical point is interacting in cases where the quantum-to-classical mapping would predict mean-field behavior. We attribute the violation of the quantum-to-classical mapping to a Berry-phase term in a continuum path-integral representation of the model.

TT 25.6 Wed 10:45 H 3010

Functional renormalization group approach to singular interactions in 2D metals — •Casper Drukier, Lorenz Bartosch, Aldo Isidori, and Peter Kopietz — Universität Frankfurt, Frankfurt am Main, Germany

Using functional renormalization group methods we study an effective low-energy model describing the breakdown of Fermi-liquid behaviour in two-dimensional metals when gapless fermions at the Fermi surface are coupled by a fluctuating bosonic order parameter.

Using a field-theoretical approach, Metlitski and Sachdev [Phys. Rev. B 82, 075127] have recently found that certain three-loop diagrams strongly modify the one-loop results, and that the conventional 1/N expansion breaks down in this problem. We show that the three-loop diagrams discovered by Metlitski and Sachdev are contained in a rather simple truncation of the functional renormalization group flow equations, containing only irreducible vertices with two and three legs. An approximate solution of these flow equations yields explicit expressions for the vertex corrections, and allows us to calculate the scale-dependent anomalous dimension beyond one-loop level.

TT 25.7 Wed 11:00 H 3010

Tuning the spin dynamics of kagome systems — •Dirk Wulferding[1], Peter Lemmens[1], Hiroyuki Yoshida[2], Yoshihiko Okamoto[3], and Zenji Hiroi[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]NIMS, Tsukuba, Japan — [3]ISSP, Tokyo, Japan

Kagome lattice systems are among the most promising candidates for realizing a quantum spin liquid state. We compare the excitation spectra of different kagome compounds and demonstrate that the ground state properties depend critically on the underlying crystal structure. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

15 min. break.

TT 25.8 Wed 11:30 H 3010

Ferromagnetic quantum criticality in the new heavy-fermion system $YbNi_4P_2$ — •Manuel Brando, Alexander Steppke, Stefan Lausberg, Robert Kuechler, Edit Lengyel, Lucia Steinke, Cornelius Krellner, Robert Borth, Michael Nicklas, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Str. 40, 01187 Dresden, Germany

We present measurements of the ac-susceptibility, specific heat (C) and thermal expansion (α) on single crystals of the new quasi-one-dimensional heavy-fermion system $YbNi_4P_2$.

$YbNi_4P_2$ is a Kondo-lattice system that orders ferromagnetically at a very low temperature $T_c = 0.17$ K [1]. Ferromagnetism can be suppressed by arsenic substitution x on phosphorus site and a ferromagnetic (FM) quantum critical point (QCP) is approached at $x = 0.08$.

We provide evidence that such a FM-QCP exists in $YbNi_4(P_{0.92}As_{0.08})_2$ by showing that (i) the magnetic transition remains ferromagnetic between $x = 0$ and $x = 0.08$, (ii) no phase transition nor Fermi-liquid ground state down to 0.02 K can be observed at $x = 0.08$, and finally (iii) the Grüneisen ratio $\Gamma = \alpha/C$ strongly diverges [2] with decreasing temperature as $\Gamma \sim T^{-0.3}$.

Part of this work has been supported by the DFG Research Unit 960 "Quantum Phase Transitions".

[1] C. Krellner *et al.*, New J. Phys. **13** (2011) 103014
[2] L. Zhu *et al.*, Phys. Rev. Lett. **91** (2003) 066404

TT 25.9 Wed 11:45 H 3010

Pressure dependence of the topological Hall effect in MnSi — •Robert Ritz, Marco Halder, Christian Franz, Michael Wagner, Andreas Bauer, Christoph Schnarr, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85748 Garching, Germany

The observation of a topological Hall signal in the A-phase of MnSi [1] provides unambiguous, quantitative evidence of the non-trivial topology of the skyrmion lattice first inferred from small angle neutron scattering [2]. We report a comprehensive study of the pressure dependence of the topological Hall signal in MnSi. We connect the behaviour reported for the pressure range 6 to 12 kbar [3] with the properties at ambient pressure and explore the importance of various aspects of the experimental set up. Careful temperature and field dependent measurements reveal that the topological Hall signal in MnSi increases monotonically from 4 nΩcm at ambient pressure and appears to limit at a large intrinsic value of ~ 50 nΩcm as the helimagnetic transition temperature decreases.

[1] A. Neubauer et al., Phys. Rev. Lett. **102**, 186602 (2010).
[2] S. Mühlbauer et al., Science, Vol **323**, 915 (2009).
[3] M. Lee et al., Phys. Rev. Lett. **102**, 186601 (2010).

TT 25.10 Wed 12:00 H 3010

Electron Spin Resonance of the Yb $4f$-moment in $Yb(Rh_{1-x}Co_x)_2Si_2$ — Thomas Gruner, •Jörg Sichelschmidt, Christoph Klingner, Cornelius Krellner, Christoph Geibel, and Frank Steglich — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden

The evolution of spin dynamics from the quantum critical system $YbRh_2Si_2$ to the stable trivalent Yb system $YbCo_2Si_2$ was investigated by Electron Spin Resonance (ESR) spectroscopy. While the Kondo temperature changes by one order of magnitude all compositions of the single crystalline series $Yb(Rh_{1-x}Co_x)_2Si_2$ show well defined ESR spectra with a clear Yb^{3+} character for temperatures below ≈ 20 K. With increasing Co-content the ESR g-factor along the c-direction strongly increases indicating a continuous change of the ground state wave function and, thus, a continuous change of the crystal electric field. The linewidth presents a complex dependence on the Co-content and is discussed in terms of the Co-doping dependence of the Kondo interaction, of the magnetic anisotropy and the influence of ferromagnetic correlations between the $4f$ states. The results provide evidence that for low Co-doping the Kondo interaction allows narrow ESR spectra despite the presence of a large magnetic anisotropy whereas at high Co-concentrations the linewidth is controlled by ferromagnetic correlations. A pronounced broadening due to critical correlations at low temperatures is only observed at the highest Co-content. This might be related to the presence of incommensurate magnetic fluctuations.

TT 25.11 Wed 12:15 H 3010

Influence of charge carrier doping on the T^*-Scale in $YbRh_2Si_2$ — •Maik-Hendrik Schubert, Manuel Mchalwat, Elias Blumenröther, H. S. Jeevan, Yoshi Tokiwa, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

$YbRh_2Si_2$ is a prototype heavy-fermion metal which displays a magnetic field-induced antiferromagnetic (AF) quantum critical point (QCP). It has attracted much attention due to an additional low-energy scale $T^\star(B)$ merging at the QCP, whose origin is controversially discussed. Here, we report measurements of the electrical resistivity

$\rho(T, B)$ on different single crystalline samples of charge-carrier doped $Yb(Rh_{1-x}T_x)_2Si_2$ (T=Fe, Ni) at temperatures down to 15 mK and in magnetic fields up to 7 T. The partial substitution of Rh by either Fe or Ni introduces holes or electrons, respectively. The evolution of the single-ion Kondo scale is similar as for isoelectronic Co substitution and in accordance with the chemical pressure effect. However, while chemical pressure has little influence on $T^\star(B)$, we observe a drastic reduction or increase of $B^\star(T = 0)$ by Fe- or Ni-doping, respectively. Most interestingly, $B^\star(T = 0)$ is always pinned at the field-induced AF QCP, in contrast to chemical pressure results. As AF order is completely suppressed by Fe-doping, a heavy Fermi liquid ground (without $T^\star(B)$ anomaly) is observed.

Work supported by the DFG through the research unit 960 (Quantum phase transitions).

TT 25.12 Wed 12:30 H 3010

Electron spin resonance on $YbRh_2Si_2$ at mK temperatures close to the quantum critical point — •Marc Scheffler[1], Conrad Clauss[1], Martin Dressel[1], Jörg Sichelschmidt[2], Cornelius Krellner[2], Christoph Geibel[2], and Frank Steglich[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

$YbRh_2Si_2$ is a prototypical heavy-fermion material close to a quantum critical point: the antiferromagnetic order can be suppressed by a small external magnetic field of 60mT. Above this quantum critical point, a broad region of the phase diagram displays signatures of quantum criticality. Furthermore, a Landau Fermi-liquid regime is found for magnetic fields higher than the quantum critical point. Previous electron spin resonance (ESR) measurements on $YbRh_2Si_2$ demonstrated that the ESR response of this Kondo lattice system is characterized by the properties of local Yb moments. So far, ESR studies on $YbRh_2Si_2$ were limited to temperatures above 500mK and could not access the quantum critical regime close to the QCP nor the antiferromagnetic phase.

Here we present ESR measurements on $YbRh_2Si_2$ single crystals performed in a dilution refrigerator down to temperatures below 100mK. With ESR frequencies of a few GHz, we can cover temperature and field regimes close to the quantum critical point. We present the temperature and field dependences of the ESR parameters, in particular the ESR g-factor, and discuss them in the context of recent theoretical models.

TT 26: Transport: Topological Insulators 3 (jointly with HL and MA)

Time: Wednesday 9:30–13:00 Location: BH 334

TT 26.1 Wed 9:30 BH 334

Spin-dependent thermoelectric transport in topological insulators — •Dietrich G. Rothe, Marine Guigou, Björn Trauzettel, and Ewelina M. Hankiewicz — Institut für Theoretische Phys. und Astrophys. Würzburg

We analyze spin-dependent thermoelectric transport of topological insulators based on (Hg,Cd)Te quantum wells using the non-equilibrium Green's function technique within the Bernevig-Hughes-Zhang model. The motivation for our work is to generate spin currents in a medium with strong spin orbit coupling by a gradient of temperature in the absence of magnetic fields. Furthermore, we would like to better understand to what extend the thermoelectric coefficients probe spectral properties of such devices.

We investigate specifically the spin Nernst effect, a transverse spin current induced by a longitudinal temperature gradient, in a four-terminal setup. Interestingly, we predict a peak in the spin Nernst signal when the device is operated in the topologically non-trivial regime. This peak is directly related to the minigap formed by overlapping edge states from opposite boundaries of our device. Hence, the spin Nernst effect is a powerful experimental tool to analyze the size and the structure of the minigap. Additionally, we see that the spin Nernst effect is rather sensitive to details of the band structure. We discuss how this effect can be used to distinguish the topologically trivial from the non-trivial regime and why the energy dependence of transport is markedly resolved in the experimental signatures of the spin Nernst signal.

TT 26.2 Wed 9:45 BH 334

Topological insulators in magnetic fields: Quantum Hall effect and edge channels with non-quantized θ-term — •Matthias Sitte[1], Achim Rosch[1], Ehud Altman[2], and Lars Fritz[1] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]Department of Condensed Matter Physics, The Weizmann Institute of Science, 76100 Rehovot, Israel

We investigate how a magnetic field induces one-dimensional edge channels when the two-dimensional surface states of three-dimensional topological insulators become gapped. The Hall effect, measured by contacting those channels, remains quantized even in situations, where the θ-term in the bulk and the associated surface Hall conductivities, σ_{xy}, are not quantized due to the breaking of time-reversal symmetry. The quantization arises as the θ-term changes by $\pm 2\pi n$ along a loop around n edge channels. Model calculations show how an interplay of orbital and Zeeman effects leads to quantum Hall transitions, where channels get redistributed along the edges of the crystal. The network of edges opens new possibilities to investigate the coupling of edge channels.

[1] M. Sitte, A. Rosch, E. Altman, and L. Fritz, arXiv:1110.1363

TT 26.3 Wed 10:00 BH 334

Fractional quantum Hall states in lattice models and their potential realization due to multiple orbitals — •Stefanos Kourtis, Jörn Venderbos, Jeroen van den Brink, and Maria Daghofer — Institute for Theoretical Solid State Physics, IFW Dresden, 01171 Dresden, Germany

It has been recently demonstrated that topologically non-trivial lattice models of interacting particles can lead to a fractional quantum Hall effect without a magnetic field as long as the band width is very narrow. This has triggered a search for possible realizations of such models in optical lattices or materials. One promising observation is that electronic orbital degrees of freedom can lead to the nearly flat bands needed for a fractional-quantum Hall ground state [1]. We map the topologically non-trivial band of such a multi-orbital system onto an effective lattice model [2]. We use exact diagonalization to obtain the ground state of the effective model taking into account Coulomb interactions and investigate its topological properties. In particular, we calculate the eigenvalue spectra, ground states and Chern numbers for a variety of filling fractions and obtain clear indications of a hierarchy of fractionally charged excitations.

[1] J. W. F. Venderbos, M. Daghofer and J. van den Brink, Phys. Rev. Lett. 107, 116401 (2011).
[2] Jörn W.F. Venderbos, Stefanos Kourtis, Jeroen van den Brink and Maria Daghofer, arXiv:1109.5955 (2011).

TT 26.4 Wed 10:15 BH 334

Quantum transport in nanostructures of Bi_2Se_3-topological insulator — •Joseph Dufouleur[1], Romain Giraud[1], Andreas Teichgräber[1], Silke Hample[1], Stephan Neuhaus[1], Barbara Eichler[2], Oliver G. Schmidt[2], and Bernd Büchner[1] — [1]Institute for Solid State Research - IFW Leibniz Institute, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Institute for Integrative Nanosciences - IFW Leibniz Institute, Helmholtzstr. 20, D-01069 Dresden, Germany

Three-dimensional topological insulators belong to a new class of semiconductors with a large spin-orbit coupling which have spin-polarized Dirac fermions at their surface. In theory, these materials are insulating in the bulk, so that charge transport is only due to electronic surface states. In pratice, the Fermi energy often stands above or below the bulk band gap, due to uncontrolled defects formed during the growth of single crystals, or of epitaxial thin films or nanostructures. This makes the electrical properties of topologically-protected surface states difficult to measure, unless ultra-thin flakes of these materials are prepared.

To overcome this difficulty, we performed quantum transport measurement in ultra-thin Bi_2Se_3 flakes grown by CVD. We used e-beam litography technics to pattern Hall bars in the topological insulator. The measurements were done at low temperature and in an in-plane and perpendicular magnetic field up to 15 T.

TT 26.5 Wed 10:30 BH 334

Interaction and disorder effects in 3D topological insula-

tor thin films — •Elio Koenig[1], Pavel Ostrovsky[2], Ivan Protopopov[2], Igor Gornyi[2], and Alexander Mirlin[1,2] — [1]Institut für Theorie der Kondensierten Materie Karlsruher Institut für Technologie Wolfgang-Gaede-Str. 1 D-76131 Karlsruhe — [2]Institut für Nanotechnologie Hermann-von-Helmholtz-Platz 1 76344 Eggenstein-Leopoldshafen

It has been recently predicted that Coulomb interaction drives a surface of a 3D topological insulator into a critical state. We employ the sigma-model formalism to investigate the effect of electron-electron interaction on the transport by surface states in topological insulator thin films. We take into account the interaction of electrons on different surfaces and also the top-bottom asymmetry of the film (different densities of states and strength of disorder on top/bottom surface). This asymmetry is naturally present in experiments where the electronic densities on the surfaces are controlled independently by means of electrostatic gates. The lack of symmetry between top and bottom surfaces is shown to have strong effect on the film conductivity. The interplay of weak antilocalization, Coulomb interaction within and between surfaces and topological protection leads to a rich flow diagram representing the low temperature behavior of the system. The connection with recent experiments on Bi_2Se_3 films is discussed.

TT 26.6 Wed 10:45 BH 334

Rashba spin-orbit interaction in the superconducting proximity effect in helical Luttinger liquid — •Pauli Virtanen and Patrik Recher — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We consider the superconducting proximity effect in a helical Luttinger liquid at the edge of a 2D topological insulator. In addition to correlations between the left and right moving modes, coupling to a s-wave superconductor can also induce correlations inside a single mode, as the spin axis of the edge modes is not necessarily constant. This can be induced controllably in HgTe/CdTe quantum wells via the Rashba spin-orbit coupling. We discuss the consequent transport signatures, and point out a long-ranged feature in a dc conductance measurement that can be used to distinguish the two types of correlations present.

TT 26.7 Wed 11:00 BH 334

Bloch–Zener Oscillations in Graphene and Topological Insulators — •Viktor Krueckl and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Conventional free electrons in a superlattice subject to an accelerating drift potential feature a periodic motion known as Bloch oscillations. This physical phenomenon is enriched for topological insulators and graphene, since the electronic structure of those materials close to the Fermi energy is governed by a linear dispersion with a vanishing bandgap between electron and hole states. As a consequence superlattices based on zero-gap semiconductors exhibit characteristic Bloch–Zener oscillations that emerge from the coherent superposition of Bloch oscillations and multiple Zener tunneling between the electron and hole branch [1]. We demonstrate this mechanism by means of wave packet dynamics in various spatially periodically modulated nanoribbons subject to an external bias field. The associated Bloch frequencies exhibit a peculiar periodic bias dependence which we explain within a two-band model. Supported by extensive numerical transport calculations, we show that this effect gives rise to distinct current oscillations observable in the I-V characteristics of graphene and mercury telluride superlattices.

[1] Viktor Krueckl and Klaus Richter, arXiv:1109.5541v1 (2011)

15 min. break.

TT 26.8 Wed 11:30 BH 334

Generalized string order in 1D symmetry protected topological phases — •Frank Pollmann[1], Ari Turner[2], and Erez Berg[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]University of Amsterdam, 1090 GL Amsterdam, The Netherlands — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

A topological phase is a phase of matter which cannot be characterized by a local order parameter. It has been shown that gapped phases in 1D systems can be completely characterized using tools related to projective representations of the symmetry groups. An example of a symmetry protected topological phase is the Haldane phase of S = 1 chains. Here the phase is protected by any of the following symmetries: dihedral group of π-rotations about two orthogonal axes, time-reversal symmetry, or bond centered inversion symmetry. We introduce non-local order parameters as generalization of string order for each case which can be simply calculated using numerical methods such as Density-Matrix Renormalization Group (DMRG). These non-local order parameters provide a practical tool for numerically detecting different phases.

TT 26.9 Wed 11:45 BH 334

Tunable quantum spin Hall effect in double quantum wells — •Paolo Michetti[1], Jan C. Budich[1], Elena G. Novik[2], and Patrik Recher[1,3] — [1]Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Physical Institute, University of Würzburg, D-97074 Würzburg, Germany — [3]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

The field of topological insulators (TIs) is rapidly growing. The quantum spin Hall effect, characterized by a single pair of helical edge modes protected by time-reversal symmetry, has been demonstrated in HgTe-based quantum wells (QWs) with an inverted bandgap. Concerning possible applications, the quest for materials with an easily controllable TI phase is a key issue.

We analyze, employing an extended version of the Bernevig-Hughes-Zhang model, the topological properties of a generically coupled HgTe-based double QW (DQW). In particular we show how in such a system a TI phase can be driven by an inter-layer bias voltage, even when the individual layers are non-inverted. We also provide a numerical estimate of the system parameters, based on k.p calculations, suggesting the experimental feasibility of the present proposal.

Consequently, a DQW composed of non-inverted QWs, which could be in principle made of suitable narrow gap semiconductors different from HgTe, can be driven into a topologically non-trivial phase with the application of a gate bias.

TT 26.10 Wed 12:00 BH 334

Strong Correlations in a Generic Topological Insulator: The Transition-Metal Oxide Na_2IrO_3 — •Manuel Laubach[1], Ronny Thomale[2], Stephan Rachel[3], and Werner Hanke[1] — [1]Theoretical Physics, University of Würzburg, D-97074 Würzburg — [2]Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045 — [3]Department of Physics, Yale University, New Haven, CT 06520, USA

A key recent advancement in condensed-matter physics is to study the interplay between nontrivial topology and electronic correlations. In 5d transition-metal oxides, both the spin-orbit interaction and the electron correlation emerge at comparable orders of magnitude. In these systems, a variety of specifically tailored crystal structures are available, enabling the design of robust topological insulators. In this work, we study theoretically a monolayer of the 5d-compound Na_2IrO_3, modeled by a Hubbard-type of Hamiltonian on a honeycomb lattice where the spin symmetry is not conserved. Based on a variational cluster approach (VCA), the zero temperature phase diagram is obtained. We can identify, through an increase of the Hubbard U, the transition from a quantum spin Hall insulator to either a spin liquid phase or an antiferromagnetic insulating phase, depending on the strength of the spin-orbit coupling. We illustrate the evolution of the quasiparticle spectral function for bulk and edge-states upon variation of system parameters.

TT 26.11 Wed 12:15 BH 334

A quantum dot in a quantum spin Hall edge: Interaction effects — •Carsten Timm — Technische Universität Dresden, Germany

The edge states of a quantum spin Hall system are topologically protected but can be gapped by a magnetic field. A quantum dot realized by two magnetic tunneling barriers in a quantum spin Hall edge is proposed and transport through this device is analyzed. The analysis goes beyond linear response and incorporates electron-electron interaction in a combination of Green-function and master-equation approaches. A partial recurrence of non-interacting behavior is found for strong interactions. The possibility of controlling the magnetization of the edge by a locally applied gate voltage is proposed.

TT 26.12 Wed 12:30 BH 334

Inelastic electron backscattering in a generic helical edge channel — •Thomas L. Schmidt[1,2], Stephan Rachel[1], Felix von Oppen[3], and Leonid I. Glazman[1] — [1]Department of Physics, Yale University, 217 Prospect Street, New Haven, CT 06520, USA —

[2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universitaet Berlin, 14195 Berlin, Germany

We calculate the low-temperature conductance of a generic one-dimensional helical liquid which exists at the edge of a two-dimensional topological insulator (quantum spin Hall insulator). In a generic case, the S_z spin-symmetry is absent, which opens a possibility of single-particle inelastic electron backscattering. We show that although time-reversal invariance is preserved, inelastic backscattering gives rise to a temperature-dependent deviation from the quantized conductance, $\delta G \propto T^4$. In addition, δG is sensitive to the position of the Fermi level in the gap of the insulator. We present an effective model for this type of helical liquid and determine its parameters explicitly from numerical solutions of microscopic models for two-dimensional topological insulators in the presence of Rashba spin-orbit coupling.

TT 26.13 Wed 12:45 BH 334

Magnetoconductance of disordered HgTe strips — •Sven Essert and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Quantum wells of HgTe show the fascinating phenomenon of edge state transport which leads to a finite conductance in an energy window where the bulk material is insulating. This edge conductance exhibits special properties. One is, that it is expected to be stable against non-magnetic disorder because of a topological protection by time-inversion symmetry.

Inspired by this, we numerically investigate how the conductance of disordered HgTe strips of finite width changes under the application of a time-reversal symmetry breaking external magnetic field. We compare our results for different disorder models to experimental data.

Additionally, we study how the so-called "topological Anderson insulator" phase of HgTe strips, i.e. the phenomenon that finite disorder drives the metallic system into a quantum spin hall state with quantized edge conductance, is affected by the application of an external magnetic field.

TT 27: Superconductivity: Cuprate Superconductors

Time: Wednesday 11:30–13:15 Location: H 2053

TT 27.1 Wed 11:30 H 2053

Quantum and classical magnetoresistance oscillations in the electron-doped cuprate superconductor $Nd_{2-x}Ce_xCuO_4$ — •Toni Helm[1], Mark V. Kartsovnik[1], Nikolaj Bittner[1], Andreas Erb[1], Rudolph Gross[1], Carsten Putzke[2], Erik Kampert[2], Frederik Wolff-Fabris[2], Iliya Sheikin[3], Stephan Lepault[3], Cyril Proust[3], Andhika Kiswandhi[4], Eun San Choi[4], and James S. Brooks[4] — [1]Walther-Meissner-Institute, Garching, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden-Rossendorf, Germany — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France — [4]National High Magnetic Field Laboratory, Tallahassee, USA

The fundamentals of high-temperature superconductivity have not been understood completely, yet. Compared to most of the hole-doped cuprates, the electron-doped compound $Nd_{2-x}Ce_xCuO_4$ (NCCO) is rather simple and has a lower critical temperature T_c. By applying sufficiently high magnetic fields superconductivity is suppressed and the normal-conducting state can be accessed for even lowest temperatures. In pulsed and steady field experiments we observed Shubnikov-de Haas (SdH) and angle-dependent magnetoresistance oscillations (AMRO) for a series of NCCO single crystals in the range of $x = 0.14 - 0.17$. Starting from optimal doping up to the higher edge of the superconducting region our results provided clear evidence for the existence of a translational symmetry breaking. Here we report on how it develops towards the underdoped side and give an explanation for the AMRO arising only for overdoped samples in very high fields.

TT 27.2 Wed 11:45 H 2053

Optical investigation of nominally undoped Pr_2CuO_4 films — •G. Chanda[1], A. V. Pronin[1], R. P. S. M. Lobo[2], J. Wosnitza[1], H. Yamamoto[3], and M. Naito[4] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]LPEM, ESPCI-ParisTech, CNRS, UPMC, Paris, France — [3]NTT Basic Research Laboratories, NTT Corporation, Kanagawa, Japan — [4]Department of Applied Physics, Tokyo University of Agriculture and Technology, Tokyo, Japan

Superconducting Pr_2CuO_4 films with T' structure and T_c beetween 25 and 27 K have been investigated by different optical methods in a wide frequency range ($5 - 55000$ cm^{-1}) and for temperatures from 2 to 300 K. From the infrared reflectivity spectra, a superconducting gap of $2\Delta_0 = 17$ meV $= 7.4\ k_BT_c$ is estimated. Absolute values of the London penetration depth (λ_L) have been calculated from phase-sensitive teraherz measurements. The zero-temperature limit of λ_L is 1.6 μm. The overall temperature dependence of λ_L shows a behavior typical for the cuprates. However, a closer look on the penetration depth at low temperatures reveals a flattening of the temperature dependence. We find $\lambda_L(T) \propto T^n$ with $n = 2.8 \pm 0.2$.

TT 27.3 Wed 12:00 H 2053

High Pressure Changes of the ^{17}O NMR Spin Shift Pseudo-Gap of $YBa_2Cu_4O_8$ — •Thomas Meissner[1], Swee K. Goh[2], Jürgen Haase[1], Grant V. M. Williams[3], and Peter B. Littlewood[2,4] — [1]Faculty of Physics and Earth Science, University of Leipzig, Leipzig, Germany — [2]Department of Physics, Cavendish Laboratory, University of Cambridge, United Kingdom — [3]The MacDiarmid Institute and Industrial Research Limited, Wellington, New Zealand — [4]Argonne National Laboratory, Argonne, Illinois, USA

The influence of high pressure up to 63 kbar on the electronic properties of the high-temperature superconductor $YBa_2Cu_4O_8$ above the superconducting transition temperature T_c was measured with an NMR anvil cell design [1]. An increase of the spin shift at all temperatures is observed and the pseudogap feature almost vanishes at 63 kbar. We show that this change of the temperature-dependent spin susceptibility can be explained by a pressure-induced decrease of a temperature-dependent component, and an increase of a temperature-independent component. The results are compared to doping effects.

[1] T. Meissner, S. K. Goh, J. Haase, G. V. M. Williams, and P. B. Littlewood, Phys. Rev. B 83, 220517(R) (2011)

TT 27.4 Wed 12:15 H 2053

Peculiar temperature and momentum dependence in the spin ladder systems $Ca_xSr_{14-x}Cu_{24}O_{41}$ — •Friedrich Roth[1], Christian Hess[1], Udo Ammerahl[2], Alexandre Revcolevschi[2], Bernd Büchner[1], and Martin Knupfer[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Laboratoire de Physico-Chimie de l'État Solide, Université Paris-Sud, 91405 Orsay, France

Electron energy-loss spectroscopy has been used to investigate the loss-function of the single crystalline two-leg ladder system $Ca_xSr_{14-x}Cu_{24}O_{41}$ with various compositions. We find a strong anisotropy of the loss function for momentum transfers along the a and c-crystallographic axis, and a remarkable linear plasmon dispersion for a momentum transfer parallel to the legs of the ladders. The investigated spectral features are attributed to localized and delocalized charge-transfer excitations and the charge carrier plasmon. The charge carrier plasmon position and dispersion in the long wave-length limit agree well with expectations based upon the band structure of the two-leg ladder, while the observed quasi-linear plasmon dispersion might be related to the peculiar properties of underdoped cuprates in general. Furthermore, a remarkable temperature dependence of the plasmon was observed.

TT 27.5 Wed 12:30 H 2053

Temperature behavior of the hole density of (Bi,Pb)-2212 single crystals — •Aliakbar Ghafari[1], Ahmad Kamal Ariffin[2], Christoph Janowitz[1], Helmut Dwelk[1], Alica Krapf[1], and Recardo Manzke[1] — [1]Institute of Physics, Humboldt University of Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Dep. of Physics, Universiti Pendidikan Sultan Idris, 35900 Tanjong Malim, Malaysia

One of the most puzzling anomalies of high-T_C cuprates is the strong temperature dependence of the Hall coefficient (R_H) and the hole density (n_H). Gor'kov and Teitel'baum (GT) showed by using experimental data of $La_{2-x}Sr_xCuO_4$ (LSCO) that the number

of holes per Cu atom, n_H, changes with temperature according to $n_H(T,x)=n_0(x)+n_1(x)\exp(-\Delta(x)/T)$ [1]. To clarify the temperature dependence of n_H we have determined n_H by x-ray absorption spectra (XAS) at the CuL_3 edge for nearly optimum and slightly underdoped (Bi,Pb)-2212 single crystals. Our results point out that the GT formula can not fit our data and therefore must be extended to the three terms.

[1] L. P. Gor'kov and G. B. Teitel'baum, Phys. Rev. B 77, 180511 (2008)

TT 27.6 Wed 12:45 H 2053

Electronic structure of $Bi_2Sr_2CaCu_2O_8$ by DFT and QMC — •Aliakbar Ghafari[1], Kaveh Haghighi mood[2], Christoph Janowitz[1], and Recardo Manzke[1] — [1]Institute of Physics, Humboldt University of Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Dep. of Physics, Science and Research Branch (IAU), Tehran, Iran

The electronic structure of high-TC cuprates superconductors (HTCS) is among the most interesting issues of condensed matter physics since their discovery by Bednorz and Müller. It has been proven that the antiferromagnetic ground state of the parent compound of the HTCS is not accessible by using local density approximation (LDA) and generalized gradient approximation (GGA) as exchange-correlation energy functionals within density functional theory (DFT). Therefore, we calculated the electronic structure of $Bi_2Sr_2CaCu_2O_8$ by adding the Hubbard parameter to DFT (GGA+U) and quantum Monte Carlo (QMC) methods. The calculations have been performed by Wien2k and Casino codes for GGA+U and QMC, respectively.

TT 27.7 Wed 13:00 H 2053

Effect of planar elastic strain on cuprate superconductivity — •Jürgen Röhler — Universität zu Köln, 50937 Köln, Germany

Elastic strain has important effects on the properties of hole doped superconducting cuprates, most significantly on T_c. While c-axis compression primarily enhances the number of hole carriers n, the intrinsic T_c^{intr} is determined by the in-plane lattice parameter a, or the area of the CuO_2 planes A. For optimal doping, $dT_c/dn = 0$, the available high pressure data suggest $T_c \propto A^{-2}$, universally within the various cuprate families [1]. This significant relationship requires $A(n)$ to exhibit an extremum around $n_{opt} = 0.16$, ubiquitously observed as "bulging" anomaly [2] riding the monotonous contraction of A from increasing covalency. We propose to express these findings in terms of the magnetoelastic strain exerted on the CuO_2 lattice by pseudogapped excitations of preformed $3a$ hole pairs with nn repulsion [2].

[1] J.S. Schilling in: Handbook of high-temperature superconductivity: theory and experiment, J.R. Schrieffer, J.S. Brooks (eds.), Springer 2007, p. 427.
[2] J. Röhler, Int. J. Mod. Phys B (2005), 19, 255.

TT 28: Correlated Electrons: Low-dimensional Systems - Materials 2

Time: Wednesday 15:00–18:30 Location: H 0104

TT 28.1 Wed 15:00 H 0104

One-dimensional quantum spin magnetism of the $CrVO_4$ structure-type — •Joseph Law and Reinhard Kremer — Max Planck Institute for Solid State Research Heisenbergstraße 1, D-70569 Stuttgart

In recent years we have investigated and characterized many new and interesting 1D quantum spin systems, as of late we have concentrated on compounds that crystallize in the $CrVO_4$ structure-type.

Here we will present new results for materials that adopt this structure-type, ranging from spin-spiral long-range magnetic order and Multiferroicity to two stage spin-Peierls transitions.

TT 28.2 Wed 15:15 H 0104

S=5/2 spin-chain Heisenberg systems $SrMn_2V_2O_8$ and $BaMn_2V_2O_8$ — •Sandra Niesen, Gerhard Kolland, Oliver Heyer, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

Low-dimensional magnetic systems are commonly studied due to their interesting magnetic properties. For small spin values ($S = 1/2$ or 1), the groundstate and the low-lying excitations are often dominated by strong quantum fluctuations, while a more classical behavior is expected for systems with larger spins. In this context, the series $AM_2X_2O_8$ (A = Ba, Sr, Pb; M = Cu, Co, Ni, Mn; X = V, As) are of particular interest. Depending on the transition metal, different spins are realized and the structure contains screw chains of octahedrally coordinated M^{2+} ions along the c axis of the tetragonal structure. These chains are spatially separated by a nonmagnetic matrix, resulting in a quasi-1D magnetic system. The Heisenberg $S = 5/2$ system $BaMn_2V_2O_8$ shows low-dimensional behavior with a broad maximum of $\chi(T)$ around 170 K but finally orders antiferromagnetically at 37 K. Up to now only few studies of polycristalline $BaMn_2V_2O_8$ were available [1]. Large single crystals of $BaMn_2V_2O_8$ and of the new compound $SrMn_2V_2O_8$ were prepared. The crystal structure and the basic physical properties of this new compound will be presented [2].

This work is supported by the DFG through SFB 608.

[1] Z. He *et al.* Solid State Comm. **141** (2007) 22
[2] S.K. Niesen *et al.* J. Mag. Mag. Mat. **323** (2011) 2575

TT 28.3 Wed 15:30 H 0104

Magnetic properties of alternating spin-1/2 chain compound $AgVOAsO_4$ — •Ramesh Nath[1], Alexander Tsirlin[2], Panchanana Khuntia[2], Michael Baenitz[2], Yurii Skourski[3], Christoph Geibel[2], and Helge Rosner[2] — [1]School of Physics, IISER, Thiruvananthapuram-695016 Kerala, India — [2]MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]HLD, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

We investigate the magnetic properties of a one-dimensional (1D) spin-1/2 alternating chain compound $AgVOAsO_4$ via magnetic susceptibility, high-field magnetization, and ^{75}As NMR measurements. Temperature dependence of the magnetic susceptibility ($\chi(T)$) and NMR shift ($K(T)$) were fitted well by the expression for the 1D spin-1/2 alternating chain. The exchange couplings along the chain are estimated to be $J \simeq 40$ K and $J' \simeq 25$ K, with a spin gap $\Delta \simeq 13$ K. The high-field magnetization measurement at 1.4 K confirms the ground state to be a non-magnetic singlet, and reveals the critical field $H_c \simeq 10$ T of the gap closing and a saturation field $\mu_0 H_s \simeq 48.5$ T. These values are largely consistent with the estimated Δ and (J, J') values based on the fit of $\chi(T)$ and $K(T)$. The ^{75}As spin-lattice relaxation rate ($1/T_1$) follows an activated behavior at low temperatures giving rise to the same Δ value. Our experimental investigations are supported by band structure calculations that additionally reveal weak and frustrated interchain couplings, thus making this compound a promising candidate for Bose-Einstein condensation of magnons in high magnetic fields.

TT 28.4 Wed 15:45 H 0104

Evidence for a Kosterlitz-Thouless transition in the quasi-2D square-lattice compound $Pb_2VO(PO_4)_2$ — •Tobias Förster, Jörg Sichelschmidt, Enrique Kaul, Christoph Geibel, and Frank Steglich — Max Planck Institute f. Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The layered vanadium-oxide-bis(phosphates) AA'$VO(PO_4)_2$ (AA'=Pb_2, SrZn, BaCd) present an interesting class of quasi-2D compounds. The crystal structure is dominated by layers of VO_5-pyramids and PO_4-tetrahedra forming a $S = 1/2$-square lattice of V^{4+} ions. In contrast to the majority of square lattice compounds these vanadium systems present a significant amount of frustration, because the ferromagnetic exchange along the sides of the squares is of the same order of magnitude as the antiferromagnetic exchange along the diagonals. Therefore one finds a good agreement of the bulk properties with the $S = 1/2$ Heisenberg J_1-J_2-model [1].

In such 2D $S = 1/2$ square-lattices quantum Monte Carlo simulations suggest that a small easy-plane anisotropy results in a crossover from Heisenberg to XY behavior [2]. With Electron Spin Resonance (ESR) measurements on single crystals of $Pb_2VO(PO_4)_2$ we show that this compound indeed presents an easy-plane anisotropy and that the spin dynamics measured via the ESR linewidth is well described by the occurrence of a Kosterlitz-Thouless transition at a temperature slightly below T_N.

[1] E. E. Kaul *et al.* J. Magn. Magn. Mater. **272-76**, 922 (2004)
[2] A. Cuccoli *et al.* Phys. Rev. Lett. **90**, 167205 (2003)

TT 28.5 Wed 16:00 H 0104

Thermodynamic properties of the 1-dimensional Spin-$\frac{1}{2}$ compound Cs_2CoCl_4 in transverse magnetic fields — •Oliver Breunig[1], Eran Sela[2], Benjamin Buldmann[2], Markus Garst[2], Petra Becker[3], Ladislav Bohatý[3], Christian Dax[1], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 is known as a an example of a spin-$\frac{1}{2}$ XXZ model crystal. It contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The ground-state doublet is separated from the first excited doublet state by approximately 15 K, in a way that at low-enough temperatures the system can be described by the one-dimensional spin-$\frac{1}{2}$ XXZ model. In literature, this model is typically studied for magnetic fields perpendicular to the easy-plane. For structural reasons, however, in Cs_2CoCl_4 the only principal magnetic field direction which is experimentally accessible lies within the easy-plane. Only few studies of the corresponding transverse field case are available so far. We compare experimental data of specific heat and thermal expansion in a temperature range from about 50 mK to 20 K to numerical calculations.

This work was supported by the DFG through SFB 608.

TT 28.6 Wed 16:15 H 0104

Combined DFT and many-body studies of charge transfer salts — •Kateryna Foyevtsova, Johannes Ferber, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Charge transfer salts are a class of strongly correlated low-dimensional organic materials which have recently gained revived attention. The appealing properties of these materials are a highly controlled quality of grown samples and a rich phase diagram where phase transitions are driven by variation of temperature and pressure (physical or chemical). We study the effects of strong electronic correlations in some representative charge transfer salts in the framework of the density functional theory combined with many-body methods. In particular, we perfom a comparative analysis for the isostructural compounds κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br, an unconventional superconductor with $T_c \sim 15$ K, and κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, an antiferromagnetic Mott insulator, in a range of temperatures and interaction strengths.

TT 28.7 Wed 16:30 H 0104

An *ab initio* Comparison of the Properties of Fabre-Bechgaard Charge Transfer Salts — •Anthony Jacko, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt, Germany

The Fabre-Bechgaard family of charge transfer salts have a rich phase diagram as a function of both physical and chemical pressure, due to strong electronic correlations and frustration [1]. We investigate the structural and electronic properties of several members of this family with density functional theory (DFT) calculations. By understanding the similarities and differences between these salts at the level of DFT, we can gain an understanding of how the choice of anion influences the effects of strong correlations and frustration on the properties of these systems, leading to the many interesting phases observed.

[1] J. Moser, M. Gabay, P. Auban-Senzier, D. Jérome, K. Bechgaard, and J.M. Fabre. Euro. Phys. J. B, 1:39-46, 1998.

15 min. break.

TT 28.8 Wed 17:00 H 0104

$(TMTTF)_2SbF_6$ at the Metal-Insulator Transition: Bulk-Sensitive Photoemission Facilitated by Aluminum Coating — Katerina Medjanik[1], Dmytro Kutnyakhov[1], Hans-Joachim Elmers[1], •Gerd Schönhense[1], Andrei Gloskovskii[2], Wolfgang Drube[3], Mariano de Souza[4], Jens Müller[5], and Michael Lang[5] — [1]Inst. f. Physik, Univ. Mainz — [2]Inst. f. Anorg. und Anal. Chemie, Univ. Mainz — [3]Deutsches Elektronen-Synchrotron, Hamburg — [4]Universidade Estadual Paulista, Rio Claro, Brazil — [5]Physikalisches Inst., Goethe Universität Frankfurt

The metal-insulator transition (MIT) in the title compound has been studied using hard X-ray photoelectron spectroscopy (HAXPES) at PETRA III (beamline P09). This material undergoes a transition from a correlated metal at ambient temperature to a Mott-Hubbard insulator at T=154 K. The latter is marked by a pronounced increase in resistivity by > 3 orders of magnitude and accompanied by a charge-order phase transition. Photoelectron spectroscopy for the bare material is hampered by strong non homogeneous surface charging visible by the sudden appearance of shifted lines in addition to the main line at the transition. The large information depth (about 20nm) of HAXPES allows coating the material by a thin (5 nm) conductive Al-layer in order to avoid charging. In this way, the intrinsic change of the spectra at the metal-insulator/charge-order transition can be observed. At the transition temperature, the S 2p signal exhibits a satellite shifted from the main line by 7.2 eV towards higher kinetic energies. Funded through Transregio SFB TR49, graduate school MAINZ and COMATT.

TT 28.9 Wed 17:15 H 0104

Analysis of the temperature dependence of the structural and electronic properties of the spin liquid candidate κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ — •Harald O. Jeschke[1], Mariano de Souza[2], Rudra Sekhar Manna[2], Michael Lang[2], Roser Valentí[1], and John A. Schlueter[3] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, United States

The interplay of the effects of electronic correlations, low dimensionality and spin frustration in the organic charge transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ is of great interest experimentally as well as theoretically. Besides the spin liquid property at very low temperatures, the material has interesting anomalies at 6K, 60K and 150K. Even though the structure of the material has been determined several times over the past 20 years, complete structural data are only available at room temperature. In our work, we precisely determine the structure at 300K, 250K, 200K, 150K, 100K, 20K and 5K. We analyze the structures using density functional theory and tight binding methods. We show that the triangular lattice Hubbard Hamiltonian parameters are temperature dependent, with the interaction strength increasing with decreasing temperature and with the frustration going through a minimum at 150 K. Our results point to the fact that the experimental determination of structures at various temperatures may be important for realistic many-body theoretical investigations of complex materials.

TT 28.10 Wed 17:30 H 0104

Single crystals and thin films of the new organic charge transfer compound (BEDT-TTF)-DTF — •Kai Ackermann[1], Milan Rudloff[1], Michael Bolte[2], Harald Jeschke[3], Matthias Wagner[2], Roser Valenti[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue-Straße 7, 60438 Frankfurt am Main — [3]Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We investigate the structural and electronic properties of the semiconducting organic charge transfer system (BEDT-TTF)-DTF [bis(ethylenedithio)-tetrathiafulvalene - 9-dicyanomethy-lene-2,4,7-trinitrofluorene]. Crystal structure analysis and X-ray diffractometry show two different phases with monoclinic and triclinic symmetry. Both have a mixed stack configuration with a 1:1 ratio of BEDT-TTF to DTF. A characteristic of the triclinic phase is the layered structure of donor and acceptor molecules. Single crystals of both phases, which are grown from solution, were characterized by temperature-dependent (1.5K - 300K) conductivity measurements in three crystallographic directions and IR-spectroscopy for determining the charge transfer degree. First results of thin film deposition experiments by using organic molecular beam deposition are presented. These films allow to measure the frequency-dependent (20Hz - 100kHz) dielectric constant. The experimental results are discussed in view of band structure calculation within the framework of density functional theory.

TT 28.11 Wed 17:45 H 0104

Field-induced length changes in the spin-liquid candidate κ-(ET)$_2$Cu$_2$(CN)$_3$ — •Rudra Sekhar Manna[1], Mariano de Souza[1,3], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA — [3]Present address: Departamento de Fisica, Unesp - Universidade Estadual Paulista, CEP 13500-970, Rio Claro (SP), Brazil

Thermal expansion measurements on the spin-liquid compound κ-$(ET)_2Cu_2(CN)_3$ show a pronounced and strongly anisotropic anomaly at 6 K, a clear signature of a second-order phase transition [1]. In order to study the effect of a magnetic field on the low-temperature spin-liquid state [2], dilatometric measurements under magnetic field have been performed. Interestingly, we find that besides the 6 K anomaly, which is insensitive to magnetic fields $B \leq 10$ T, the maximum field applied, field-induced anomalies show up for fields aligned along the crystallographic b-axis. The effects become particularly clear in measurements of the magnetostriction where two step-like anomalies were observed. One of these anomalies lies close to the phase boundary between quantum critical (QC_H) and weak antiferromagnetic (WAF_H) phases derived from μSR measurements [2].
[1] R. S. Manna et al., PRL **104**, 016403 (2010).
[2] F. L. Pratt et al., Nature **471**, 612 (2011).

TT 28.12 Wed 18:00 H 0104

Charge-carrier dynamics at the multiferroic transition in the organic charge-transfer salt κ-$(ET)_2$-Cu[N$(CN)_2$]Cl studied by fluctuation (noise) spectroscopy — •Benedikt Hartmann[1], Robert Rommel[1], John Schlueter[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt (M) — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

The organic molecular conductors (BEDT-TTF)$_2$X are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. The quasi-2D triangular lattice Mott insulator κ-$(ET)_2$Cu[N$(CN)_2$]Cl (κ-Cl) undergoes an antiferromagnetic transition at $T_N \approx 27\,K$. Recently, clear evidence for charge-order driven ferroelectircity coinciding with the onset of magnetic-ordering has been found [1], making κ-Cl a multiferroic material.
We report on fluctuation (noise) spectroscopy, a suitable technique to study the low-frequency charge-carrier dynamics of κ-Cl. We discuss the temperature dependence of the $1/f$-type fluctuations in order to get insight in the electronic energy scale involved in the ordering mechanism. We observe deviations of $1/f$ noise at temperatures around 27 K which may be attributed to the formation of charge-order domains.
[1] P. Lunkenheimer, J. Müller et al., arXiv:1111.2752v2 (2011)

TT 28.13 Wed 18:15 H 0104

The anomalous metallic properties of quasi two-dimensional organic superconductors studied by non-linear transport — •Robert Rommel[1], Benedikt Hartmann[1], Jens Brandenburg[1], John Schlueter[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt am Main — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

In ac transport measurements the technique of measuring higher harmonics, in particular the third ($R_{3\omega}$), may be used as an additional, powerful tool probing the microgeometry of the current distribution in a bulk sample. $R_{3\omega}$ has been used, e.g., to determine the superconducting transition temperature of high-T_c cuprates or to estimate the number of correlated polarons in manganites. We apply this technique to the quasi two-dimensional organic charge-transfer salt κ-$(H_8$-$ET)_2$Cu[N$(CN)_2$]Br and its fully deuterated analogue. We studied the dependence of $R_{3\omega}$ on temperature, current, frequency, magnetic field and the degree of disorder and analyze the data with respect to the vicinity of the 1st order Mott metal-insulator transition line in the complex phase diagram of this class of materials. We show that the signal allows for an accurate determination of $T_c(B)$ and found a good estimate for the upper critical magnetic field B_{c2} of these extreme type-II superconductors. We furthermore gain information about changes in the transport mechanism, which we will discuss in terms of the anomalous properties of the metallic state in these materials.

TT 29: Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 1

Time: Wednesday 15:00–18:30 Location: H 2053

TT 29.1 Wed 15:00 H 2053

Tunable double well potential for fractional Josephson two-vortex molecule — •D. M. Heim[1], K. Vogel[1], W. P. Schleich[1], E. Goldobin[2], D. Koelle[2], and R. Kleiner[2] — [1]Institut für Quantenphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, D-72076 Tübingen, Germany

We study a fractional Josephson two-vortex molecule in a long Josephson 0-κ-2κ junction. The ground state is degenerate, corresponding to two configurations with topological charges $(\kappa, \kappa-2\pi)$ and $(\kappa-2\pi, \kappa)$ of fractional vortices. We propose to use such a system to study macroscopic quantum phenomena involving fractional vortices. Similar to the previous proposal based on a 0-π-0 junction [1], the two-vortex-molecule states can be mapped to a double well potential. However, by changing the value of κ during experiment we are able to tune the energy barrier separating the two classical ground states. We calculate characteristic properties (e.g. barrier height, eigenfrequency) and demonstrate that a controlled transition into the quantum regime is possible in such a system.
[1] E. Goldobin et al., Phys. Rev. B **72**, 054527 (2005).

TT 29.2 Wed 15:15 H 2053

Current-voltage dependence of a one-dimensional Josephson junction array in the Coulomb blockade regime — •Nicolas Vogt[1], Alexander Shnirman[1,2], and Alexey V. Ustinov[3,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN) , Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Physikalisches Institus, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

We theoretically investigate the transport characteristics of a one-dimensional Josephson junction array in the Cooper pair Coulomb blockade regime. Explanations for the hysteresis in the current-voltage characteristics and threshold voltage have been previously proposed within the mean field sine-Gordon model. This approach fails, however, to explain the recent experimental data. Experiments show a quadratic dependence of the differential conductance on the Josephson coupling energy which depends on the magnetic field. We introduce various models of dissipation into the mean field theory in order to numerically simulate the time resolved behavior of the voltage biased array.

TT 29.3 Wed 15:30 H 2053

Further investigations on dc-SQUID gradiometers based on growth modified bi-crystal grain boundaries — •Peter Michalowski, Christian Katzer, Daniel Kuhwald, Stefanie Koch, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The properties of grain boundaries of $YBa_2Cu_3O_{7-\delta}$ (YBCO) films grown on bi-crystal substrates can be modified by gold nano crystallites self-assembling from an intermediate gold layer during pulsed laser deposition [1]. These gold particles act as additional pinning centers in the YBCO layer [2]. Using a new layout, which enables us to restrict the gold nano crystallites only to the Superconducting QUantum Interference Device (SQUID) or the antenna structures, we fabricated dc-SQUID gradiometers. We present results of the temperature dependence of the London penetration depth as well as of noise measurements carried out with ac- and dc-bias. In addition we investigated the dependence of the superconducting properties on the thickness of the initial gold layer.
[1] P. Michalowski et al., Physica Status Solidi - Rapid Research Letters **5** (2011) 268-270.
[2] Katzer et al., EPL **95** (2011) 68005.

TT 29.4 Wed 15:45 H 2053

Temperature Dependence of Driven Duffing Oscillator — •Lingzhen Guo[1,4], Michael Marthaler[1,2], Vittorio Peano[1,3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN),Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [3]Department of Physics and Astronomy, Michigan State University, East Lansing,

Michigan 48824, USA — [4]Department of Physics, Beijing Normal University, Beijing 100875, China

We investigate the temperature dependence of the stationary distribution for the Driven Duffing Oscillator (DDO). We focus on the fragility of the zero temperature solution. This unusual phenomenon means that the probabilities over the two stable vibrational states will endure an abrupt change in the presence of a small temperature. In this work, we first numerically demonstrate the fragility of the zero temperature solution. Realizing that this is due to the violation of the detailed balance condition, we find a condition for the divergency of the small temperature perturbation theory. Then an analytical expression for a critical temperature is obtained. Our results reveal that this fragility is more and more prominent as the number of states in the quasienergy potential wells increases which indicates a semiclassical regime. The fragile regime can be investigated with currently existing experimental setups.

TT 29.5 Wed 16:00 H 2053

Subgap density of states in the superconductor Aluminum — •Andreas Heimes[1], Michael Marthaler[1], Juha Leppäkangas[2], Jens Michelsen[1], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

In recent years great effort in screening envoironmental decoherence sources lead to an increased coherence time of Josephson based qubits. However there are still intrinsic mechanisms in the bulk superconductors that set a natural limit. According to that recent experiments measure a finite electronic density of states below the superconducting gap leading to incoherent quasiparticle tunneling. At the same time it was proposed that non-magnetic impurities at the superconductor-substrate interface or in the oxide tunneling barrier can cause magnetic impurities with a certain surface concentration which are believed amongst other to cause the $1/f$ flux noise. Here we propose that such surface spins could also be the reason for the observed subgap density of states in the phonon-mediated superconductor aluminum. We find that magnetic scattering in the bulk superconductor leads to a subgap tunneling rate that can be compared to the mentioned experimental observations.

TT 29.6 Wed 16:15 H 2053

Understanding the Josephson current through Kondo-correlated quantum dots — •David J. Luitz[1], Fakher F. Assaad[1], Tomaš Novotný[2], and Volker Meden[3] — [1]Institut für theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Condensed Matter Physics, Charles University Prague, Czech Republic — [3]Institut für Theorie der Statistischen Physik, RWTH Aachen, Germany

We study the Josephson current 0-π transition through correlated carbon-nanotube quantum dots tuned to the Kondo regime. The physics dominated by an interplay of two complex many-body effects, namely superconductivity and Kondo correlations, can be quantitatively captured by the numerically exact continuous time quantum Monte Carlo method within the single-impurity Anderson model with two superconducting leads. Comparison to existing experiments with the model parameters determined from the normal state linear conductance shows excellent agreement for the dependence of the critical Josephson current on the dot level position ϵ experimentally tuned by the gate voltage.

15 min. break.

Invited Talk TT 29.7 Wed 16:45 H 2053

Novel Josephson effect in triplet Josephson junctions: the story begins — •Dirk Manske — Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, 70569 Stuttgart

In the theoretical study of Josephson junctions, it is usually assumed that the properties of the tunneling barrier are fixed. This assumption breaks down when considering tunneling between two triplet superconductors with *misaligned* **d**-vectors in a TFT-junction (triplet–ferromagnet–triplet) [1,2]. Such a situation breaks time-reversal symmetry, which radically alters the behaviour of the junction, stabilizing it in a fractional state, i.e. the free energy minimum lies at a phase difference intermediate between 0 and π. Fractional flux quanta are then permitted at the junction [3]. A further consequence of the **d**-vector misalignment is the appearance of a Josephson spin current, which flows even in the absence of an equilibrium charge current. Not only do our calculations enhance the physical understanding of transport through triplet superconductor junctions, but they also open the possibility of novel spintronic Josephson devices [4].

[1] B. Kastening, D.K. Morr, D. Manske, and K.H. Bennemann, Phys. Rev. Lett. 96, 047009 (2006)
[2] P. M. R. Brydon, B. Kastening, D. K. Morr and D. Manske, Phys. Rev. B **77**, 104504 (2008).
[3] P.M.R. Brydon, C. Iniotakis, D. Manske, and M. Sigrist, Phys. Rev. Lett. 104, 197001 (2010).
[4] P.M.R. Brydon and D. Manske, Phys. Rev. Lett. 103, 147001 (2009).

TT 29.8 Wed 17:15 H 2053

Grain boundary junctions with Co-doped Ba-122 — •Stefan Schmidt[1], Sebastian Döring[1], Frank Schmidl[1], Fritz Kurth[2], Kazumasa Iida[2], Silvia Haindl[2], Bernhard Holzapfel[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institut für metallische Werkstoffe, Helmholtzstrasse 20, 01069 Dresden, Germany

Josephson junctions are a strong tool to investigate fundamental superconducting properties, such as gap behaviour, dependencies from external fields and the order parameter symmetry. Finding secure values enables the possibility of theoretical descriptions to understand the physical processes within the new iron-based superconductors. The superconducting quantum interference device (SQUID) symmetry provides a phase-sensitive tool to examine flux behaviour in a very precise.

Based on Co-doped $Ba(Fe_{0.9}Co_{0.1})_2As_2$ (Co:Ba-122) thin films produced via pulsed laser deposition (PLD) on $SrTiO_3$ bicrystal substrates (mismatch angles from 9° to 36°), we manufactured grain boundary junctions by using photolithography and ion beam etching. Based on the grain boundary junctions, SQUID structures can be realized.

We present first measurements on Co:Ba-122 grain boundary Josephson junctions and their temperature dependence.

This work was partially supported by the EU within project IRONSEA, no. FP7-283141 and the Landesgraduiertenförderung Thüringen.

TT 29.9 Wed 17:30 H 2053

Andreev Reflexion studies on planar hybrid SNS-junctions based on 122-thin films — •Sebastian Döring[1], Stefan Schmidt[1], Frank Schmidl[1], Volker Tympel[1], Silvia Haindl[2], Fritz Kurth[2], Kazumasa Iida[2], Bernard Holzapfel[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institur für Festkörperphysik, Helmholtzweg 5, 07745 Jena — [2]IFW Dresden, Institut für metallische Werkstoffe, Helmholtzstraße 20, 01069 Dresden

To investigate the properties of iron-based superconductors, we prepared hybrid junctions in thin film technique [1]. Therefore two geometries were prepared, a planar SNS-junction and an edge junction. The base electrode was made of $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin films [2], a sputtered gold layer acts as normal barrier for the planar junction and for the counter electrode we used the conventional superconductor lead. We measured the electrical properties of each electrode, as well as the junctions itself. To obtain information about the order parameter symmetry, we show the differential conductance and compare with different variations of an extended BTK-model. We will show differences and commonalities between the results of both junction geometries.

This work was partially supported by DFG under project nos. HA5934/3-1 and SE664/15-1, the EU under project no. FP7-283141 (IRONSEA) and the Landesgraduiertenförderung Thüringen.
[1] S. Schmidt et al. APL. 97 (2010) 172504
[2] K. Iida et al. SST 24 (2011) 125009

TT 29.10 Wed 17:45 H 2053

Carrier injection into pnictide superconductors — •C. Steiner[1], S. Probst[1], Y. Simsek[1], Y. Koval[1], S. Wurmehl[2], B. Büchner[2], and P. Müller[1] — [1]Department of Physics and Interdisciplinary Center of Molecular Materials, Universität Erlangen-Nürnberg — [2]Institute for Solid State Research, IFW-Dresden

1111 pnictides have a layered structure consisting of FeAs planes separated by LaO layers. Doping is achieved by partial replacement of oxygen by fluorine. We have already shown that layered high-T_c cuprates can be doped by carrier injection along c-axis direction [1]. For our c-axis transport measurements of pnictides we selected very small single crystals (approximately $5 \times 5 \times 1\ \mu m^3$) from powder samples of $LaO_{1-x}F_xFeAs$ with $x = 0.06$ and $x = 0.1$. Mesa structures were pre-

pared by electron beam lithography. Above a certain bias threshold, low temperature IV characteristics showed switching from a low resistive state to a high resistive state and back, indicating charge carrier trapping and release. By this type of switching, the resistance at T_c was changed approximately by a factor of 2. The c-axis critical current belonging to the low resistive state was higher by a similar ratio. This increase of critical current was accompanied by a T_c increase of ca. 2 K. We interpret these results by electron trapping in the LaO layers and compensation of this additional charge by a decrease of electron concentration in the FeAs layers.
[1] Y. Koval, X. Y. Jin, C. Bergmann, Y. Simsek, L. Özyüzer, P. Müller, H. B. Wang, G. Behr, B. Büchner Appl. Phys. Lett. **2010**, 96, 082507

TT 29.11 Wed 18:00 H 2053

Transport measurements of lateral $MgB_2/Fe/MgB_2$ junctions — •Savio Fabretti, Patrick Thomas, Markus Schäfers, Oliver Schebaum, and Andy Thomas — Bielefeld University

We fabricated $MgB_2/Fe/MgB_2$ lateral junctions by rf-dc co-sputtering. The MgB_2 films have a thickness of about 30nm and a critical temperature of up to 33 K. The samples were annealed in-situ between 450°C and 750°C. Our MgB_2 films were sputtered on different substrates such as (100) MgO and r-cut sapphire . Their crystalline structure and magnetic anisotropy were investigated. For transport measurement a thin iron cross strip of about 30 nm was placed between the MgB_2 strip. The MgB_2 strip was relieved by a groove of about 5 μm. The superconductivity of MgB_2 is suppressed due to the proximity effect near the junction area and builds a natural metallic barrier. With this configuration, we get a magnetoresistance due to the domain wall scattering in iron where the magnetoresistance was measured perpendicular and in plane of this array. Further, we investigated their I-V and dI/dV characteristics in dependence of an applied magnetic field up to 4T. The sigma gap as well as the pi gap was observed.

TT 29.12 Wed 18:15 H 2053

Superconductivity induced by current injection into non-superconducting $Bi_2Sr_2CaCu_2O_8$ — •Y. Simsek[1], Y. Koval[1], S. Probst[1], X.Y. Jin[2], C. Steiner[1], and P. Müller[1] — [1]Department of Physic and Interdisciplinary Center for Molecular Materials (ICMM) Universität Erlangen-Nürnberg, Germany — [2]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

Unlike doping by oxygen excess, we are able to change the carrier concentration of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) single crystals by carrier injection. The electrons injected along c-axis of Bi2212 are trapped in BiO and SrO layers which increases the hole concentration in CuO layers. This method gives an opportunity to observe the evolution of c-axis transport properties of Bi2212 from the antiferromagnetic state to the superconducting overdoped phase on the same sample. In order to eliminate the contact resistance, we have fabricated double cross-bar crystal stacks on fully oxygen depleted Bi2212 single crystal which was not superconducting above 4.2 K. We have observed that by carrier injection the conductivity can be increased until superconductivity above 4.2 K is reached. Continuing the doping by carrier injection, optimum-doped and even overdoped states were obtained. In the superconducting phase, the critical current density exponentially increases by doping level. At the same time, the variation of the critical temperature with doping shows a well known parabolic behavior. Doping by carrier injection offers an unique opportunity of tuning the properties of high-T_c electronic devices in situ.

TT 30: Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 1

Time: Wednesday 15:00–18:45 Location: H 3005

Invited Talk TT 30.1 Wed 15:00 H 3005

Bose-Einstein condensation of Photons — •Martin Weitz — Institut für Angewandte Physik, Universität Bonn, Wegelerstr. 8, D-53115 Bonn

Bose-Einstein condensation, the macroscopic ground state accumulation of particles with integer spin (bosons) at low temperature and high density, has been observed in several physical systems, including cold atomic gases and solid state physics quasiparticles. However, the most omnipresent Bose gas, blackbody radiation (radiation in thermal equilibrium with the cavity walls), does not show this phase transition. The photon number here is not conserved (vanishing chemical potential), and at low temperatures photons disappear in the cavity walls instead of occupying the cavity ground state. In my talk, I will describe an experiment observing a Bose-Einstein condensation of photons in a dye-filled microscopic optical resonator [1]. The phase transition to a macroscopically occupied ground state occurs at room temperature. In my talk, I will begin with a general introduction and give an account of current work and future plans of the Bonn photon gas experiment.
[1] J. Klaers, J. Schmitt, F. Vewinger, and M. Weitz, Nature 468, 545 (2010).

TT 30.2 Wed 15:30 H 3005

Stroboscopic observation of quantum many-body dynamics — •Stefan Kessler[1], Andreas Holzner[2], Ian McCulloch[3], Jan von Delft[2], and Florian Marquardt[1,4] — [1]Institute for Theoretical Physics, Friedrich-Alexander-Universiät Erlangen-Nürnberg, Erlangen, Germany — [2]Physics Department, ASC, CeNS, Ludwig-Maximilians-Universität München, München, Germany — [3]School of Physical Sciences, University of Queensland, Brisbane, Australia — [4]Max Planck Institute for the Science of Light, Erlangen, Germany

Recent experiments have demonstrated single-site resolved observation of cold atoms in optical lattices. Thus, in the future it may be possible to take repeated snapshots of an interacting quantum many-body system during the course of its evolution. Here we address the impact of the resulting quantum (anti-)Zeno physics on the many-body dynamics. We use time-dependent DMRG to obtain the time evolution of the full wave function, that is then periodically projected in order to simulate realizations of stroboscopic measurements. For the example of a 1-D lattice of spinless fermions with nearest-neighbor interactions, we find regimes for which many-particle configurations are stabilized or destabilized, depending on the interaction strength and the time between observations. We show that similar effects are expected for other models, such as the 1-D Fermi- and Bose-Hubbard model.

TT 30.3 Wed 15:45 H 3005

Universal probes for antiferromagnetic correlations and entropy in cold fermions on optical lattices — •E.V. Gorelik[1], D. Rost[1], T. Paiva[2], R. Scalettar[3], A. Klümper[4], and N. Blümer[1] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil — [3]Department of Physics, UC Davis, USA — [4]University of Wuppertal, Germany

A major hurdle on the way of using ultracold fermionic atoms on optical lattices as "quantum simulators" of correlated solids is the verification of antiferromagnetic (AF) signatures. Current experimental efforts focus on nearest-neighbor (NN) spin correlation functions and on cooling below a central entropy per site of $s < \log(2)/2$.

Our calculations in the strong-coupling regime of the half-filled Hubbard model using DMFT, determinantal QMC, and Bethe ansatz [1] reveal AF signatures in the double occupancy, spin correlations, and kinetic energy already at $s \lesssim \log(2)$ with surprising universality regarding dimensionality, when viewed as a function of entropy (which is appropriate in the cold-atom context). Both the onset of next-nearest neighbor spin correlations and a minimum in the double occupancy clearly separate the AF Heisenberg regime (at $s \lesssim \log(2)$) from dominant charge physics and should be used experimentally to probe both the AF correlations and the entropy of the system.
[1] E. V. Gorelik, D. Rost, T. Paiva, R. Scalettar, A. Klümper, N. Blümer, arXiv:1105.3356

TT 30.4 Wed 16:00 H 3005

Constant forces induce negative absolute temperatures in optical lattices — •Stephan Mandt[1], Akos Rapp[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Institute for Theoretical Physics, University of Hanover, Germany

Ultracold atoms in optical lattices offer a novel possibility to explore transport properties of model Hamiltonians, such as the Hubbard model for Fermions, in absence of impurities, lattice defects or phonons. The fact that the Hubbard model describes a thermally isolated system has got severe consequences on its transport properties: a cloud of interacting fermionic atoms in an optical lattice in presence of a gravitational potential, e.g., doesn't simply "fall downwards". Instead, we show that it diffuses symmetrically upwards and downwards, while its radius grows subdiffusively in time according to $R \propto t^{1/3}$. We also show that negative absolute temperatures naturally emerge in such a situation, and how equilibrated negative temperatures can be realized in optical lattices.

TT 30.5 Wed 16:15 H 3005

Ultracold atomic gases at negative absolute temperatures — •Akos Rapp — Institut f. Theoretische Physik, Leibniz Universität, Hannover, Deutchland

Ultracold atomic clouds are used to simulate a broad range of complex quantum systems with a high degree of experimental control. We will discuss that current techniques allow for a realization of an out-of-equilibrium situation where the system relaxes to a state with negative absolute temperature, T<0. Under these conditions, higher energy levels are more likely occupied than lower energy levels. As a consequence, bosonic atoms in an optical lattice condense at finite momenta, at the maxima instead of the minimum of the kinetic energy. A further interesting possibility of using T<0 is that one can experimentally reach new parameter regimes. This idea could be applied to simulate the SU(3) attractive Hubbard model with repulsively interacting atoms, which can prove useful to understand some puzzles of quantum chromodynamics.

TT 30.6 Wed 16:30 H 3005

Spin-1 Bosons in Optical Superlattices — •Andreas Wagner[1], Andreas Nunnenkamp[1], Eugene Demler[2], and Christoph Bruder[1] — [1]University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Harvard University, Cambridge, MA 02138, USA

We examine spinor Bose-Einstein condensates in optical period-2 superlattices theoretically using a Bose-Hubbard Hamiltonian which takes spin effects into account. The system shows quantum phase transitions between Mott-insulating and superfluid phases. In particular, we study the spin-dependent effects on the phase diagram. Within the Mott phase the extended superlattice corresponds to an array of isolated double-well potentials. For these systems we study single-particle tunneling which occurs when one lattice site is ramped up relatively to a neighboring site [1]. Spin-dependent effects modify the tunneling events in a qualitative and a quantitative way. Depending on the asymmetry of the double well different types of magnetic order occur, making the system of spin-1 bosons in an optical superlattice a model for mesoscopic magnetism. Homogeneous and inhomogeneous magnetic fields are applied and the effects of the linear and the quadratic Zeeman shifts are examined.We also investigate the bipartite entanglement between the sites and construct states of maximal entanglement. The entanglement in our system is due to both orbital and spin degrees of freedom. We calculate the contribution of orbital and spin entanglement and show that the sum of these two terms gives a lower bound for the total entanglement.
[1] A. Wagner, C. Bruder, and E. Demler, arXiv:1110.1968

TT 30.7 Wed 16:45 H 3005

Interaction Effects in One-Dimensional Many-Body Bosonic Transport — •Arturo Argüelles, Julien Dujardin, and Peter Schlagheck — Université de Liège, Liège, Belgium

We calculate the transport properties of an ultracold gas of Bose-Einstein condensed atoms that is coupled from a magnetic trap into a one-dimensional waveguide[1,2]. A central aim of such guided atom lasers[1] is to study the role of atom-atom interaction in many-body transport processes across finite scattering regions within the waveguide resembling tunnel junctions and quantum dots. Our numerical approach to solve this many-body scattering problem is based on the Matrix Product State ansatz where we adapt absorbing boundary conditions and a external source of particles. We discuss the current, the density profiles and the transmission coefficient in the steady-state regime as functions of the interaction for varous scattering geometries.
[1] W. Guerin et al., PRL 97, 200402 (2006).
[2] T. Ernst et al., PRA 81, 013631 (2010).

15 min. break.

Invited Talk TT 30.8 Wed 17:15 H 3005

Topological superfluids confined in a regular nano-scale slab geometry — •John Saunders[1], Robert Bennett[1], Lev Levitin[1], Andrew Casey[1], Brian Cowan[1], Jeevak Parpia[2], Dietmar Drung[3], and Thomas Schurig[3] — [1]Department of Physics, Royal Holloway University of London, Egham, Surrey, TW20 0EX — [2]Department of Physics, Cornell University, Ithaca, NY 14853, USA — [3]Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, D-19587, Berlin, Germany

Superfluid 3He confined in a regular nano-fabricated slab geometry provides a model system for the investigation of surface and thin film effects in a p-wave superfluid. We have fabricated and cooled such samples to well below 1 mK for the first time, and investigated their NMR response, exploiting a SQUID NMR spectrometer of exquisite sensitivity. We have used NMR on a 650 nm thick superfluid slab to identify the profound effect of confinement on the relative stability of the A and B phases and to make quantitative measurements of the suppression and surface induced distortion of the order parameter.

In these systems the effective confinement length scale (slab thickness/superfluid coherence length) is the new tuning parameter. Increasing confinement should stabilize new p-wave superfluid states of matter, such as the quasi-2D gapped A phase or the planar phase. Nanofluidic samples of superfluid 3He promise a route to explore topological superfluids and their surface, edge and defect-bound excitations under well controlled conditions.

TT 30.9 Wed 17:45 H 3005

Supersolid phase transitions for hard-core bosons on a triangular lattice — •Xue-Feng Zhang[1,2], Raoul Dillenschneider[1], Yue Yu[2], and Sebastian Eggert[1] — [1]Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany — [2]Institute of Theoretical Physics, Chinese Academy of Sciences, P.O. Box 2735, Beijing 100190, China

Hard-core bosons on a triangular lattice with nearest-neighbor repulsion are a prototypical example of a system with supersolid behavior on a lattice. We show that in this model the physical origin of the supersolid phase can be understood quantitatively and analytically by constructing quasiparticle excitations of defects that are moving on an ordered background. The location of the solid to supersolid phase transition line is predicted from the effective model for both positive and negative (frustrated) hopping parameters. For positive hopping parameters the calculations agree very accurately with numerical quantum Monte Carlo simulations. The numerical results indicate that the supersolid to superfluid transition is first order.

TT 30.10 Wed 18:00 H 3005

Dislocation-induced superfluidity in a model supersolid — •Debajit Goswami[1], Kinjal Dasbiswas[2], Chi-Deuk Yoo[3], and Alan Dorsey[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]University of Florida, Gainesville, USA — [3]University of Minnesota, Minneapolis, USA

Motivated by recent experiments on the supersolid behavior of ^{4}He, we study the effect of an edge dislocation in promoting superfluidity in a Bose crystal. Using Landau theory, we couple the elastic strain field of the dislocation to the superfluid density, and use a linear analysis to show that superfluidity nucleates on the dislocation before occurring in the bulk of the solid. Moving beyond the linear analysis, we develop a systematic perturbation theory in the weakly nonlinear regime, and use this method to integrate out transverse degrees of freedom and derive a one-dimensional Landau equation for the superfluid order parameter. We then extend our analysis to a network of dislocation lines, and derive an XY model for the dislocation network by integrating over fluctuations in the order parameter. Our results show that the ordering temperature for the network has a sensitive dependence on the dislocation density, consistent with numerous experiments that find a clear connection between the sample quality and the supersolid response.

TT 30.11 Wed 18:15 H 3005

Half-Vortex Unbinding and Ising Transition in Two-Dimensional Superfluids — •Lars Bonnes[1,2] and Stefan Wessel[3] — [1]Institut für Theoretische Physik, Universität Innsbruck, Österreich — [2]Institut für Theoretische Physik III, Universität Stuttgart — [3]Institut für Theoretische Festkörperphysik, RWTH Aachen

We analyze the thermodynamics of the atomic and (nematic) pair superfluids appearing in the attractive two-dimensional Bose-Hubbard model with a three-body hard-core constraint that has been derived as an effective model for cold atoms subject to strong three-body losses in optical lattices. We show that the thermal disintegration of the pair superfluidity is governed by the proliferation of fractional half-vortices leading to an unconventional Berezinskii-Kosterlitz-Thousless transition. In addition to the (conventional) Berezinskii-Kosterlitz-Thousless transition out of the atomic superfluid, we furthermore identify a direct thermal phase transition separating the pair and the atomic superfluid phases, and show that this transition is continuous with critical scaling exponents consistent with those of the two-dimensional Ising universality class. Our results make a direct connection between the partial loss of quasi long-range order at the Ising transition between the two superfluids and the parity selection of the atomic winding number fluctuations that distinguish the atomic and pair superfluid.

TT 30.12 Wed 18:30 H 3005

Interaction of helium-3 impurities with point defects and deformation fileds in solid helium-4. — •Yaroslav Lutsyshyn — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Interaction between defects and impurities is widely believed to be at the root of a wide range of effects which had been observed in recent years in hcp solid helium-4. In particular, several theories place special role on the dislocation network pinning by helium-3 impurities.

We will report quantum Monte Carlo simulations of a helium-3 impurity in crystalline helium-4. Calculations are performed with the diffusion Monte Carlo method. This is a first principles approach which allows to obtain exact ground state of many-body bosonic systems. The results show that while vacancies are attracted to the impurity, the vacancy-He3 pair is not bound at low density. Additional impurity properties are extracted by simulating it in a strained crystal. Motion in the elastic deformation field can be used to describe the long-range interaction of helium-3 with various lattice defects, especially the dislocation lines.

TT 31: Correlated Electrons: Quantum-Critical Phenomena 2

Time: Wednesday 15:00–16:15 Location: H 3010

TT 31.1 Wed 15:00 H 3010

Ferromagnetic quantum phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider, Vasily Moshnyaga, Sebastian Esser, and Philipp Gegenwart — Georg-August Universität-Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

The $Sr_{1-x}Ca_xRuO_3$ series recently received a lot of attention because of a continuous evolution from itinerant electron magnetism towards a paramagnetic metallic state. We focus on the region near the quantum phase transition at x=0.7. Using metal-organic aerosol deposition, we have grown high-quality epitaxial thin films. For pure $CaRuO_3$ (x=1), grown on $NdGaO_3$, the residual resistivity ratio (RRR) approaches 55, i.e. the highest value reported up to now. Pronounced non-Fermi liquid effects are observed in the temperature dependence of the electrical resistivity, which could be suppressed by the application of large magnetic fields.

This work is supported by the German Science foundation through SFB 602, TP A19.

TT 31.2 Wed 15:15 H 3010

Thermodynamics of Phase Formation and Heavy Quasiparticles in $Sr_3Ru_2O_7$ — •Andreas W. Rost[1], Santiago A. Grigera[1,2], Jan A.N. Bruin[1], Robin S. Perry[3], Demian Tian[1], Sri Raghu[4], Steve A. Kivelson[5], and Andrew P. Mackenzie[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews KY169SS, UK — [2]Instituto de Física de Líquidos y Sistemas Biológicos, UNLP-CONICET, La Plata 1900, Argentina — [3]SUPA, School of Physics, University of Edinburgh, Mayfield Road, Edinburgh EH93JZ, UK — [4]Department of Physics and Astronomy, Rice University, Houston, Texas, 77005, USA — [5]Department of Physics, Stanford University, Stanford, California, 94305, USA

The itinerant metamagnet $Sr_3Ru_2O_7$ has motivated a wide range of experimental and theoretical work in recent years because of the discovery of an unusual low temperature phase which is forming in the vicinity of a proposed quantum critical point. A major challenge is the investigation of the thermodynamic properties of both this unusual phase and the fluctuations associated with the quantum critical point. Here we will report on new specific heat measurements extending previous work to the wider phase diagram. Our results shed light on two important aspects of the system. First we will discuss the entropic details of the formation of heavy quasiparticles as a function of temperature in this compound relevant for a wide class of materials. Secondly we will present thermodynamic evidence for the anomalous low temperature phase forming directly out of the critical high temperature phase.

TT 31.3 Wed 15:30 H 3010

Crystal Growth and Magnetic Order of Ni-doped CePdAl — •Veronika Fritsch[1], Sarah Woitschach[2], Oliver Stockert[2], and Hilbert v. Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Max-Planck-Institut für Chemische Physik feste Stoffe, 01187 Dresden, Germany — [3]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76344 Karlsruhe, Germany

CePdAl is a stoichiometric, antiferromagnetic compound, which can be tuned to a quantum critical point (QCP) by hydrostatic [1] or chemical pressure [2]. The latter can be achieved by substituting Ni for Pd. Neutron-scattering experiments [3] pointed towards a partial frustration of the Ce moments in CePdAl, making this system a promising candidate for investigating the influence of frustration on quantum criticality. We have grown large single crystals of $CePd_{1-x}Ni_xAl$ by the Czochralski method. The samples were characterized by x-ray powder diffraction, atomic absorption spectroscopy and x-ray Laue diffraction. Magnetization measurements of undoped CePdAl display a strong magnetic anisotropy, which is preserved in the Ni-doped compounds, where the magnetic order is suppressed. Neutron-diffraction experiments indicate that short-range correlations are present well above the Néel temperature T_N. Below T_N one third of the Ce moments displays short-range order only, confirming the frustration in this system.

[1] T. Goto *et al.*, J. Phys. Chem. of Solids **63**, 1159 (2002)
[2] Y. Isikawa *et al.*, J. Phys. Soc. Jpn. **65**, 117 (1996)
[3] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996)

TT 31.4 Wed 15:45 H 3010

Spin excitations in CePdAl — •S. Woitschach[1], O. Stockert[1], M. Koza[2], V. Fritsch[3], H. v. Löhneysen[3], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

The heavy-fermion compound CePdAl orders antiferromagnetically below the Néel temperature $T_N = 2.7$ K. Heat capacity measurements reveal a Kondo temperature of $T_K \approx 5$ K. Magnetic order can be continuously suppressed by Ni doping on the Pd site or application of hydrostatic pressure and a quantum critical point is approached. Moreover, as inferred from neutron scattering, geometrical frustration is present in CePdAl. So far, no detailed microscopic measurements have been published on the crystalline electric field (CEF) excitations in CePdAl. Here, we report on our inelastic neutron scattering on CePdAl powder samples to study the characteristic energy scales. The measurements yield the CEF excitations and the quasielastic spin fluctuations. Two excited CEF levels have been detected at ≈ 240 K and > 400 K. The results are compared to the thermodynamic measurements.

TT 31.5 Wed 16:00 H 3010

Quantum Phase transitions in $CeTi_{1-x}V_xGe_3$ — •Wolfram Kittler[1], Veronika Fritsch[1], Frank Weber[2], and Hilbert Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany

$CeTiGe_3$ is a low-temperature ferromagnet with a $T_c \approx 14$ K. It crystallizes in a hexagonal structure with space group P63/mmc. The magnetic moments are located at the Ce atoms and point along the c-axis. T_c can be driven to $T_c = 0$ by V doping on the Ti sites. Thus $CeTi_{1-x}V_xGe_3$ seems to be one of the few ferromagnetic systems that

can be driven to a quantum critical point where $T_c = 0$ by concentration tuning, in this case at $x_c \approx 0.35$.

The magnetic structure of pure $CeTiGe_3$ was determined in detail by powder neutron diffraction. Physical properties of the doped system were investigated with specific-heat, magnetization and resistivity measurements in order to determine the $T_c(x) \sim |x - x_c|^p$ dependence in detail. Our data are comparible with an exponent $p = 3/4$ expected for a three-dimensional ferromagnet. However $p = 1$ is also possible.

TT 32: Transport: Nanoelectronics III - Molecular Electronics 1

Time: Wednesday 15:00–17:30 Location: BH 334

TT 32.1 Wed 15:00 BH 334

Influence of disorder and dephasing events on the electron transport through conjugated molecular wires in molecular junctions — •Daijiro Nozaki[1], Claudia Gomes da Rocha[1], Horacio M. Pastawski[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Instituto de Fisíca Enrique Gaviola (CONICET) and FaMAF, Universidad Nacional de Córdoba, Argentina

Understanding electron transport mechanisms on the molecular scale is a central issue in the field of molecular electronics. Among them, the dephasing effect, causing the tunneling-to-hopping transition, has a great importance for applications as well as from the fundamental point of view. In this study, we analyzed the coherent and incoherent electron transmission through conjugated molecular wires by means of a first principle approach within D'Amato-Pastawski model [1]. Our approach can study explicitly the structure/transport relationship in molecular junctions in a dephasing environment using only a single tuning parameter. We investigated the length dependence and the influence of thermal disorder on the transport and reproduced the well-known tunneling-to-hopping transition [2]. This approach will be a powerful tool for the interpretation of recent conductance measurements of molecular wires.

[1] J. L. D'Amato and H. M. Pastawski, Phys. Rev. B 41, 7411 (1990).
[2] D. Nozaki, C. G. Rocha, H. M. Pastawski, and G. Cuniberti, submitted.

TT 32.2 Wed 15:15 BH 334

Master-equation approach for simulating STM images of single molecules — •Tim Ludwig[1], Carsten Timm[1], Torsten Hahn[2], and Jens Kortus[2] — [1]TU Dresden, Dresden, Germany — [2]TU Freiberg, Freiberg, Germany

The power of STM imaging of single molecules lies in the spatial resolution and a well-defined contact with highly controllable contact strength. Therefore a wide range of molecule-substrate combinations are investigated by this technique. Traditional methods for simulating STM images, e.g., DFT + Tersoff-Hamann, use a static single-particle density-of-states description of the scanned object. This can be inappropriate for the investigation of single molecules, as for example Coulomb blockade may occur. In contrast a master-equation approach models the full many-body dynamics on the molecule, including, e.g., spin blockade and vibrational coupling. Furthermore it can be used for arbitrarily high bias voltages. We report on the first attempt for simulating STM images of single molecules by using a master-equation description.

TT 32.3 Wed 15:30 BH 334

Molecular orbital switching in photochromic single molecular junctions — •Youngsang Kim[1], Torsten Pietsch[1], Elke Scheer[1], Thomas Hellmuth[2], Fabian Pauly[2], Dmitro Sysoiev[3], Thomas Huhn[3], Thomas Exner[3], Ulrich Groth[3], Ulrich Steiner[3], and Artur Erbe[4] — [1]Department of Physics, Universität Konstanz, 78467 Konstanz, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Department of Chemistry, Universität Konstanz, 78467 Konstanz, Germany — [4]Helmholtz-Zentrum Dresden Rossendorf, 01328 Dresden, Germany

Photoswitchable molecules gain significant interest due to the applicability in data storage media, as optical switches, and in novel logic circuits [1]. The molecular energy levels and their coupling to the metal electrodes determine both the single-molecule conductance and the switching ratio between the two states of a switch molecule. Here, we show the preferential conductance of individual, specifically designed sulfur-free diarylethene [2] molecules bridging mechanically controlled break-junction (MCBJ) electrodes at low temperatures. These molecules undergo a ring-opening/ring closure transition upon irradiation with light of suitable wave-length. We discuss the changes of molecular energy levels and electrode couplings in both isomers obtained by evaluating the current-voltage (I-V) characteristics using the single-level model [3].

[1] M. Del Valle etal., Nat Nanotechnol 2, 176 (2007).
[2] D. Sysoiev etal., Chem. Eur. J. 17, 6663 (2011).
[3] Y. Kim etal., Nano Lett. 11, 3734 (2011); L. Zotti et al., Small 6, 1529 (2010).

TT 32.4 Wed 15:45 BH 334

Vibrationally dependent electron-electron interactions in single-molecule junctions: A mechanism for asymmetric gate-voltage dependence of the current in symmetrically coupled junctions — •Rainer Härtle, Andre Erpenbeck, and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058, Germany

The influence of non-adiabatic effects due to vibrationally dependent electron-electron interactions on the transport characteristics of single-molecule junctions is investigated. Non-adiabatic effects in single-molecule junctions result from the dependence of the electronic states of the molecular bridge on the nuclear coordinates. This includes a direct coupling between electronic states, which is important, for example, in the presence of avoided level-crossings or conical intersections, but involves also vibrationally dependent electron-electron interactions. We demonstrate that the latter gives rise to an effective electronic-vibrational coupling, which depends on the population of the electronic states. As a result, the current-voltage characteristics of a single-molecule junction can be asymmetric with respect to a gate voltage, even if the molecular bridge is symmetrically coupled to the leads. To describe these effects, we employ a master equation approach that is based on a second-order expansion in the coupling between the molecule and the leads.

TT 32.5 Wed 16:00 BH 334

Transport through π-stacked benzene rings and evaluation of their IETS — •Thomas Hellmuth, Marius Bürkle, Fabian Pauly, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Motivated by recent experiments [1], we study the electric transport through wires with multiple π-π-stacked benzene rings connected to gold electrodes. In our density-functional-theory-based calculations we analyze various junction geometries and study both the elastic transmission and inelastic electron tunneling spectra (IETS). Transmission eigenchannels show that the current is mostly carried by the π-system, but the gold-benzene binding affects the transmission path notably. Features in the inelastic tunneling spectra are identified with their corresponding vibrational modes.

[1] S. T. Schneebeli et al., J. Am. Chem. Soc. 133, 2136 (2011)

15 min. break.

TT 32.6 Wed 16:30 BH 334

Coulomb blockade in molecular junctions with intermediate coupling to the leads — •Dmitry Ryndyk, Andrea Donarini, Milena Grifoni, and Klaus Richter — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

An ab initio based theoretical approach to describe nonequilibrium many-body effects in molecular transport is developed. In particular, an Anderson-Hubbard cluster model on the basis of localized molecular orbitals is derived for single-molecule junctions with intermediate coupling to the leads. As an example we consider the Coulomb blockade in a benzenedithiol junction with gold electrodes. An effective few-level model is obtained, transformed into the many-body eigenstate basis and solved within the master equation approach. It is shown

that transport through asymmetrically coupled molecular edge states results in strongly suppressed peaks of the differential conductance at small voltage.

TT 32.7 Wed 16:45 BH 334

Spin-polarized transport through single molecules: insight from theory — •Alexei Bagrets[1,2] and Ferdinand Evers[2,3] — [1]Steinbuch Center for Computing, Karlsruher Institut für Technologie (KIT), Germany — [2]Institut für Nanotechnologie, KIT, Germany — [3]Institut für Theorie der Kondensierten Materie, KIT, Germany

In this talk, a short overview will be given on our recent advances in DFT modeling of spin-polarized electron transport across single molecules bridged between magnetic reservoirs. In particular, we will discuss implementation of the non-equilibrium Green's function formalism, where efficient absorbing boundary conditions encoded into self-energy function are extended to account for the spin-polarized electronic structure of magnetic electrodes. We will demonstrate an ability, within our approach, to treat a variety of different magnetic configurations (e.g. nano-scale domain walls) which could appear when a molecule with few spin-centers (d-ions) is brought in contact with a magnetic surface and a tip of the spin-polarized-STM. Recent experiments [1,2] on spin-transport and magnetoresistance effect observed in hydrogen-phtalocyanine STM molecular junctions will be discussed in detail.

[1] S. Schmaus, A. Bagrets, Y. Nahas, T. K. Yamada, A. Bork, M. Bowen, E. Beaurepaire, F. Evers, W. Wulfhekel, Nature Nanotechnology **6**, 185 (2011).
[2] A. Bagrets, A. Jaafar, S. Schmaus, M. Alouani, W. Wulfhekel, F. Evers, preprint (2011)

TT 32.8 Wed 17:00 BH 334

Optical response of a single-molecule junction: current switching, negative differential resistance and plasmon induced conductance enhancement — •Yaroslav Zelinskyy[1,2] and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for theoretical physics National Academy of Science of Ukraine, Metrologichna str. 14b, UA-03683, Kiev, Ukraine

Based on a generalized master equation approach the conductive properties of a current-carrying molecular junction driven by an external optical excitation are studied [1]. The description incorporates vibrational states of the molecule and related relaxation processes with the latter being crucial for the strength of the actual current. A photoinduced switch of the current, the appearance of a negative differential resistance and its photoinduced suppression are predicted [2]. The nano-electrode plasmon control of the single molecule conductivity appearing at the simultaneous optical excitation of the molecule and the electrodes is also considered [3]. A remarkable enhancement of the current is achieved in this case.

[1] L. Wang, V. May, Phys.Chem.Chem.Phys., 13, 8755 (2011).
[2] Ya.R. Zelinskyy, E.G. Petrov, Ukr.J.Phys. 54, 707 (2009).
[3] Y. Zelinskyy, V. May, Nano Lett. (submitted).

TT 32.9 Wed 17:15 BH 334

Resonant photoconductance of molecular junctions formed in Gold nano-particle arrays — M. Mangold[1], •J. Schopka[1], M. Calame[2], M. Mayor[3], and A.W. Holleitner[1] — [1]Walter Schottky Insitut and Physik-Department, Technische Universitaet Muenchen, 85748 Garching — [2]Departement Physik, Universitaet Basel, 4056 Basel, Switzerland — [3]Departement Chemie, Universitaet Basel, 4056 Basel, Switzerland

We report on a molecular phototransistor effect based on oligo(phenylene vinylene) (OPV) incorporated in gold nanoparticle arrays. We find a pronounced photoconductance arising upon resonant excitation of the OPV molecules. We determine the typical response time and the irradiation intensity dependence of this resonant photoconductance. Our results suggest that the charge carriers, which are resonantly excited in the OPV molecules, directly contribute to the current flow through the nanoparticle arrays. We can consistently model the dynamics of the resonant photoconductance by considering the filling and recombination of trap states in the nanoparticle arrays. Our results verify that individual molecules in metal-molecule-metal junctions can be functional modules of optoelectronic devices [1].

[1] M. Mangold, M. Calame, M. Mayor, A.W. Holleitner, J. Am. Chem. Soc. 133, 12185-12191 (2011).

TT 33: Superconductivity, Measuring Devices, Matter at Low Temperature: Poster Session

We recommend to hang up the posters already during the morning sessions.

Time: Wednesday 15:00–19:00 Location: Poster B

TT 33.1 Wed 15:00 Poster B

Magnetic investigations on $EuFe_2(As_{1-x}P_x)_2$ single crystals — •Felix Klingert[1], Sina Zapf[1], Dan Wu[1], Shuai Jiang[1,2], Hirale S. Jeevan[2], Philipp Gegenwart[2], and Martin Dressel[1] — [1]1.Physikalisches Institut, Universität Stuttgart, Germany — [2]I.Physikalisches Institut, Universität Göttingen, Germany

Magnetic susceptibility measurements on a series of $EuFe_2(As_{1-x}P_x)_2$ single crystals (x = 0, 0.05, 0.12, 0.25, 0.35) show, how the isovalent P substitution on the As site influences the magnetic ordering of the Eu^{2+} spins, which appears at low temperatures additionally to the spin-density-wave (SDW) or superconducting (SC) phase of the Fe subsystem. Thus this system provides an extraordinary possibility to study the interplay of magnetism and SC.

The Eu^{2+} moments order ferromagnetic (FM) in the ab-plane, but depending on the P content the interlayer coupling develops from antiferromagnetic (in the SDW- and SC-phase) to ferromagnetic coupling (for high substitution). We have previously reported low field magnetization measurements, showing an additional canting of Eu^{2+} spins out of the plane, which leads to a FM component along the c-direction and gets stronger with the suppression of the SDW ordering of Fe [1]. We have now performed a detailed study on a series of samples, which includes angle dependent magnetization measurements, investigating in detail the interplay of Fe and Eu magnetic ordering.

[1] S. Zapf et al., PRB(R) 84, 140503

TT 33.2 Wed 15:00 Poster B

Temperature dependent ellipsometric Studies on Iron-Pnictides — •Mathias Eichler, Dan Wu, Bruno Gompf, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Iron-pnictides indicate a strong temperature dependence in their optical properties even at high energies. The aim of the present work is spectroscopic ellipsometry measurements on iron-pnictides performed as a function of temperature. To accomplish this task we use a Woollam Variable Angle Spectroscopic Ellipsometer (VASE) operating in the spectroscopic range from 4,000cm^{-1} to 40,000cm^{-1}. The setup is equipped with a customized Janis ST-400 liquid helium cryostat that allows us to measure at temperatures down to 5 K. In order to measure small samples with 1×1 mm^2 in size the setup was improved by upgrading the sample stage geometry to yield an undisturbed signal. The final design also allows us to compensate thermal expansion effects and to easily align the crystal within the cryostat. With this advanced setup, we have investigated several families of 122-pnictides, for example the series $EuFe_2(As_{1-x}P_x)_2$. We find a significant shift of the spectral weight with temperature. The results on other compounds will be also discussed, e.g. different doping levels.

TT 33.3 Wed 15:00 Poster B

Isovalent substitution on the iron site in pnictides - an optical study — •Daniel Pröpper[1], Aliaksei Charnukha[1], Ma Jin Eom[2], Jun Sung Kim[2], Bernhard Keimer[1], and Alexander Boris[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, Pohang University of Science and Technology, Pohang, Korea

Here we report on the full complex dielectric function $\epsilon(\omega)$ in the *ab* plane of $Ba(Fe_{1-x}Ru_x)_2As_2$ applying spectroscopic ellipsometry in the broad range of 60 meV to 6 eV. The investigated set of samples spans the whole range from the parent compound $BaFe_2As_2$ deep into the overdoped regime (x = 0.74), not reported so far, showing superconductivity with T_c up to 20 K at optimally doping (x = 0.35). By classical dispersion analysis of Drude-Lorentz type we detect an increase in

the bare plasma frequency ω_p, associated with the free carrier response, and a significant decrease of the low-energy dielectric permittivity ϵ_∞ upon doping. The main contribution to ϵ_∞ arises from the lowest lying interband transitions at $\sim 0.5\,\mathrm{eV}$, assigned to be from Fe(Ru)-d/As-p to Fe(Ru)-d hybrid states [1]. This gives rise to anomalously high $\epsilon_\infty \approx 60 - 80$ among all other high-T_c superconductors. This, in conjunction with increased Fe(Ru)-d bandwidth with x due to stronger hybridization with As-p states [2], hints to a strong decrease in the high polarizability of Fe-As bonds, which is thought to play a crucial role in establishing and controlling superconductivity in iron pnictides.
[1] A. Charnukha et al., Nat. Comm. 2 (2011), 219
[2] L. Zhang et al., PRB 79 (2009), 174530

TT 33.4 Wed 15:00 Poster B

Evidence for vortex lattice melting in $Ba_{1-x}K_xFe_2As_2$ seen by thermal expansion — •Philipp Burger[1,2], Anna Böhmer[1,2], Frédéric Hardy[1], Peter Adelmann[1], Doris Ernst[1], Rainer Fromknecht[1], Peter Schweiss[1], Thomas Wolf[1], Hilbert von Löhneysen[1,3], and Christoph Meingast[1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [3]Physikalisches Institut, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

Low temperature thermal expansion measurements have been performed on underdoped (T_c=30.6 K) and overdoped (T_c=33.8 K) $Ba_{1-x}K_xFe_2As_2$ single crystals in magnetic fields up to 10T applied perpendicular to the Fe-As layers. The superconducting transition for the underdoped sample broadens strongly with increasing magnetic field due to strong fluctuations, whereas for the overdoped sample it simply shifts to lower temperatures. Upon heating (after cooling in constant field) we observe a sharp peak in the expansion coefficients at a temperature slightly lower than T_c. These peaks are absent in the cooling curves. We associate these peaks with an underlying thermodynamic melting of the vortex lattice, since our results are very similiar to previous thermal expansion data [1] of YBCO, which clearly exhibits a first-order vortex melting transition.
[1] R. Lortz *et al.*, J. Low Temp. Phys **147**, 365 (2007)

TT 33.5 Wed 15:00 Poster B

Thermal expansion and magnetostriction studies on Fe-based pnictides — •Christopher Dietl[1], Norman Leps[1], Liran Wang[2], Ulrike Stockert[3], Luminita Harnagea[4], Sabine Wurmehl[4], Bernd Büchner[4], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institute for Physics,University of Heidelberg, Heidelberg, Germany — [2]National High Magnetic Field Laboratory, Tallahassee,Florida, USA — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany

We investigate the thermal expansion coefficient α and the magnetostriction β of single crystalline $Ca(Fe_{1-x}Co_x)_2As_2$ and polycrystalline $RFeAsO_{1-x}F_x$. The data are obtained by means of a high-resolution capacitive dilatometer consisting of silver. For $CaFe_2As_2$, the SDW-type magnetic and structural phase transition causes a pronounced anomaly which shifts, splits, and broadens upon doping. The structural phase diagram is constructed and particular emphasis is given to the paramagnetic tetragonal phase where a linear temperature dependence of the length changes is observed.

TT 33.6 Wed 15:00 Poster B

Coherent excitations and e-ph coupling in 122 FeAs compounds investigated by time-resolved ARPES — •I. Avigo[1], R. Cortés[2,3], L. Rettig[1,2], S. Thirupathaiah[4], H. S. Jeevan[5], P. Gegenwart[5], T. Wolf[6], M. Ligges[1], M. Wolf[2,3], J. Fink[4], and U. Bovensiepen[1,2] — [1]Universität Duisburg-Essen — [2]Freie Universität Berlin — [3]Fritz-Haber-Institut d. MPG, Berlin — [4]IFW Dresden — [5]Georg-August Universität Göttingen — [6]Karlsruhe Institute of Technology

We investigate the coupling of low energy electrons to lattice vibrations in iron based high-T_c superconductors to shed light on the mechanisms leading to superconductivity. Femtosecond time and angle-resolved photoemission spectroscopy was employed to analyze the response of the electronic system of 122 iron pnictide compounds to optical excitation. Oscillations of the spectral weight around the Fermi level were observed showing three different coherently excited phonon modes. We identify the symmetric A_{1g} mode at 5.6 THz, corresponding to the displacement of the As atoms perpendicular to the Fe-plane, and two further modes at 3.3 THz and 2.6 THz. Our observations are consistent with calculations predicting strong e-ph coupling for the A_{1g} mode. By analyzing the rate of energy relaxation of excited electrons we estimate the moment-averaged e-ph coupling constant to $\lambda < 0.2$ which makes simple e-ph interaction an unlikely pairing candidate for superconductivity. This work has been funded by the DFG through BO 1823/2 and SPP 1458. R.C. acknowledges the Alexander von Humboldt Foundation.

TT 33.7 Wed 15:00 Poster B

Three-dimiensional Fermi surface of Iron-pnictide superconductor $Ba_{1-x}K_xFe_2As_2$ — •Masaki Kobayashi[1,2], Vladimir N. Strocov[1], Elia Razzoli[1,3], Ming Shi[1], Thorsten Schmitt[1], Xiaoping Wang[1,4], Yaobo Huang[4], Hong Ding[4], Masaharu Oshima[2], and Luc Patthey[1] — [1]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [2]Department of Applied Chemistry, University of Tokyo, Tokyo, Japan — [3]Laboratory for Synchrotron and Neutron Spectroscopy, EPFL, Lausanne, Switzerland — [4]Institute of Physics, Chinese Academy of Science, Beijing, China

Iron-based superconductors have attracted much attention because of the unexpected high transition temperatures of the superconducting state. Investigation of bulk three-dimensional electronic structure will provide further understanding of the superconducting properties of $Ba_{1-x}K_xFe_2As_2$ (BKFA). Here, we report investigations of the shape and k_z-dependence of the Fermi surface (FS) in BKFA with soft X-ray ARPES, taking into advantage enhanced bulk sensitivity and intrinsic k_z resolution achieved in the soft-X-ray range.

The experimental FS measured at energies around 900 eV show modulations along the k_z direction corresponding to the Brillouin zone periodicity in BKFA. The in-plane FS shapes alternate between a circle-like and flower-like appearances when going from the Γ point to the higher Brillouin zones. Furthermore, we observed clear polarization dependences of the FS, allowing separation of different valence bands. The results provide with experimental information on the dimensionality and orbital character of FSs of BKFA.

TT 33.8 Wed 15:00 Poster B

Pinning in $CaFe_{2-x}Co_xAs_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals as studied by MWA — •Nadezda Panarina[1,2], Niyaz Beysengulov[1], Yuri Talanov[1], Tatyana Shaposhnikova[1], Evgenia Vavilova[1], Luminita Harnagea[2], Saicharan Aswartham[2], Claudia Nacke[2], Sabine Wurmehl[2], Christian Hess[2], Vladislav Kataev[2], and Bernd Büchner[2] — [1]Zavoisky Physical-Technical Institute, Kazan, Russia — [2]IFW Dresden, Germany

Modulated microwave absorption studies were performed on a series of $CaFe_{2-x}Co_xAs_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals with different Co content. Investigation of pinning features in these samples is of particular interest since there is a significantly wide region of Co concentration, where the superconducting and magnetic orders coexist. Depending on the scale of such electron phase separation, the nonsuperconducting inclusions present in the samples at certain Co concentration may act as additional pinning centers and influence the pinning strength. To estimate the values of the critical current density, an appropriate theoretical model was applied. By analyzing the magnetic field and temperature dependence of the critical current density, we were able to discriminate different types of pinning (small-bundle and large-bundle pinning) in single crystals of $CaFe_{2-x}Co_xAs_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$. The most effective pinning centers are present in the $CaFe_{2-x}Co_xAs_2$ sample at Co concentration corresponding to the boundary of the coexistence of SDW and superconductivity states. This is due to the best correlation of the sizes of additional nonsuperconducting inclusions with the sizes of vortex cores.

TT 33.9 Wed 15:00 Poster B

In-plane/out-of-plane resistivity anisotropy of Co-doped $BaFe_2As_2$ — •Oleksii Vakaliuk, Manoj Kumar, Saicharan Aswartham, Sabine Wurmehl, Christian Hess, and Bernd Büchner — IFW Dresden

We present an experimental study of the in-plane and out-of-plane electrical resistivities (ρ_{ab}, ρ_c respectively) of $Ba(Fe_{1-x}Co_x)_2As_2$ with x=0; 0.05; 0.075; 0.1; 0.125. The anisotropy $\gamma = \rho_c/\rho_{ab}$ is temperature independent. This suggests an isotropic electron scattering mechanism. We observe a monotonic decrease of γ with changing the doping, suggestive of 2D-3D crossover of the electron structures.

TT 33.10 Wed 15:00 Poster B

Systematic NMR/NQR investigation of the local charge environment in iron pnictides — •Uwe Gräfe[1], Eva-

Maria Brüning[1], Guillaume Lang[1], Louis Veyrat[1], Seung-Ho Baek[1], Hans-Joachim Grafe[1], Dalibor Paar[1,2], Franziska Hammerath[1], Katarina Manthey[1], Günther Behr[1], Jochen Werner[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dept. of Physics, Faculty of Science, Univ. of Zagreb, P.O. Box 331, HR-10002 Zagreb, Croatia

As iron-based superconductors are a striking example of a system featuring unconventional superconductivity close to a region of static magnetism in the phase diagram, much attention has been devoted to the study of ground-state coexistence and/or competition. In this regard, a more general question is the existence and the role played by electronic inhomogeneities, whether in ordered states or in the paramagnetic state. A powerful tool to investigate these issues is Nuclear Magnetic/Quadrupole Resonance, which allows to probe locally the electric charge environment and the spin fluctuations. Here, we present a summary of recents results and on-going studies at the As site of 1111 iron pnictides.

TT 33.11 Wed 15:00 Poster B

Superconducting LiFeAs as seen by Scanning Tunneling Microscopy/Spectroscopy — •Rico Pohle, Martha Scheffler, Ronny Schlegel, Torben Hänke, Danny Baumann, Anne Bachmann, Dirk Bombor, Steffen Sykora, Luminita Harnagea, Sabine Wurmehl, Christian Hess, and Bernd Büchner — Institut für Festkörperforschung IFW Dresden

Among the entire class of iron-based superconductors the material LiFeAs is of particular interest since an absence of nesting between electron and hole pockets suggests an unconventional type of pairing in this material. Using Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS) we investigate topographic properties of the surface as well as the temperature dependency of the superconducting gap. The good agreement of our results with model calculations for the tunnelling conductance allows us to draw conclusions about the low energy properties of the superconducting system. Furthermore, we compare our results with Transport- and NMR-measurements.

TT 33.12 Wed 15:00 Poster B

Electronic Transport Properties of LiFeAs and Transition Metal doped LiFeAs in comparison to doped and undoped NaFeAs — •Dirk Bombor[1], Anne Bachmann[1], Luminita Harnagea[1], Claudia Nacke[1], Saicharan Aswaratham[1], Igor Morozov[2], Maria Roslowa[2], Sabine Wurmehl[1], Christian Hess[1], and Bernd Büchner[1] — [1]Leibnitz Institute for Solid State and Materials Research, IFW Dresden, Germany — [2]Moscow State University, Moscow 119991, Russia

Electronic transport properties of the unconventional 111-superconductors LiFeAs and NaFeAs as well as its transition metal doped compounds have been studied. Unlike in other iron arsenide superconductors the stoichiometric LiFeAs doesn't show any nesting of the Fermi surface and therefore exhibits no spin density wave but even the undoped compound becomes superconducting below 18 K. We find that doping by substitution of iron with Co, Ni, Cr or Rh suppresses superconductivity. Ferromagnetism in Li-deficient samples is discussed. The isostructural NaFeAs also exhibits superconductivity in its undoped state, but in contrast to LiFeAs a structural and SDW-transitions are found. With Co-doping the SDW-transition can be suppressed and the superconducting transition temperature increased.

TT 33.13 Wed 15:00 Poster B

Superconductivity in LiFeAs — •Johanna Brand[1], Sabine Wurmehl[2], Bernd Büchner[2], Anne Stunault[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Leibniz-Institut, Dresden — [3]Institut Laue Langevin, Grenoble

LiFeAs is a member of the family of FeAs based superconductors and is remarkable as it exhibits superconductivity without doping or application of pressure with a sizeable transition temperature, $T_c = 18\,K$. It is still an open question whether the superconducting phase in LiFeAs is characterized by spin singlets or by spin triplets. There are two ways to analyze the magnetic response in the superconducting state as a simple magnetometer study is not possible due to the superconducting shielding: Knight shift and polarized neutron diffraction experiment. We measured flipping ratios with polarized neutron diffraction to follow the spin-susceptibility across T_c. For the magnetic field applied parallel and perpendicular to the c axis we find a drop in the local spin susceptibility which is comparable to the observation for Co-doped $BaFe_2As_2$ suggesting a spin singlet state in LiFeAs.

TT 33.14 Wed 15:00 Poster B

Gutzwiller theory of band magnetism in LaOFeAs — •Tobias Schickling[1], Florian Gebhard[1], Jörg Bünemann[2], Lilia Boeri[3], Ole K. Andersen[3], and Werner Weber[4] — [1]Fachbereich Physik, Philipps Universität, D-35037 Marburg, Germany — [2]Institut für Physik, BTU Cottbus, D-03013 Cottbus, Germany — [3]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [4]Fakultät Physik, TU Dortmund, D-44221 Dortmund, Germany

For the iron pnictide LaOFeAs we investigate multi-band Hubbard models which are assumed to capture the relevant physics [1, 2]. In our calculations, we employ the Gutzwiller variational theory which is a genuine many particle approach. We will present results both on the paramagnetic and antiferromagnetic phases of our model systems. These results show that a five band-model is not adequate to capture the relevant physics in LaOFeAs [3]. However, our results for the eight band-model which includes the arsenic 4p bands reproduce the experimental data, especially the small magnetic moment, for a broad parameter regime [4].

[1] S. Graser et al., New J. Phys. 11, 025016 (2009).
[2] O. K. Andersen, L. Boeri. Annalen der Physik, 523:8-50 (2011).
[3] T. Schickling et al., PRL, 106:146402 (2011).
[4] T. Schickling et al., arXiv: 1109.0929.

TT 33.15 Wed 15:00 Poster B

Preemptive Nematic Order, Pseudogap, and Orbital Order in the Iron Pnictides — •Johannes Knolle[1], Ilya Eremin[2], Rafael M. Fernandes[3], Andrey V. Chubukov[4], and Jorg Schmalian[5] — [1]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [3]Department of Physics, Columbia University, New York, New York 10027, USA — [4]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA — [5]Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany

Starting from a microscopic itinerant model, we derive and analyze the effective low-energy model for collective magnetic excitations in the iron pnictides. We show that the stripe magnetic order is generally preempted by an Ising-nematic order which breaks C4 lattice symmetry but preserves O(3) spin-rotational symmetry. This leads to a rich phase diagram as function of doping, pressure, and elastic moduli, displaying split magnetic and nematic tri-critical points. The nematic transition may instantly bring the system to the verge of a magnetic transition, or it may occur first, being followed by a magnetic transition at a lower temperature. In the latter case, the preemptive nematic transition is accompanied by either a jump or a rapid increase of the magnetic correlation length, triggering a pseudogap behavior associated with magnetic precursors. Furthermore, due to the distinct orbital character of each Fermi pocket, the nematic transition also induces orbital order. We compare our results to various experiments.

TT 33.16 Wed 15:00 Poster B

Quasiparticle properties in iron arsenides — •Guido Klingschat and Carsten Honerkamp — RWTH Aachen

We calculate the quasiparticle scattering rates and renormalization factors around the various Fermi pockets in multi-band models for iron arsenide superconductors by perturbation theory. The existence of a fifth Fermi pocket is found to have an important influence on the anisotropy of the scattering. We furthermore compare the anisotropies and pocket dependences of the scattering rates with those of the superconducting gaps found in the functional renormalization group and discuss the role of Hund's coupling on these observables.

TT 33.17 Wed 15:00 Poster B

Ultrafast non-equilibrium dynamics in SDW metals — •Bhaskar Kamble[1], Alireza Akbari[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum — [2]Max Planck Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany

We employ a density-matrix theory to analyze the ultrafast dynamics of metallic two-dimensional spin density wave systems on short time scales far away from thermal equilibrium. In particular, we study a non-adiabatic regime where the full account for the time evolution of anomalous expectation values and the coherences between different

quasiparticle states are required. We calculate the time evolution of the SDW mean-field order parameter and compare its behavior with that of a superconductor. In addition, we discuss the transition between the adiabatic and the non-adiabatic regimes, where the order parameter oscillates, and a description in terms of the quasiparticle occupations becomes insufficient.

TT 33.18 Wed 15:00 Poster B

Robustness of surface states in noncentrosymmetric superconductors — •Raquel Queiroz and Andreas Schnyder — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Noncentrosymmetric superconductors, where spin singlet and triplet pairing states are mixed, exhibit topologically protected zero-energy flat bands localized on the surface [1-3]. The region of the surface Brillouin zone where these states appear is bounded by the projections of the nodal lines of the bulk gap. Using both analytical analysis and numerical simulations, we study the robustness of these surface states against surface roughness and disorder. We show that time-reversal preserving disorder leaves the surface states mostly unaffected. Time-reversal breaking perturbations, on the other hand, such as magnetic impurities, result in a shift of the surface states away from zero energy, but do not change the total amount of ingap states.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504(R) (2011).
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B 84, 020501(R) (2011).
[3] A. P. Schnyder, P. M. R. Brydon, and C. Timm, arXiv/1111.1207 (unpublished).

TT 33.19 Wed 15:00 Poster B

Mössbauer investigation of magnetic and structural phase transitions in $Fe_{1+x}Te$ — •Philipp Materne[1], Cevriye Coz[2], Sahana Rössler[2], Ulrich K. Rössler[3], Mathias Doerr[1], Steffen Wirth[2], Ulrich Schwarz[2], Til Goltz[1], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [3]IFW Dresden, Postfach 270016, 01171 Dresden, Germany

$Fe_{1+x}Te$, the antiferromagnetic parent compound of the Fe-chalcogenide superconductors, displays separated magnetic (T_N) and structural (T_s) transitions with $T_N > T_s$ for $x > 0.12$ [1]. Such behavior, namely the magnetic transition preceeding the structural transition upon cooling, is uncommon for the parent systems of pnictide superconductors. We performed Mössbauer spectroscopy on samples with two representative levels of iron excess: i) $Fe_{1.06}Te$ with simultaneous magnetic and structural transitions at $T_N = T_s$ =69 K and ii) $Fe_{1.13}Te$ with separated transitions at $T_N = 57$ K followed by $T_s = 46$ K. Mössbauer data, analyzed by taking into account two different Fe-sites clearly, display a precursor magnetic state which is only present in $Fe_{1.13}Te$. Further, a complex magnetic phase has been observed in the temperature range 75 K $\gtrsim T \gtrsim$ 40 K in $Fe_{1.13}Te$. We discuss our Mössbauer results in the context of recently published thermodynamic and neutron scattering data on $Fe_{1+x}Te$.

[1] S. Rößler *et al.*, Phys. Rev. B. **84** (2011) 174506.

TT 33.20 Wed 15:00 Poster B

Noise spectroscopy of superconducting systems δ'-FeSe and $FeSe_{0.5}Te_{0.5}$ — •Adham Amyan[1], Amir-Abbas Haghighirad[1], Pintu Das[1], Sahana Rössler[2], Steffen Wirth[2], Dona Cherian[3], Suja Elizabeth[3], Wolf Assmus[1], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt am Main, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [3]Dep. of Physics, Indian Institute of Science, Bangalore, India

One of the most recent interesting and surprising phenomena is superconductivity in Fe-based compound (i.e. pnictides and chalcogenides), where FeSe has the most simple structure of the diverse family of these materials. The $FeSe_{1-x}Te_x$ system shows superconductivity up to $T_c \sim 14$ K. The Fe planar structure may be crucial for understanding the mechanism of superconductivity in these systems: it was suggested that a low temperature structural distortion is closely associated with the superconductiing properties of this material [1]. We employ fluctuation (noise) spectroscopy to study the intrinsic charge carriers dynamics and their correlation with the structural properties. In both superconducting compounds δ'-FeSe and $FeSe_{0.5}Te_{0.5}$ we observe a maximum in the normalized noise power spectral density at 107 K and 110 K respectively, where a structural transition from tetragonal to orthorhombic occurs [2].

[1] M. J. Wang et al, PRL 103, 117002 (2009)
[2] M. de Souza et al, Eur. Phys. J. B 77, 101-107 (2010)

TT 33.21 Wed 15:00 Poster B

Superconductor-insulator transition in disordered FeSe thin films — •Rudolf Schneider, Alexander G. Zaitsev, and Dirk Fuchs — Karlsruher Institut für Technologie, Institut für Festkörperphysik, Karlsruhe, Germany

The evolution of the temperature-dependent sheet resistance with increasing disorder in epitaxial c-axis oriented FeSe thin films was studied. Disorder was induced by decreasing the thickness of identically prepared stoichiometric films. At critical values of the thickness and sheet resistance a transition from the superconducting to the insulating state occurred. The critical sheet resistance was three times the supposed universal quantum resistance for pairs of electrons. Finite-size scaling analysis in the critical regime according to the Bose-glass model revealed a critical exponent product of 7/3 compatible with the prediction of a quantum percolation transition.

TT 33.22 Wed 15:00 Poster B

Superconducting oyxpnictide thin films — •Andreas Reisner[1], Martin Kidszun[1], Thomas Thersleff[2], Elke Reich[1], Bernhard Holzapfel[1], Ludwig Schultz[1], and Silvia Haindl[1] — [1]IFW Dresden, Institute of Metallic Materials, 01069 Dresden, Germany — [2]Uppsala University, Angstrom Laboratory, Box 524, S-751 20 Uppsala, Sweden

We present an overview on the oxypnictide thin film preparation. So far, only $LaAlO_3$ (001) single crystalline substrates provided a successful growth using pulsed laser deposition in combination with a post annealing process. Further experiments on the in-situ deposition will be reported. The structure of the films was investigated by X-ray diffractometry and transmission electron microscopy. Transport properties were measured with different applied fields to obtain a magnetic phase diagram for this new type of superconductor.

TT 33.23 Wed 15:00 Poster B

Unusual flux jumps in MgB_2 thin films — •Sebastian Treiber[1], Claudia Stahl[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Hochschule Aalen, Beethovenstraße 1, 73430 Aalen, Germany

Most superconductors exhibit flux jump phenomena, for example the so called flux avalanches. Below a material dependent threshold temperature - about 10K in case of MgB_2 - flux penetration changes from deterministic to chaotic. In this case, very fast moving vortices form dendritic flux patterns, destroying the critical state along their path. Magneto - optical images show characteristic features of this destruction, like a current - free path of an avalanche. Our experiments have shown, that avalanche behavior can be very different in MgB_2 films with an irregular microstructure [1]. In this contribution, we report on large flux jumps which occur in samples with irregular microstructure at higher temperatures than the classical avalanche temperature. Up to 14K very fast and chaotic flux penetration forms dendritic patterns without destroying the critical state. While SQUID measurements suggest a regular behavior, magneto - optical imaging clearly indicates the presence of large flux jumps.

[1] S. Treiber et al., Phys. Rev. B 84, 094533 (2011)

TT 33.24 Wed 15:00 Poster B

Two concepts of introducing thin-film superconductivity in Ge and Si by use of Ga-ion implantation — •Richard Skrotzki[1,2], Thomas Herrmannsdörfer[1], Jan Fiedler[1], Viton Heera[1], Matthias Voelskow[1], Arndt Mücklich[1], Bernd Schmidt[1], Wolfgang Skorupa[1], Manfred Helm[1], and Joachim Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD) and Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 51 01 19, D-01314 Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany

We report on two unconventional routes of embedding superconducting nanolayers in a semiconducting environment. Ion implantation and subsequent annealing have been used for preparation of superconducting thin-films of Ga-doped germanium (Ge:Ga) [1] as well as 10 nm thin amorphous Ga-rich layers in silicon (Si:Ga) [2]. Structural investigations by means of XTEM, EDX, RBS/C, and SIMS have been per-

formed in addition to low-temperature electrical transport and magnetization measurements. Regarding Ge:Ga, we unravel the evolution of T_c with charge-charrier concentration while for Si:Ga recently implemented microstructuring renders critical-current densities or more than 50 kA/cm^2. Combined with a superconducting onset at around 10 K, this calls for onchip application in novel heterostructured devices.
This work was supported by EuroMagNET, EU contract 228043.
[1] R. Skrotzki et al., *Low Temp. Phys.* **37**, 1098 (2011)
[2] R. Skrotzki et al., *Appl. Phys. Lett.* **97**, 192505 (2010)

TT 33.25 Wed 15:00 Poster B

Synthesis, structural characterization and superconductivity in La_2Sb — •Stephan Knöner, Elena Gati, Markus Kuhnt, Mariano de Souza, Amir Haghighirad, Wolf Assmus, and Michael Lang — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), Germany

The discovery of superconductivity in Fe-pnictides has attracted enormous interest to this class of materials [1]. In this contribution, we report on synthesis, structural characterization and magnetic properties of La_2Sb. So far, only little is known on the superconductivity of La_2Sb [2]. This compound possesses a layered quasi-2D structure and crystallizes in a tetragonal structure with space group $I4/mmm$, which is isostructural to the 122-family of the iron pnictides. Since La_2Sb does not contain magnetic ions, it may serve as a reference material to explore the role of magnetic and structural degrees of freedom for superconductivity in iron-pnictides. EPMA and x-ray analyses indicate the phase purity of the samples, which show a superconducting transition at 4.6 K. We will discuss transport and magnetic properties of polycrystalline La_2Sb samples as a function of temperature and will address the effect of hydrostatic pressure.
[1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (08)
[2] H. Mizoguchi and H. Hosono, Chem. Commun., **47**, 3778 (11)

TT 33.26 Wed 15:00 Poster B

High-field and low-temperature study of the nanostructured ferromagnetic superconductor Bi_3Ni — •Thomas Herrmannsdörfer[1], Richard Skrotzki[1,2], Rico Schönemann[1], Iurii Scurschii[1], Jochen Wosnitza[1], Daniel Köhler[2], Regine Boldt[3], and Michael Ruck[2] — [1]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Department of Chemistry and Food Chemistry, TU Dresden, Dresden — [3]Leibniz Institute of Polymer Research, Dresden

We have demonstrated the coexistence of superconductivity and ferromagnetism in Bi_3Ni nanostructures which have been prepared by making use of novel chemical-reaction paths [1]. Here, we present recent experiments on novel nanostructures, such as monodisperse spherical clusters with a diameter of 8 nm as well as nanofibers. We have investigated their magnetic and electrical-transport properties by means of SQUID magnetometry, pulsed-field susceptometry, and ac-resistance measurements in a wide field and temperature range. Pulsed-field susceptibility data up to 60 T allow for a determination of the saturation magnetization of Bi_3Ni nanostructures. Resistivity measurements performed on moderately compacted Bi_3Ni nano fibers down to sub-Kelvin temperatures have shown clear evidence for the existence of an isosbestic point. These results will be presented in the context of a coexistence of superconductivity and ferromagnetism. Part of this work was supported by EuroMagNET, EU-contract No. 228043.
[1] T. Herrmannsdörfer, R. Skrotzki, J. Wosnitza, D. Köhler, R. Boldt, M. Ruck, Phys. Rev. B 83, 140501 (R) (2011).

TT 33.27 Wed 15:00 Poster B

Fermi-surface change in Yb-doped $CeCoIn_5$ — •A. Polyakov[1], O. Ignatchik[1], B. Bergk[1], A.D. Bianchi[2], S. Blackburn[2], B. Prevost[2], M. Cote[2], G. Seyfarth[3], D. Hurt[3], Z. Fisk[3], R.G. Goodrich[4], M. Richter[5], I. Sheikin[6], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Department of Physics, University of Montreal, Canada — [3]Department of Physics and Astronomy, University of California Irvine, USA — [4]Department of Physics, George Washington University, USA — [5]IFW Dresden, Leibniz Institute for Solid State and Materials Research, Germany — [6]LNCMI-Grenoble, France

The evolution of the band-structure parameters of $Ce_{1-x}Yb_xCoIn_5$ was studied as a function of Yb doping by systematic de Haas–van Alphen (dHvA) measurements. We found only a small change of the dHvA frequencies and effective masses of $CeCoIn_5$ for a low Yb concentrations ($x = 0.1$). A drastic change of the Fermi surface appears for high dilution, i.e., for $x \geq 0.55$. The experimentally observed Fermi-surface topology of $YbCoIn_5$ is in perfect agreement with the calculated band structure. For small x, the effective masses remain strongly renormalized, whereas for $x \geq 0.55$ the masses are reduced dramatically.
Work supported in part by EuroMagNET, EU contract No. 228043.

TT 33.28 Wed 15:00 Poster B

Unconventional strain dependence of superconductivity in Sr_2RuO_4 — •Sebastian Zaum[1,2], Kai Grube[1], Roland Schäfer[1], Florian Hübler[1], Christoph Meingast[1], Yoshiteru Maeno[3], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [3]Department of Physics, Kyoto University, Kyoto 606-8502, Japan

In the transition-metal oxide Sr_2RuO_4 unconventional superconductivity emerges presumably near a ferromagnetic ground state. As a result it is generally believed that critical magnetic fluctuations form the pairing mechanism leading to p-wave symmetry of the order parameter. To investigate the coupling of superconductivity to the crystal lattice we measured the thermal expansion of Sr_2RuO_4 single crystals in a temperature range between 20 mK and 10 K. The uniaxial pressure and strain dependences of the superconducting transition temperature along the tetragonal a and c axes were determined by using the Ehrenfest relation and the elastic constants. Although the layered crystal structure suggests a strongly anisotropic behavior, the strain dependences of T_c are nearly of the same size for both axes. In contrast to many conventional superconductors, the temperature dependence of the linear thermal expansion coefficients along the a and c axes are not proportional to each other. Such a difference indicates that the superconducting ground state is controlled by more than one characteristic energy scale.

TT 33.29 Wed 15:00 Poster B

Berry curvature and orbital magnetization of the triplet superconductor Sr_2RuO_4 — •Martin Gradhad, James F. Annett, and Balazs L. Györffy — University of Bristol, H.H. Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

The strong experimental evidence of spin triplet pairing in the superconducting phase of Sr_2RuO_4 prompts an interest in a detailed material dependent study of orbital magnetization in this exotic superconductor. [1] Evidently, the modern theory of orbital magnetization for metals, when generalized for the case of superconductors, would shed interesting light on the superconducting state which brakes time-reversal symmetry.

Here we present first principles as well as tight binding calculations of the Berry curvature in the normal state of Sr_2RuO_4 to show the reliability of the tight binding model. Since spin-orbit coupling is an essential ingredients of the problem a fully relativistic Greens-function method is applied to the calculation of the Berry curvature. [2] In a next step the tight binding model is used to describe the superconducting phase by solving the Bogolubov-de Gennes equation [3] and new contributions to the Berry curvature will be discussed.
[1] Y. Maeno et al. Phys. Today **54** (1), 42 (2001)
[2] M. Gradhand et al. Phys. Rev. B **84**, 075113 (2011)
[3] J.F. Annett et al. Phys. Rev. B **66**, 134514 (2002)

TT 33.30 Wed 15:00 Poster B

Direct observation of the superconducting energy-gap opening in the optical conductivity spectra of $LuNi_2B_2C$ — •Theo Fischer[1], A. V. Pronin[1], D. Stehr[1], J. Wosnitza[1], T. Niemeier[2], and B. Holzapfel[2] — [1]Hochfeld-Magnetlabor Dresden (HLD) and Institute of Ion Beam Physics and Materials Research, HZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]IFW Dresden, Leibniz Institute for Solid State and Materials Research, Germany

At frequencies between 100 GHz and 2.5 THz, we have accurately measured the complex transmission coefficient of $LuNi_2B_2C$ films on MgO substrates using two different setups: a time-domain terahertz spectrometer and a setup based on backward-wave oscillators. For the first time, the development of the superconducting energy gap is directly observed in the optical spectra. From the measured data, we have calculated the optical conductivity and the penetration depth. We have compared the results with the BCS theory, and found an additional absorption at low frequencies. The origin of this absorption may be related to the complex gap structure of the compound with possible nodes. Theoretical calculations are currently under way. Part of this work has been supported by EuroMagNET, EU contract 228043.

TT 33.31 Wed 15:00 Poster B

Fluctuation conductivity in small superconducting cylinders — •Brian Tarasinski and Georg Schwiete — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

By threading a magnetic flux through mesoscopic superconducting cylinders with diameter comparable to the superconducting coherence length ξ, it is possible to suppress superconductivity, leading to a destructive regime around half integer flux quanta.

Recently, transport experiments on small superconducting cylinders have been reported, in which the destructive regime could be observed [1,2]. We study theoretically the fluctuation conductivity on the normal side of the transition with particular emphasis on the low temperature regime.

[1] Y. Liu et al., Science 294, 2332 (2001).
[2] I. Sternfeld et al., Phys. Rev. Lett. 107, 037001 (2011)

TT 33.32 Wed 15:00 Poster B

Anisotropic magneto-transport in a Bi-2201 high-T_c superconductor — •Thorsten Jacobs[1], Sven-Olof Katterwe[1], Andreas Rydh[1], Holger Motzkau[1], Toni Helm[2], Mark V. Kartsovnik[2], Andrey Maljuk[3], Erik Kampert[4], Frederik Wolff-Fabris[4], and Vladimir M. Krasnov[1] — [1]Department of Physics, Stockholm University, AlbaNova University Center, 10691 Stockholm, Sweden — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748, Garching, Germany — [3]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01171 Dresden, Germany — [4]Hochfeld-Magnetlabor Dresden, Helmholtz Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

The single-CuO_2 plane cuprate superconductor $Bi_{2+x}Sr_{2-y}CuO_{6+\delta}$ is characterized by a relatively low critical temperature and upper critical field. This allows for a complete suppression of superconductivity at low T and thus opens a possibility to study the normal-state properties with a low interference of thermal fluctuations.

We present magnetotransport measurements of small mesa structures (1 to 25 μm^2) of Bi-2201 single crystals with a T_c of only ~ 4 K. The tunneling conductance in the superconducting state exhibits gap-like characteristics that vanish at T_c or at a modest $H_{c2} \sim 10$ T. However, a profound negative c-axis magnetoresistance persists in the normal-state without saturating at fields up to $H = 65$ T. This is likely due to a magnetic field suppression of an antiferromagnetic or spin/charge density wave order and provides evidence for a different origin of superconductivity and the pseudogap in cuprates.

TT 33.33 Wed 15:00 Poster B

Asymmetric resistive switching in $Bi_2Sr_2CaCu_2O_{8+x}$ single crystals — •Holger Motzkau, Thorsten Jacobs, Sven-Olof Katterwe, Andreas Rydh, and Vladimir M. Krasnov — Experimental Condensed Matter Physics, Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden

We study resistive switching phenomena in small mesa structures on top of $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212) and $Bi_{1.75}Pb_{0.25}Sr_2CaCu_2O_{8+x}$ (Bi(Pb)-2212) single crystals. We manipulate the normal state resistance of the mesa by a bias voltage as well as short current pulses, and study current-voltage characteristics, magnetoresistance, and the temperature dependence of the resistance. Indications of several different switching mechanisms are found, including asymmetric, current directional dependent changes of the resistance, and filamentary breakdown. We find that resistive changes from a fairly gentle biasing is accompanied by a clear influence on the superconducting properties, including critical current, critical temperature, and gap voltage. Our findings indicate that ion transport may occur at the conditions where resistive switching takes place, and therefore should not be neglected in the interpretation of resistive switching mechanisms of Bi-2212.

TT 33.34 Wed 15:00 Poster B

Polarization dependence of (Bi,Pb)-2201 and (Bi,Pb)-2212 low energy excitations by variable polarization ARPES — •Peter Hlawenka, Robin Weyrich, Aliakbar Ghafari, Christoph Janowitz, Helmut Dwelk, Alica Krapf, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Deutschland

The low energy excitations at the M-points of the four quadrants of the first Brillouin zone of superstructure free (Bi,Pb)-2201 and (Bi,Pb)-2212 single crystals have been investigated systematically with respect to their polarization dependence. A new spectrometer with a SCIENTA SES100 and HeI radiation from a duoplasmatron source was used. A polarizer with focusing capability enabled a continuous variation of the polarization vector in the CuO_2- plane. Like previously reported[1] the topmost emission consists of two peaks, whose relative intensity varies with the selected polarization and also the M-point under study, showing the M points to be essentially not equivalent. Possible reasons will be discussed taking also the results of temperature and photon energy dependent measurements into account.

[1] R. Manzke, R. Müller, C. Janowitz, M. Schneider, A. Krapf, H. Dwelk; Phys. Rev. B 63, R100504 (2001)

TT 33.35 Wed 15:00 Poster B

Momentum-dependend quasiparticle relaxation dynamics in Bi2212 investigated by trARPES above and below T_c — •S. Freutel[1], R. Cortés[1,2], L. Rettig[1,2], Y. Yoshida[3], H. Eisaki[3], M. Ligges[3], M. Wolf[4], and U. Bovensiepen[1,2] — [1]Univ. Duisburg-Essen — [2]Freie Univ. Berlin — [3]NIAIST, Tsukuba, Japan — [4]Fritz-Haber-Institut d.MPG, Berlin

After more than two decades of research, the understanding of high temperature superconductivity is still one of the most challenging problems of solid state physics. Femtosecond, time- and angle-resolved photo electron spectroscopy has proven to be a powerful technique to investigate the quasiparticle dynamics after optical excitation of these materials. Recent work on the optimally doped high-T_c superconductor $Bi_2Sr_2CaCu_2O_{2+\delta}$ [1] studied the decay times of photoexcited quasiparticles well below the transition temperature T_c at different electron momenta along the Fermi surface. At $T < T_c$ the relaxation times exhibit no sign of a momentum dependency which was explained by blocked electron-electron scattering channel towards the nodal region due to phase space restrictions originating from the superconducting gap. Here we report independent evidence of this explanation. Since the gap vanishes at $T > T_c$ an onset of a momentum dependence in the relaxation time would support our earlier conclusion [1]. Analyzing Bi2212 at 100 K we find a clear decrease of the relaxation time towards the nodel line from 800fs at a Fermi Surface angle of 18° to 300fs at 45°.

[1] Cortés et al., Phys. Rev. Lett., 107, 097002 (2011)

TT 33.36 Wed 15:00 Poster B

Correlated heterostructures with dynamical mean field theory — •Christoph Schütte and Achim Rosch — Institut für theoretische Physik, Universität zu Köln, Germany.

The interfaces between different materials in three-dimensional nanostructures give rise to interesting electronic phenomena such as metallic or even superconducting layers between insulators. We calculate various transport coefficients for different heterostructures as a function of temperature. The interactions in the structure may be described by the Hubbard model with an additional self-consistent treatment of long-range Coulomb interactions in a Hartree approximation. Inhomogeneous Dynamical Mean Field Theory (DMFT) is employed to calculate the electronic structure of such a multilayered device in three spatial dimensions. The subsequent single impurity Anderson model (SIAM) is solved with the numerical renormalisation group (NRG), a non-perturbative method which yields the accurate low-temperature properties.

TT 33.37 Wed 15:00 Poster B

Charge carrier density at the (Na/K)TaO_3/$SrTiO_3$ interfaces — •Udo Schwingenschlögl and Safdar Nazir — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The formation of a quasi two-dimensional electron gas between the band insulators $NaTaO_3$ and $SrTiO_3$ as well as $KTaO_3$ and $SrTiO_3$ is studied by means of the full-potential linearized augmented plane-wave method of density functional theory. Optimization of the atomic positions points to only small changes in the chemical bonding at the interface. The creation of metallic interface states thus is not affected by structural relaxation but can be explained by charge transfer between transition metal and oxygen atoms. It is to be expected that a charge transfer is likewise important for related interfaces such as $LaAlO_3/SrTiO_3$. Both the p-type $(NaO)^-/(TiO_2)^0$ and n-type $(TaO_2)^+/(SrO)^0$ interfaces in $NaTaO_3/SrTiO_3$ are found to be metallic with strongly enhanced charge carrier densities as compared to the respective interfaces in $KTaO_3/SrTiO_3$. The effects of O vacancies are discussed. Spin-polarized calculations point to the formation of isolated O 2p magnetic moments, located in the metallic region of the p-type interface. The systems under investigation are suitable for disentangling the complex behavior of metallic interface states, since the structural relaxation is small.

TT 33.38 Wed 15:00 Poster B

Preparation and characterization of $LaAlO_3/SrTiO_3$ heterostructures — •Ahmed Sleem[1,2], Dirk Fuchs[1], Rudolf Schneider[1], and Hilbert von Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Fakultät für Physik, 76031 Karlsruhe, Germany — [3]Karlsruher Institut für Technologie, Physikalisches Institut, 76031 Karlsruhe, Germany

Thin films of $LaAlO_3$ were grown epitaxially by pulsed laser deposition on TiO_2 terminated <001> oriented $SrTiO_3$ substrates. The deposition parameters, i. e., substrate temperature T_S, oxygen partial pressure $P(O_2)$ and the laser fluence F on the target were optimized with respect to the interface conductivity of the heterostructure. For this purpose, contacts through the $LaAlO_3$ layer were prepared by argon ion-etching down to the interface and subsequent hole-filling with Pt or direct bonding of Al-wires. Metallic behavior down to $T = 4.2$ K was found only in a very narrow range of T_S, F and $P(O_2)$. Experimental results with respect to the characterization of the surface and substrate termination, the structural properties and interface conductivity obtained by atomic force microscopy, x-ray diffraction and high resolution electron microscopy, and resistivity measurements, respectively, will be presented and discussed.

TT 33.39 Wed 15:00 Poster B

Torque magnetometry on $SrTiO_3$-$LaAlO_3$ heterostructures — •Matthias Brasse[1], Rainer Jany[2], Marc A. Wilde[1], and Dirk Grundler[1] — [1]Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str.1, D-85747 Garching b. München, Germany — [2]Experimentalphysik VI, Institut für Physik, Universität Augsburg

Two-dimensional electron systems (2-DESs) have been found to form at the interface between the otherwise insulating oxides $LaAlO_3$ and $SrTiO_3$. The strongly correlated electron system shows a metallic phase and coexistence of superconductivity and magnetism at low temperatures. To explore the nature of the magnetic phase we use highly sensitive micromechanical torque magnetometry. This technique allows us to address different phenomena such as the de Haas-van Alphen effect, dia- and paramagnetism in superconducting states as well as magnetic hysteresis and anisotropy in case of correlated magnetism. Methods and results of ongoing measurements will be presented. We thank R. Jany and the group of J. Mannhart from the University of Augsburg for sample preparation. This work is supported by the DFG via TRR 80.

TT 33.40 Wed 15:00 Poster B

Thin film $YBa_2Cu_3O_7$ junctions with $La_{2/3}Ca_{1/3}MnO_3$ barrier — •Matthias Hepting, Andreas Stöhr, Robert Werner, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut – Experimentalphysik II and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

We report on the fabrication and electric transport properties of thin film $YBa_2Cu_3O_7$ (YBCO) junctions with $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) barrier. Heteroepitaxial YBCO/LCMO/YBCO multilayers were grown in-situ by pulsed laser deposition and subsequently patterned by photolithography and Ar ion milling to form rectangular junctions with typical area $5\,\mu m \times 30\,\mu m$. A self-alignment process was used for electrical contact via an Au wiring layer to the upper YBCO electrode, smilarly as decribed in [1]. Samples were characterized at temperature $T = 4.2$ K either in magnetically shielded environment or in in-plane magnetic fields B up to the Tesla range. We will present and discuss current-voltage-characteristics and measurements of critical current vs B.

[1] J. Tomaschko et al., Phys. Rev. B **84**, 064521 (2011).

TT 33.41 Wed 15:00 Poster B

$YBa_2Cu_3O_7$ nanoSQUIDs for detection of small spin systems — •Tobias Schwarz[1], Joachim Nagel[1], Roman Wölbing[1], Matthias Kemmler[1], Siegfried Menzel[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany

We report on the fabrication and characterization of nanopatterned $YBa_2Cu_3O_7$ (YBCO) SQUIDs with grain boundary junctions (GBJs) for the investigation of small spin systems at 4 K and below. We use photolithography and Ar ion milling to prepattern bridges (several μm wide) in a YBCO/Au (50 nm/60 nm) bilayer across the grain boundary of a $SrTiO_3$ bicrystal substrate. Subsequently the final SQUID geometry with junction widths down to 80 nm is patterned by focused ion beam (FIB) milling, without significant reduction of critical current density ($j_c > 10^5$ A/cm^2 at 4.2 K) [1]. The Au layer serves as a shunt resistor to provide overdamped GBJs and protects the YBCO during the FIB process. We obtained a flux noise down to $S_\Phi^{1/2} \approx 600\,n\Phi_0/Hz^{1/2}$, corresponding to an estimated spin sensitivity $S_\mu^{1/2} \approx 65\,\mu_B/Hz^{1/2}$

[1] J. Nagel *et al.*, Supercond. Sci. Technol. **24**, 015015 (2011).

TT 33.42 Wed 15:00 Poster B

Wachstumsbedingungen und Eigenschaften von YBCO-Schichten mit Au-Nano Partikeln — •Markus Westerhausen[1], Christian Katzer[1], Romina Diener[1], Ingo Uschmann[2], Frank Schmidl[1], Markus Rettenmayr[3] und Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Deutschland — [2]Friedrich-Schiller-Universität Jena, Institut für Optik und Quantenelektronik, Max-Wien-Platz 1, 07743 Jena, Deutschland — [3]Friedrich-Schiller-Universität Jena, Institut für Materialwissenschaft und Werkstofftechnologie, Löbdergraben 32, 07743 Jena, Deutschland

Gegenstand der vorgestellten Untersuchungen ist die Herstellung und Charakterisierung dünner $YBa_2Cu_3O_{7-x}$ (YBCO) Schichten, die unter dem Einfluss von Au-Nanopartikeln auf einkristallinen STO-Substraten aufwachsen. Durch Variation der Beschichtungsparameter der lasergestützten Abscheidung ($P(O_2)$, TS, Laserenergie, Au-Ausgangsschichtdicke, YBCO-Schichtdicke) ist es möglich, sowohl die elektrischen Eigenschaften der YBCO-Schicht als auch die Größe und Verteilung der Au-Partikel zu verändern. Wir stellen strukturelle Untersuchungen (X-Ray, REM, AFM ,TEM) ebenso wie elektrische (J_c, T_c) Messungen an den hergestellten Schichten vor.

TT 33.43 Wed 15:00 Poster B

Grain boundary high-T_c dc-SQUIDs with self-organized nanocrystals — •Stefanie Koch, Peter Michalowski, Christian Katzer, Markus Westerhausen, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Deutschland

We fabricated and investigated direct current superconducting quantum interference devices (dc-SQUIDs) based on $YBa_2Cu_3O_{7-x}$ (YBCO) grain boundary Josephson junctions. Directed embedding of gold nanoparticles different sizes can modify the crystalline structure and thus the superconducting properties of the YBCO thin films and grain boundaries. We investigated the growth conditions of these particles as well as their influence on the properties of the YBCO thin films. The variation of the size and distribution of the gold nanoparticles changes the electrical properties of the dc-SQUIDs. For this kind of device the normal resistance, critical current density, the resulting I_cR_N-product, the London penetration depth and transfer function are analyzed. Furthermore we will show noise properties for such modified dc-SQUIDs.

TT 33.44 Wed 15:00 Poster B

Characterization of directly coupled $YBa_2Cu_3O_{7-x}$ SQUID magnetometers — •Alexander Guillaume, Verena Beister, Jan M. Scholtyssek, Frank Ludwig und Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany.

Superconducting Quantum Interference Devices (SQUIDs) can be employed as highly sensitive magnetic field sensors in a variety of applications such as magnetoencephalography or magnetic nanoparticle detection. We fabricated SQUIDs from the high-T_c superconductor $YBa_2Cu_3O_{7-x}$ on symmetric $SrTiO_3$-bicrystal substrates by pulsed laser deposition and argon ion etching. The layout consists of two directly coupled magnetometers on one chip which are attached to a rectangular pickup loop.

The measurements were carried out in a liquid nitrogen container using a variable temperature insert. The temperature at the magnetically shielded sample holder can be adjusted between 77 K and 100 K. Here, we present measurements of the I-V-curves under the influence of a magnetic field for different sample temperatures. Also, the influence of the temperature and the influence of the bias current on the V-

Φ-curves were investigated. From these measurements, parameters of the SQUID were calculated and compared to the theoretical estimations. Additionally, noise spectra were recorded for different bias reversal frequencies by using a direct-coupled flux-locked loop electronics from Magnicon GmbH.

TT 33.45 Wed 15:00 Poster B

Cooper pair and quasiparticle transport in Josephson junction chains — •Roland Schäfer[2], Andreas Fiebig[1], Birgit Kiessig[2,1], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology — [2]Institut für Festkörperphysik, Karlsruhe Institue of Technology

We present measurements of IV characteristics of daisy-chained mesoscopic SQUID loops where the charging energy is of the same order as the Josephson coupling energy at zero magnetic field. At low voltages the transport is suppressed to a level below the detection limit. Above a threshold V_{sw} the system jumps to a resistive brunch. The effective Josephson coupling along the chain can be modulated by a magnetic field. The field dependence of the IV characteristics gives evidence that the current is carried dominantly by Cooper pairs. Yet, the smooth transition to quasiparticle dominated transport at large bias hints towards a dissipation mechanism that involves generation and incoherent transport of the latter at any finite current even for voltages well bellow $2N\Delta$, where N is the number of Josephson junctions in the chain and Δ is the superconducting energy gap.

TT 33.46 Wed 15:00 Poster B

Fabrication of Flux Qubits and Resonators for their Dispersive Readout — •Anastasia V. Shcherbakova[1], Kirill G. Fedorov[1], Roland Schäfer[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut and DFG-Centrum für Funktionelle Nanostrukturen (CFN), Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76344 Eggenstein-Leopoldshafen, Germany

The dispersive readout of a superconducting qubit gives the possibility to read it out without damaging the quantum state space. The idea of dispersive readout with the help of a resonator is based on the shift of the resonator frequency depending on the state of the qubit coupled to it. This work is devoted to the fabrication of flux qubits coupled to different types of resonators - linear $\lambda/4$ resonators and non-linear resonators. We will present preliminary results on measurements of superconducting quantum bits in these schemes. We are also concerned with developing a scalable readout scheme using a quantum cavity bus.

TT 33.47 Wed 15:00 Poster B

Influence of mechanical strain on coherent atomic tunneling systems investigated by Josephson phase qubits — •Torben Peichl[1], Grigorij J. Grabovskij[1], Jürgen Lisenfeld[1], Georg Weiss[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, KIT, 76131 Karlsruhe — [2]DFG Centrum für Funktionelle Nanostrukturen, KIT, 76131 Karlsruhe

Forty years ago Zeller and Pohl discovered a fundamental difference of the heat capacity of glassy materials compared to their crystalline counterparts. Only one year later Anderson, Halperin and Varma attributed this behavior to two-level systems (TLSs), which are formed by the two lowest energy states of atoms tunneling in a double-well potential. This idea was the basis for the so-called tunneling model which despite its totally empiric nature proved to be very successful in describing the universal properties of dissordered materials at temperatures below 1 K. — It is believed that those TLSs also present in the thin disordered oxide barrier of Josephon junctions, used e.g. in the design of phase qubits, are the main reason for decoherence and thus limit the lifetime of the macroscopic quantum state.

Here we present a method that for the first time allowed the investigation of individual coherent atomic TLSs. We apply strain by in situ bending the chip with the phase qubits and studying the so-called "avoided-level-crossings" in the qubit spectrum that are caused by the resonant coupling between the phase eigenstates and coherent TLSs. As a result we can extract their properties that are in good agreement with the tunneling model.

TT 33.48 Wed 15:00 Poster B

Comparing coherence time of Josephson junction phase qubits made of different materials — •Kirill Lakhmanskiy[1,2], Jürgen Lisenfeld[2], and Alexey V. Ustinov[2] — [1]Kotel'nikov Institute of Radio Engineering and Electronics, Russian Academy of Sciences, 125009 Moscow, Russia — [2]Physikalisches Institut, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

Superconducting phase qubits suffer from energy relaxation which occurs predominantly in the dielectrics used to insulate the qubit junction or to make a shunt capacitor. This is verified from our measurements on phase qubits made using either SiO_x or SiN_x dielectrics. The latter circuits achieve an energy relaxation time T_1 of about 40 ns which is 8 times longer than for the identically made SiO_x circuits. We also plan to explore an alternative idea to replace the lossy tunnel junction by a nanowire, leaving the shunt capacitor unchanged. Such a qubit circuit can be fabricated without junction dielectric and should thus achieve longer coherence times.

TT 33.49 Wed 15:00 Poster B

Charge transport through 1D arrays of small capacitance Josephson junctions — •Jochen Zimmer[1], Andreas Fiebig[1], Roland Schäfer[2], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology — [2]Institut für Festkörperphysik, Karlsruhe Institute of Technology

We investigate one-dimensional arrays of small capacitance Josephson junctions, fabricated by conventional e-beam lithography techniques. These arrays can serve as model systems for the study of superconductor-insulator transitions as found in thin disordered superconducting films. For sufficiently low Josephson energy, the arrays we fabricated exhibit a pronounced Coulomb blockade, i.e. insulating behavior. We studied the transport properties of the arrays in a voltage-bias setup. Data taken at several array lengths and different temperatures in the Coulomb blockade regime and at finite conductance will be presented.

TT 33.50 Wed 15:00 Poster B

Supercurrent in Nb/Au-nanowire/Nb Josephson junctions — •Nick Borgwardt[1,2], Yusuf H. Günel[1,2], Huijun Yao[1,3], Gregor Panaitov[4], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2,5] — [1]Peter Grünberg Institute -9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, People's Republic of China — [4]Peter Grünberg Institute -8, Forschungszentrum Jülich, 52425 Jülich, Germany — [5]II. Physikalisches Institut, RWTH Aachen University,52056 Aachen, Germany

Josephson junctions and SQUIDs were fabricated using single crystalline gold nanowires (NWs), grown by electrochemical deposition. The diameter of the NWs ranged from 80 to 140nm with a length of several μm. Devices with an electrode distance ranging from 80 to 300nm were fabricated by electron beam lithography and subsequent Nb sputtering.

Electrical measurements were carried out in a ^{3}He cryostat at temperatures between 0.3 and 6K. From the current-voltage characteristics of the junctions a critical current as high as I_c 60μA at 0.4K was deduced. Measurements of the critical current depending on temperature and magnetic field give insights into the fundamental transport properties. Analyzing the differential resistance we observed pronounced sub-gap peaks which we assigned to Andreev reflections.

TT 33.51 Wed 15:00 Poster B

Mesoscopic conductance and critical current fluctuations in Nb/InAs-nanowire/Nb Josephson Junctions — Yusuf H. Günel[1,2], •Igor Batov[3], Hilde Hardtdegen[1,2], Kamil Sladek[1,2], Andreas Winden[1,2], Karl Weis[1,2], Gregor Panaitov[4,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2,5] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432 Moscow district, Russia — [4]Peter Grünberg Institut (PGI-8), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [5]II. Physikalisches Institut, RWTH Aachen, 52056 Aachen, Germany

We report on the experimental study of mesoscopic Josephson junctions based on InAs nanowires and niobium superconducting electrodes. The gate voltage and magnetic field dependent measurements revealed pronounced conductance and critical current fluctuations. We found that the pattern of the conductance fluctuations as a function of gate voltage follows precisely the fluctuations of the Josephson critical current. It has been found that the conductance fluctuation amplitude in Nb/InAs-nanowire/Nb samples significantly exceeds the amplitude of the normal-state universal conductance fluctuations (UCF) in the

reference samples with normal conducting Au/Ti contacts. We attribute the enhancement of the conductance fluctuations in nanowires contacted with superconductors to the contribution of phase-coherent Andreev reflection.

TT 33.52 Wed 15:00 Poster B

Kritische Stromdichte von Josephson-Kontakten mit NbSi-Barriere in Abhängigkeit von Temperatur, Magnetfeld und Zusammensetzung — •Thomas Scheller, Müller Franz, Wendisch Rüdiger, Kieler Oliver, Störr Kathrin, Weimann Thomas, Egeling Bert und Kohlmann Johannes — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig

Josephson-Kontakte werden u.a. zur Erzeugung von quantengenauen Referenzspannungen eingesetzt. An der PTB werden dazu seit einigen Jahren überdämpfte Josephson-Kontakte mit einer Barriere aus amorphem Nb_xSi_{1-x} eingesetzt. Dieses Material zeigt einen Metall-Halbleiter-Übergang bei x=11,5%. Durch Anpassung der Barrierendicke d und des Niob-Gehaltes x können kritische Stromdichte und charakteristische Spannung des Josephson-Kontaktes nahezu unabhängig voneinander eingestellt werden. Wir haben Kontakte mit Barrierenzusammensetzungen auf beiden Seiten des Metall-Halbleiter-Überganges untersucht und die Abhängigkeit der kritischen Stromdichte von Temperatur und externem Magnetfeld gemessen. Dabei haben wir festgestellt, dass dieser Typ von Josephson-Kontakten je nach Zusammensetzung der Barrieren als Tunnelkontakt oder als weak link arbeitet. Die Magnetfeldabhängigkeit der kritischen Stromdichte zeigt zum Teil deutliche Abweichungen vom Fraunhofer-Muster eines Kontaktes mit homogener Josephson-Stromverteilung.

Teilweise finanziert durch die EU. (ERA-NET Plus, Nr. 217257, JoSy-Projekt).

TT 33.53 Wed 15:00 Poster B

Nb/HfTi/Nb nanoSQUIDs with optimized spin sensitivity — •Matthias Rudolph[1], Roman Wölbing[1], Joachim Nagel[1], Matthias Kemmler[1], Reinhold Kleiner[1], Dieter Koelle[1], Oliver Kieler[2], Thomas Weimann[2], Johannes Kohlmann[2], and Alexander Zorin[2] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, 72076 Tübingen, Germany — [2]Fachbereich 2.4 , Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Nowadays the downscaling of SQUIDs to the submicron range is mainly motivated by applications for magnetization measurements of small magnetic systems like single magnetic molecules. We use SQUIDs based on Nb/HfTi/Nb junctions, which do not require bulky resistive shunts. The parameters of the junctions can be optimized for flux sensitive SQUIDs and the used nanolithography technique (e-beam) allows the realization of SQUID loops in the submicron range and junction sizes on the order of 100 nm. For some SQUIDs we implemented coils on the chip that are galvanically coupled to the SQUID loop. These coils allow to modulate the SQUIDs without the need of external coils with relatively small currents. This might be useful for the flux-locked operation of our SQUIDs using conventional SQUID electronics.

We present a detailed study of the transport properties and the flux noise characteristics of several SQUIDs with different designs (magnetometer-type or gradiometric) in low magnetic fields as well as magnetic fields up to 100 mT. For our best SQUID geometries we obtain a spin sensitivity $S_\mu^{1/2} = 29\,\mu_B/\mathrm{Hz}^{1/2}$.

TT 33.54 Wed 15:00 Poster B

Nonequilibrium Josephson and quasi-particle currents through hybrid superconductor-quantum dot devices — •Sascha Ratz and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We present a real-time diagrammatic theory for investigating the Josephson current through an interacting quantum dot coupled to two biased superconducting leads showing a phase difference Φ. Our nonequilibrium transport theory is based on the time evolution of the reduced density matrix obtained by integrating out the fermionic degrees of freedom in the leads. As an example we study a system described as a single-level Anderson impurity model in a two-terminal transistor geometry in the weak coupling regime. Here we investigate the interplay between quasiparticle cotunneling current and phase-driven Cooper-pair tunneling in second order in the tunnel-coupling strength Γ as well as in the limit of large superconducting gaps in the leads.

TT 33.55 Wed 15:00 Poster B

Transport through Andreev bound states in a triplet superconductor - ferromagnet - singlet superconductor Josephson junction — •Wei Chen[1], Philip M. R. Brydon[2], Yasuhiro Asano[3], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden — [3]Department of Applied Physics, Hokkaido University, Sapporo, 060-8628, Japan

We use microscopic Bogoliubov-de Gennes theory to study a model triplet superconductor - ferromagnet - singlet superconductor Josephson junction. We obtain analytic expressions for the Andreev bound state spectrum, and hence calculate the free energy minimum of the junction, and the spontaneous charge and spin currents. We find that these properties of the junction strongly depend upon the orbital pairing state of the two superconductors. The results are interpreted with the assistance of a tunneling Hamiltonian theory.

TT 33.56 Wed 15:00 Poster B

Proximity effects at the interface between chiral p-wave superconductors and ferromagnets — •Damien Terrade[1], Mario Cuoco[2], Paola Gentile[2], and Dirk Manske[1] — [1]Max Planck Institute For Solid State Research, Stuttgart, Germany — [2]CNR-SPIN, Fisciano (Salerno), Italy

We focus on an interface along the (001) direction. The system is made by a stack of two-dimensional layers, with a $\vec{d}$-vector perpendicular to the plane, which should be the first experimental configuration of the predicted Josephson junctions involving component like Sr_2RuO_4. The SC is described with an extended Hubbard model and the ferromagnetism is based either on a Stoner-like model [1,2] or on a change in the relative bandwidth of electrons for the two different spin polarizations[3]. We compute self-consistently the pairing potentials, the magnetization and the free energy as a function of the exchange field strength as well as the angle between the exchange field and the $\vec{d}$-vector. We have generalized the work done in [3] by including spin-flip process and magnetic impurities at the interface as well as a temperature dependence. We obtain in the FM layers no induced singlet components unlike interface along the (100) direction and strongly reduced oscillations for the triplet components.

[1] K. Kuboki. J. Phys. Soc. Jap. **70**, 9 (2001).
[2] B. M.Andersen, *et al.* Phys. Rev. B **77**, 054501 (2008).
[3] M. Cuoco, *et al.* Phys. Rev. B **78**, 054503 (2008).

TT 33.57 Wed 15:00 Poster B

Josephson-like spin current in junctions composed of antiferromagnets and ferromagnets — •Andreas Moor, Anatoly Volkov, and Konstantin Efetov — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We study Josephson-like junctions formed by materials with antiferromagnetic (AF) order parameters. As an antiferromagnet, we consider a two-band material in which a spin density wave (SDW) arises, e.g., the Fe-based pnictides in the temperature interval $T_c \leq T \leq T_N$, where T_c and T_N are the critical temperatures for the superconducting (S) and antiferromagnetic transitions, respectively. We have generalized the theory of quasiclassical Green's functions to two-band superconductors, in which superconducting and antiferromagnetic ordering may coexist, and derived the equations for the quasiclassical Green's functions. Especially, we are interested in the Josephson-like spin current in the AF/F/AF (F means a ferromagnet) structures, where the short- and long-range components can be identified. This is an analogy with the case of the Josephson current in an S/F/S junction with a non-homogeneous magnetization where short- and long-range condensate components are induced in the F-layer. However, the analogy is not complete due to the fact that the spin current in AF/F/AF junctions is not constant in space, but oscillates in the ballistic F-layer.

[1] A. Moor, A. F. Volkov, and K. B. Efetov, Phys. Rev. B **83**, 134524 (2011);
[2] A. M., A. F. V., and K. B. E., arXiv:1111.5582;
[3] F. S. Bergeret, A. F. Volkov, K. B. Efetov, Rev. Mod. Phys. **77**, 1321 (2005);
[4] M. Eschrig, Physics Today, **64**, 43 (2011).

TT 33.58 Wed 15:00 Poster B

AC Josephson current through quantum dots — •Bastian Hiltscher[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE — [2]School of Chemical and Physical Sciences and MacDiarmid Institute

for Advanced Materials and Nanotechnology, Victoria University of Wellington

We consider a setup consisting of two superconductors linked by a single-level quantum dot with strong Coulomb repulsion. An AC Josephson current is generated by applying a bias voltage to the superconductors. Our formalism bases on a diagramatic perturbation expansion in tunnel coupling [1], where the quasiparticle states are traced out from the total density matrix and the quantum dot as well as the Cooper pair condensates are treated explicitly. The Coulomb repulsion is taken into account nonperturbatively. We find that the first harmonic dominates the higher ones. Furthermore, we discuss the differences between the AC and the DC Josephson effect.
[1] M. Governale, M. G. Pala, and J. König, PRB 77, 134513 (2008).

TT 33.59 Wed 15:00 Poster B

Influence of finite superconducting gaps on the proximity effect in interacting quantum dots — •David Futterer[1], Jacek Swiebodzinski[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg Essen and CeNIDE, 47048 Duisburg, Germany — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington, New Zealand

The tunnel coupling of superconductors to an interacting quantum dot leads to the formation of Andreev-bound states (ABS), which are the excitation energies of the proximized dot. In the limit of large superconducting gaps in the leads, $\Delta \to \infty$, the hybrid system of dot and superconductors can be described exactly by an effective Hamiltonian.

Since in real systems the superconducting gap is usually not a large quantity it is an interesting question whether the predictions of the $\Delta \to \infty$ calculations still have significance for real systems with finite gaps. In order to investigate this question we perform two different calculations: first, a systematic $1/\Delta$ expansion where we find that the occurring currents show only small changes but we find indications that a finite Δ renormalizes the ABSs. To quantify the last statement we perform a second calculation where we resum the coupling to the superconductors at arbitrary values for Δ neglecting vertex corrections.

TT 33.60 Wed 15:00 Poster B

Josephson current through a quantum dot coupled to a nanomagnet — •Pascal Stadler, Cecilia Holmqvist, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Magnetically tunable nanoscale Josephson junctions have recently drawn increased attention since they offer interesting perspectives for superconducting spintronics [1]. We theoretically study the transport through a junction consisting of two superconducting electrodes and a quantum dot which is coupled to a nanomagnet. A magnetic field applied to the central region lifts the spin degeneracy of the energy levels on the dot and starts a precession of the nanomagnet's magnetization with the Larmor frequency. This precession induces spin flips as well as a renormalization of the Zeeman splitting on the dot. The transport properties are calculated using a non-equilibrium Green's function approach. We show how the density of states on the dot is modified due to the nanomagnet and present the results for the current-phase relation. The current can be either suppressed or enhanced depending on the precession frequency, the coupling strength and the angle between the direction of the nanomagnet's magnetization and the magnetic field. Tuning the precession frequency can also cause the junction to undergo a 0 to π transition.
[1] C. Holmqvist, S. Teber, and M. Fogelström, Phys. Rev. B **83**, 104521 (2011)

TT 33.61 Wed 15:00 Poster B

Multiply gapped density of states in a normal metal in contact with a superconductor — •Johannes Reutlinger[1], Yuli V. Nazarov[2], Leonid I. Glazman[3], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Kavli Institute of Nanoscience Delft, Delft University of Technology, 2628 CJ Delft, Netherlands — [3]Department of Physics, Yale University, New Haven CT 06511-8499, USA

The spectral properties of a normal metal adjacent to a superconductor are strongly dependent on the characteristic mesoscopic energy scale - the Thouless energy E_{Th} - and the strength of the connection. In this work, we predict that the local density of states (LDOS), besides the well know minigap $\sim E_{Th}$, can exhibit a multiple gap structure, which strongly depends on the type of the contact. For ballistic contacts we calculate these secondary gaps analytically in the framework of quantum circuit theory of mesoscopic transport. The secondary gaps are absent in the case of tunnel contacts. In the general case the equations are solved numerically for more realistic contacts, like for example diffusive connectors or dirty interfaces, which are characterized by continuous distributions of transmission eigenvalues between 0 and 1. We find that the gap vanishes in these cases, but the density of states is still suppressed around the superconducting gap edge. Distribution functions with a stronger weight at higher transmissions can be modeled through asymmetric ballistic double junctions, which even exhibit multiple gaps. Such spectral signatures are fundamental to disordered nanoscopic conductors and experimentally accessible.

TT 33.62 Wed 15:00 Poster B

Long-range spin transport in superconductors — •Detlef Beckmann[1], Florian Hübler[2], Michael J. Wolf[1], and Hilbert von Löhneysen[2,3] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [3]Physikalisches Institut, Karlsruher Institut für Technologie

Recently, there has been some controversy about spin-polarized quasiparticle transport and relaxation in superconductors, with reports of both anomalously short [1] or anomalously long [2] relaxation times as compared to the normal state. Here, we report on non-local transport in multiterminal superconductor-ferromagnet structures. We find signatures of spin transport over distances much larger than the normal-state spin-diffusion length in the presence of a large Zeeman splitting of the quasiparticle states. The relaxation length shows a nearly linear increase with magnetic field, hinting at a freeze-out of spin relaxation by the Zeeman splitting.
[1] Poli et al., Phys. Rev. Lett. **100**, 136601 (2008)
[2] Yang et al., Nature Materials **9**, 586 (2010)

TT 33.63 Wed 15:00 Poster B

Proximity effect between a ferromagnetic insulator and a superconductor — •Michael J. Wolf[1], Florian Hübler[1,2], Christoph Sürgers[3], Detlef Beckmann[1], and Hilbert v. Löhneysen[2,3] — [1]Institut für Nanotechnologie, KIT — [2]Institut für Festkörperphysik, KIT — [3]Physikalisches Institut, KIT

Electron transfer through spin-active interfaces can be modeled by the transmission amplitudes and a relative phase shift between spin-up and spin-down wavefunctions, the spin-mixing angle [1]. Recently, Andreev bound states have been observed in F/S tunnel contacts which imply a non-zero spin-mixing angle of the ultrathin F/S barrier [2]. In order to separate the spin-active interface from the detector tunnel contact, we have fabricated normal metal / superconductor tunnel contacts on top of a ferromagnetic insulator. We prepared EuS thin films (d $\approx$ 20 nm) on top of Si(111) substrates by means of e-beam evaporation and created Al / Al-Oxide / Cu tunnel contacts by means of shadow evaporation. In an applied magnetic field, the tunnel spectra show an enhanced Zeeman splitting which is due to the presence of the exchange field of the EuS layer [3]. Furthermore, we observe small peaks in the subgap region of the tunnel spectra which may be attributed to Andreev bound states due to a non-zero spin-mixing angle at the EuS / Al interface. The results suggest the use of EuS thin films for generating equal-spin triplet superconductivity.
[1] T.Tokayasu *et al.* Phys. Rev. B **38**, 8823 (1988)
[2] F. Hübler *et al.* arXiv:1012.3867 (2010)
[3] X. Hao *et al.* Phys. Rev. Lett. **67**, 1342 (1991)

TT 33.64 Wed 15:00 Poster B

Ferromagnet/superconductor hybrids with out-of-plane magnetization: comparison of current-in-plane and current-out-of-plane measurements — •Richard Montbrun[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruhe Institute of Technology, Physikalisches Institut and Center for Functional Nanostructures, D-76049 Karlsruhe — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik, D-76021 Karlsruhe

Ferromagnet (F)/superconductor (S)/F hybrid structures - with S = Nb and Co/Pt multilayers as F electrodes - were fabricated by e-beam lithography and reactive ion-etching using silicon-nitride shadow masks on Si/SiO_2. The sample layout allows four-point resistivity measurements with the current perpendicular to the F/S interface. In addition, planar F/S/F multilayers were prepared for current-in-plane measurements. The dependence of the superconductive transition temperature T_c on the relative orientation of the two F-layer magnetizations (par-

allel or antiparallel) was investigated for different S-layer thicknesses and transport currents. For current out of the plane T_c is always higher in the antiparallel configuration than in the parallel configuration whereas for current in the plane we observe a peculiar influence of the transport current amplitude on the spin-switch behavior. This indicates a different pair breaking in the two layouts.

TT 33.65 Wed 15:00 Poster B

Long-range triplet pairing in superconductor-ferromagnet proximity effect heterostructures — •V. Zdravkov[1,2], J. Kehrle[1], G. Obermeier[1], D. Lenk[1], H.-A. Krug von Nidda[1], C. Müller[1], M.Yu. Kupriyanov[3], A.S. Sidorenko[2], S. Horn[1], R. Tidecks[1], and L.R. Tagirov[1,4] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]Institute of Electronic Engineering and Nanotechnologies ASM, Kishinev MD-2028, Moldova — [3]Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow 119992, Russia — [4]Solid State Physics Department, Kazan Federal University, 420008 Kazan, Russia

For superconductor-ferromagnet (S-F) heterostructures with two or more F-layers, the generation of a long-range, odd-in-frequency triplet pairing at non-collinear (NOC) alignment of the F-layers magnetizations is predicted [1]. Here, we report on the first experimental observation of the triplet pairing in a $Nb/Cu_{41}Ni_{59}/Nb/Co/CoO_x$ spin-valve type proximity effect heterostructure, where a very thin Nb layer between the F materials acts as a normal conducting spacer. Measuring the resistance of the samples as a function of an external magnetic field, we observed a sequence of transitions through normal conducting (NC) and superconducting (SC) phases, when the system goes along the magnetic hysteresis loop. The scenario found during the NOC regime is consistent with the theoretical picture of the singlet superconductivity suppression by the long-range triplet pairing generation [2].

[1] F.S. Bergeret, et al. Rev. Mod. Phys. 77, 1321 (2005).
[2] Ya.V. Fominov, et al. JETP Lett. 91, 308 (2010).

TT 33.66 Wed 15:00 Poster B

Development of a large-area detector for position and energy resolving detection of molecular fragments — •Alexandra Kampkötter, Andreas Fleischmann, Loredana Gastaldo, Sebastian Kempf, Andreas Pabinger, Christian Pies, Sönke Schäfer, Thomas Wolf, and Christian Enss — Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

The recombination of a molecular cation with an electron, followed by fragmentation, is a fundamental reaction in cold, dilute plasmas and plays a key role in interstellar chemistry. To investigate such reactions in laboratory environment with full quantum control, the Max-Planck Institute for Nuclear Physics in Heidelberg is building a cryogenic storage ring to prepare molecular ions in their groundstate. The full kinematics of these recombination processes can be resolved by a position and energy sensitive detection of the reaction products/molecule fragments. We describe the development of a new large-area MMC for position sensitive detection of massive particles with kinetic energies down to a few keV. The detector encompasses sixteen pie-shaped large-area absorbers to form a circular whole with a diameter of 36mm. The temperature sensor is positioned on the outer edge of each absorber. The rise-time of the detector signals varies with the impact location of the particle due to diffusive expansion of heat in the absorbers. We present results of first test measurements where energy was deposited in the absorber at different positions by light pulses from three LEDs. The observed position dependence of the signal shapes agrees well with the one expected from detailed thermal simulations.

TT 33.67 Wed 15:00 Poster B

Low temperature particle detectors with magnetic penetration thermometers — •N. Foerster, D. Hengstler, A. Kampkötter, S. Kempf, C. Pies, G. Pizzigoni, P. Ranitzsch, S. Schäfer, S. Uhl, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

We present low temperature micro-calorimeters based on a novel sensor concept, the Magnetic Penetration Thermometers (MPTs). The MPTs make use of the temperature dependence of the critical magnetic field and the penetration depth of a superconducting sensor. The superconducting sensor is inductively coupled to a superconducting pick-up coil which also provides a bias magnetic field. The flux in the pick-up coil depends on the position of the interface between normal and superconducting regions in the sensor which in turn is a steep function of temperature. The change of magnetic flux upon the absorption of a particle is read-out by low-noise high-bandwidth dc-SQUIDs. Similar to metallic magnetic calorimeters, MPTs operate in a wide range of temperature and without intrinsic bias power dissipation.

We present the results of numerical simulations for the signal size and energy resolution for various superconducting films based on a simple thermo-dynamical model, as well as first experimental results.

TT 33.68 Wed 15:00 Poster B

Study of the Energy Thermalisation in Superconducting Absorbers by Means of Low Temperature Magnetic Calorimeters — •Daniel Hengstler, Philipp C.-O. Ranitzsch, Jan-Patrick Porst, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University INF 227, 69120 Heidelberg, Germany

The use of superconducting particle absorbers for low temperature micro-calorimeters promises several advantages like the possibility to combine high stopping power with low heat capacity. Due to the still not well understood thermalization of the energy released by the interacting particle, superconducting absorbers are used only in special cases. We investigated by means of metallic magnetic calorimeters the temperature response of the paramagnetic sensor following the absorption of an x-ray in a superconducting absorber. We analyzed the pulse shape as function of temperature for different absorber materials: rhenium, aluminum and aluminum doped with 600ppm manganese, zinc and zinc doped with 24ppm Mn. The doping with manganese was performed in order to understand the role of magnetic impurities in the thermalization of energy. We discuss the temperature dependence of the energy thermalization in superconducting absorbers at the light of presently available theories.

TT 33.69 Wed 15:00 Poster B

A high-resolution mK-calorimeter applying SQUID-thermometry — •Andreas Reifenberger, Norman Leps, Andreas Fleischmann, Christian Pies, Christian Enss, and Rüdiger Klingeler — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227,69120 Heidelberg, Germany

A new calorimeter for measuring single-crystalline samples of mg-size at ultra-low temperatures is described. Thermometry is done by means of a paramagnetic sensor material (Er-doped Au) in a low magnetic field. A temperature change results in a magnetization change which can be read out as change in magnetic flux by a superconducting quantum interference device (SQUID). This enables measurements in a wide temperature range (theoretically from 1 mK - 1 K) with very high sensitivities. The bolometric design exhibits low addenda heat capacity and allows measurements of heat capacities from nJ/K to μJ/K by means of a temperature-relaxation method. The performance of the device is compared to a commercially available Quantum Design calorimeter in elsewise unchanged experimental settings in the temperature range from 15 mK to 500 mK.

TT 33.70 Wed 15:00 Poster B

A Low-Temperature Scanning Polarizing Microscope for Magneto-Optical Imaging — •Matthias Grünzweig, Stefan Guénon, Matthias Kemmler, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

We present the design and preliminary results on the performance of a low-temperature scanning polarizing microscope (LTSPM), which has been developed for research on thin film devices based on ferromagnets (F), superconductors (S) and S-F-hybrid structures. The LTSPM is based on confocal laser microscopy for imaging at temperatures from 4 K to 300 K in magnetic fields up to 0.5 T (in plane) and 5 T (out-of-plane). The LTSPM allows to combine imaging of electrical transport properties (via beam-induced voltage change) with imaging of magnetic structures (via Kerr-/Faraday-effect).

The LTSPM can be applied to research on a broad variety of devices, such as Kerr microscopy on ferromagnetic thin film structures, e.g. magnetic tunnel junctions or S-F heterostructures. Using a magneto-optical sensor layer (e.g. EuSe or an Fe-garnet single crystal) for imaging the magnetic stray field above the sample, the LTSPM shall be used for the investigation of vortex distributions in type-II superconductor thin film devices.

TT 33.71 Wed 15:00 Poster B

Modulated Intensity Spin Echo: μeV resolution for dynamics in magnetic samples — •Georg Brandl[1,2], Robert

Georgii[2], Wolfgang Häussler[2], and Peter Böni[1] — [1]Physik Department E21, Technische Universität München, D-85748 Garching — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, D-85748 Garching

The MIEZE technique (Modulation of IntEnsity by Zero Effort) [1,2] is a variant of the neutron spin echo technique [3] that achieves the same very high energy resolution by converting a neutron spin oscillation into a high-frequency modulation of the neutron beam. Because all beam preparation is done before the sample, MIEZE is well suited to measuring magnetic samples, even in high magnetic fields, both of which are unfavorable conditions for measurements with conventional neutron spin echo. Here, an introduction is given to the MIEZE principle and presents setup and measurements performed with MIEZE in magnetic fields, both at the FRM II in Munich [4] and at the HFIR in Oak Ridge [5]. Also discussed is the design of a drop-in MIEZE module that can be added to existing neutron instruments.

[1] R. Golub and R. Gähler, Phys. Lett. A 123(1), 43, 1987.
[2] R. Gähler, R. Golub and T. Keller, Physica B 180-181(2), 899, 1992.
[3] F. Mezei, Z. Phys. A 255(2), 146, 1972.
[4] R. Georgii, G. Brandl, N. Arend, A. Tischendorf, W. Häußler, C. Pfleiderer, P. Böni and J. Lal, Appl. Phys. Lett. 98(8), 2011.
[5] G. Brandl, J. Lal, J. Carpenter, L. Crow, L. Robertson, R. Georgii, P. Böni and M. Bleuel, accepted by Nucl. Inst. Meth. A, 2011.

TT 33.72 Wed 15:00 Poster B

Coherent broadband THz spectrometer using photomixers for accurate determination of complex dielectric function — •Malte Langenbach[1], Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Ernesto Vidal[1], Jennifer Marx[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Axel Roggenbuck[3], Anselm Deninger[3], Joachim Hemberger[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany; — [2]Max-Planck-Institut für Radioastronomie, Bonn, Germany; — [3]Toptica Photonics AG, Gräfelfing, Germany

We report on a novel cw THz spectrometer for measurements in high magnetic fields and at low temperatures. The spectrometer employs photomixing of two NIR lasers for generation and phase-sensitive detection of THz radiation from 60 GHz to 1.8 THz. A fast phase-modulation technique using two fiber stretchers is used to determine the amplitude and the phase at a given frequency with excellent reliability. The phase accuracy is increased with further implementation of a third laser which enables correction of phase drifts mainly caused by thermal drifts. Thus, the complex dielectric function can be determined very accurately with a very high resolution in the MHz range. This compact spectrometer in combination with the magneto-cryostat allows for investigations in magnetic fields up to 8 T and temperatures down to 3 K with excellent reliability. Various aspects of the above-mentioned developments will be outlined.

TT 33.73 Wed 15:00 Poster B

Broadband dielectric spectroscopy on transition metal oxides: Is $LuFe_2O_4$ ferroelectric? — •Daniel Niermann[1], Joost de Groot[2], Manuel Angst[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, 50937 Köln — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The mixed valence system $LuFe_2O_4$ was proposed to show a novel type of ferroelectricity based on charge order within triangular Fe-O-double layers at 330 K [1]. However, an unambiguous evidence for ferroelectricity by means of dielectric polarization measurement, e.g. hysteretical P-E-loops, is difficult to give due to the relatively high residual conductivity in this material. We show results of temperature-dependent dielectric measurements on the potentially multiferroic material $LuFe_2O_4$ in a broad frequency range from mHz to GHz. Our measurements on a singlecrystalline sample [2] show very high magnitudes of both real and imaginary part of complex permittivity, decreasing towards low temperatures and high frequencies according to those reported in literature [1]. However in the temperature range from 200 - 400 K this dispersive behaviour is well-described by a standard equivalent-circuit model considering Maxwell-Wagner-type contacts and variable range hopping AC-conductivity, without a pronounced contribution of intrinsic dipolar polarization and thus the ferroelectric character of the charge order in $LuFe_2O_4$ has to be questioned. (*Work supported by DFG through SFB 608.*

[1] N. Ikeda et al., Nature **436**, 1136 (2005)
[2] M. Angst et al., PRL **101** (2008), 227601

TT 33.74 Wed 15:00 Poster B

High-magnetic-field investigation of $CoCr_2O_4$ — •A. V. Pronin[1], M. Uhlarz[1], R. Beyer[1], T. Fischer[1], J. Wosnitza[1], B. P. Gorshunov[2,3,4], G. A. Komandin[2], A. S. Prokhorov[2,3], M. Dressel[4], A. A. Bush[5], and V. I. Torgashev[6] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]A. M. Prokhorov Institute of General Physics, Russian Academy of Sciences, Moscow, Russia — [3]Moscow Institute of Physics and Technology (State University), Russia — [4]1. Physikalisches Institut, Universität Stuttgart, Germany — [5]Moscow Institute of Radiotechnics, Electronics, and Automation, Russia — [6]Faculty of Physics, Southern Federal University, Rostov-on-Don, Russia

We report on magnetic, optical, and thermodynamic properties of multiferroic $CoCr_2O_4$ in magnetic fields up to 14 T. We have found indications of a new phase transition at $T^* = 5 - 6$ K. The phase between T^* and the lock-in transition at 15 K is characterized by magnetic irreversibility. At higher fields the irreversibility increases. Heat-capacity measurements confirm the transition at T^*, and also show the irreversible behaviour. We construct a field-temperature phase diagram of $CoCr_2O_4$. Below the ferrimagnetic transition (94 K), the low-frequency (terahertz) optical response is dominated by a magnetic exchange mode, which shows an anomalous temperature dependence and a softening at the structural transition (26 K).

Part of this work has been supported by EuroMagNET under the EU contract no. 228043.

TT 34: Correlated Electrons: Metal-Insulator Transition 1

Time: Wednesday 16:30–18:00 Location: H 3010

TT 34.1 Wed 16:30 H 3010

Periodized Matsubara Green's functions — •Andro Sabashvili, Mats Granath, and Stellan Östlund — Department of Physics, University of Gothenburg, Gothenburg, Sweden

A new formalism for Fermionic thermal Green's functions that are periodized in imaginary (Matsubara) frequency space is developed. The periodization requires a generalisation of the Dyson equation and Luttinger-Ward-Baym-Kadanoff functional. Due to the Matsubara Green's function periodicity imaginary frequency space is relatively small which allows calculations at the extremely high precision which is necessary to perform a reliable analytic continuation. The formalism was tested on dynamical mean field theory calculations using iterated perturbation theory for the paramagnetic Hubbard model [1]. Currently the method together with the DRPA (dressed random phase approximation) is being used to study particular 2D models.

[1] arXiv:1103.3516v2

TT 34.2 Wed 16:45 H 3010

Emergence of a joint low-energy scale close to the orbital-selective Mott transition — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretical Physics III, Electronic Correlations and Magnetism, Universität Augsburg

We investigate the microscopic precondition for the appearance of kinks in the self-energy [1] and their relation to low-energy spin-excitations [2] within the framework of Dynamical Mean Field Theory. To this end we investigate the two-band Hubbard model with unhybridized, differently correlated orbitals close to the orbital selective Mott transition [3]. We find the emergence of one common energy-scale which is shared by the self-energy kinks and the diagonal spin-susceptibilities. A physical explanation of this energy-scale is obtained from a minimal Kondo-type model.

[1] K. Byczuk *et al.*, Nat. Phys. **3**, 168 (2007).
[2] C. Raas, P. Grete, and G. Uhrig, Phys. Rev. Lett. **102**, 076406 (2009).
[3] C. Knecht, N. Blümer, and P. G. J. van Dongen, Phys. Rev. Lett. **72**, 081103 (2005).

TT 34.3 Wed 17:00 H 3010

Correlated multiorbital systems, a Gutzwiller study — Nicola Lanata'[1], •Hugo U. R. Strand[1], Xi Dai[2], and Bo Hellsing[1] — [1]University of Gothenburg, SE-412 96 Gothenburg, Sweden — [2]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We present a numerical method for the minimization of general multi-orbital Gutzwiller variational wavefunctions in the Gutzwiller approximation [1]. The method is general in the sense that it can treat any type of local interaction, in particular spin-flip and pair-hopping interactions. To construct the variational wavefunction, we apply the ϕ-matrix formalism [2], and present a general approach for how to reduce the variational space by imposing lattice point group symmetries.

Using our numerical method we study the multiorbital Hubbard model for d-electron systems with rotational invariant Kanamori-interaction. The variational wavefunction is restricted to cubic symmetry and the properties of the model is studied with respect to; total electron filling, e_g-t_{2g} crystal field splitting and interaction strength.

This work is an extension of the Gutzwiller solver, used in the first principles LDA+Gutzwiller method [3], to general local interactions.

[1] N. Lanatà, H. U. R. Strand, X. Dai, B. Hellsing, (arXiv:1108.0180)
[2] N. Lanatà, P. Barone, M. Fabrizio, Phys. Rev. B **78**, 155127 (2008)
[3] X. Y. Deng, L. Wang, X. Dai, Z. Fang, Phys. Rev. B **79**, 075114 (2009)

TT 34.4 Wed 17:15 H 3010

The role of rotational symmetry in the magnetism of multiorbital Hubbard model — •Andrey Antipov[1,2] and Alexey Rubtsov[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Moscow State University, Department of Physics, 1-2 Leninskiye Gory, 119991 Moscow, Russia

The effects associated with orbital fluctuations play an important role in the physics of strongly correlated electron systems. Examples worth noting are the orbital ordering effects and the orbital-selective Mott transition. A full quantitative description of these systems require taking into account the complete Coulomb interaction between the valence band electrons, a difficult task for quantum impurity solvers. This complexity often leads to taking into account only the density-density part of the Coulomb interaction which is diagonal in the orbital space. As it was shown in [1] this reduction can lead to a breakdown of a Kondo-peak in the metallic density of states of a multiorbital Hubbard model due to the change in the degree of the degeneracy of the ground state.

In order to access the finite-temperature regime the interaction-expansion quantum Monte Carlo impurity solver was employed. It is shown that taking into account the full rotationally invariant Coulomb interaction leads to double decrease of the metal-insulator transition temperature in a doubly-occupied three-band model and to a 20% change in a half-filled two-band and three-band models. The change in the density of states is compatible with the results of [1].

[1] Th. Pruschke and R. Bulla, Eur. Phys. J. B 44, 217 (2005)

TT 34.5 Wed 17:30 H 3010

Model study of the Dzyaloshinskii-Moriya interaction in strongly correlated itinerant systems — •Sergej Schuwalow, Christoph Piefke, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

In low symmetry systems, the combination of spin-orbit interaction and broken inversion symmetry may give rise to effective noncollinear magnetic interactions first described in [1,2]. With the recently increasing interest in the effects of spin-orbit coupling, it becomes important to assess the role of such effects in the scope of complex solid state systems with different competing interactions.

Within this work, we investigate the interplay between strong electronic correlations and noncollinear magnetism induced by the Dzyaloshinskii-Moriya interaction in an itinerant model system within the framework of the Rotationally-Invariant Slave-Boson formalism (RISB)[3,4]. It allows us to capture the low-energy physics of the interacting system while retaining full rotational degrees of freedom which are essential for the magnetic structure at hand. Our main focus lies on determining the magnetic properties of the system and their behaviour under the influence of a finite Hubbard U.

[1] Dzyaloshinskii, J. Phys. Chem. Solids **4**, 241 (1958).
[2] Moriya, Phys. Rev. **120**, 91 (1960).
[3] Lechermann, Georges, Kotliar, Parcollet, PRB **76**, 155102 (2007).
[4] Piefke, Boehnke, Georges, Lechermann, PRB **82**, 165118 (2010).

TT 34.6 Wed 17:45 H 3010

Heat transport in a disordered and interacting electron system — •Georg Schwiete[1] and Alexander Finkelstein[2,3] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany — [2]Texas A&M University, Texas, USA — [3]The Weizmann Institute of Science, Rehovot, Israel

We study thermal conductivity in a disordered two dimensional electron gas at low temperatures. To this end we calculate the heat density correlation function. In comparison to the case of the well-studied charge density correlation function additional logarithmic corrections appear. Particular care is taken to confirm the compatibility of these corrections with the energy conservation law. The purpose of this study is to develop a renormalization group treatment for heat transport. This would allow to describe thermal transport near the metal-insulator transition.

TT 35: Focused Session: Charge and Spin Transport through Junctions at the Nanometre Scale

Time: Thursday 9:30–13:00 Location: H 0104

Invited Talk TT 35.1 Thu 9:30 H 0104

The information is the noise: shot noise a tool for investigating atomic and molecular nanowires — •Jan van Ruitenbeek — Kamerlingh Onnes Laboratory, Leiden University, Netherlands

Shot noise is the intrinsic noise in an electron current arising from the discrete character of the electron charge. It carries information on the quantum mechanical electronic structure of nanoscale conductors. In atomic wires shot noise can be exploited for obtaining information on the number of conductance channels and their transmission probability. We have applied shot noise analysis to single-molecule junctions. The outstanding property that distinguishes a molecule from a quantum dot is its floppy character. This leads to the observation of electron scattering on vibration modes of the molecule, known as Inelastic Electron Tunneling Spectroscopy (IETS). While IETS is now being exploited by many groups for the study and characterization of metal-molecule junctions, the influence of inelastic scattering is expected to affect electron transport more deeply. The conductance can be viewed as the first moment in the probability distribution of a charge q being transmitted through the junction during a given period of time. The second moment is the shot noise in the current. For bias voltages above the vibration mode energy corrections to shot noise have recently been predicted by several groups. As a first test of these predictions measurements will be discussed in terms of two-electron effects.

Invited Talk TT 35.2 Thu 10:10 H 0104

Electronic transport and magnetism in one-atom contacts — •Carlos Untiedt — Dep. Fisica Aplicada. Facultad de Ciencias (Fase II). Universidad de Alicante. Alicante. Spain

The smallest object that we could connect to an electronic circuit will be formed by just a single atom. With the use of the Scanning Tunneling Microscope (STM) we can fabricate and modify such bridges. There has been a great advance in the understanding of the electronic properties of these [1]. However it has been very difficult to extract consequences of the magnetism on their transport properties.

Recently we reported the observation of an effective Kondo screening of the magnetic moment of one-atom contacts between pure ferromagnetic metals by the conduction electrons [2]. Using a STM or Electromigrated Break Junctions we fabricated atomic contacts on these ferromagnetic materials and Fano-Kondo resonances where found in the conductance with the characteristic behavior of a Kondo system.

One of the advantages of our set-up configuration is the capability of the STM to study and analyze hundreds of atomic contacts. This has

given us the unique opportunity of performing statistics on the Fano parameters of our conductance curves. A statistical analysis allow us to discuss on the dependence of the Kondo system with the different degrees of couplings to the environment. Finally we will show some of our latest results including Pt chains suggesting a magnetic moment being developed.

[1] Agraït,Yeyati, Ruitenbeek, Phys. Rep. 377 (2003)
[2] Nature 458, 1150(2009)

Topical Talk TT 35.3 Thu 10:50 H 0104

Metallic atomic-size contacts: The role of absorbed noble gas atoms and anisotropic magnetoresistance — •Juan Carlos Cuevas — Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

In this talk I will review our efforts to resolve two basic puzzles in the context of metallic atomic-size contacts. First, I will discuss how the presence of noble gas atoms affects the electronic transport through atomic contacts. In particular, I will present ab initio results for the conductance of atomic junctions comprising single noble gas atoms (He, Ne, Ar, Kr, and Xe) coupled to gold electrodes. These results show that for the lightest elements (He and Ne) no significant current flows through the noble gas atoms and their effect is to reduce the conductance of the junctions by screening the interaction between the gold electrodes. This explains the observations reported in atomic contacts with adsorbed He atoms. Conversely, the heaviest atoms (Kr and Xe) increase the conductance because of the additional current path provided by their valence p states.

On the other hand, I will address the origin of the anomalous anisotropic magnetoresistance (AMR) observed in different experiments in ferromagnetic atomic-size contacts, which is still under debate. I will present theoretical results that strongly suggest that the anomalous AMR stems from the reduced symmetry of the atomic contact geometries. This reduced symmetry leads to both a great enhancement of the AMR magnitude and an anomalous angular dependence, as compared to bulk devices.

10 min. break.

Topical Talk TT 35.4 Thu 11:40 H 0104

Spin transport through organic molecules — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, Germany

We demonstrate that with the help of spin-polarized Scanning Tunneling Microscopy the spin transport across single organic molecules can be investigated and a molecular GMR junction can be realized. For this, single hydrogen phthalocyanine molecules were contacted by two ferromagnetic electrodes, i.e. a magnetic substrate and a magnetic STM tip. As substrate, ferromagnetic Co nano-islands grown Cu(111) were used, onto which the molecules were deposited. The magnetic state of the islands was determined by spin-polarized Scanning Tunneling Spectroscopy (STS) with Co tips. Then, the tip of the STM was approached in a controlled way towards a single molecule to contact the molecule. Below 0.4 nm distance, an attractive interaction between the tip and the molecule leads to a jump to contact of one of the side groups of the molecule, leading to a well defined molecular junction. Through the contacted molecule a GMR of 60% was observed which is one order of magnitude larger than the magnetoresistance without the molecule. This is explained on basis of ab initio calculations showing a selective hybridization of the molecular states with minority states of the electrodes. Finally, one of the electrodes has been replaced by an antiferromagnet forming an ideally hard magnetic layer. Due to the local character of the hybridization with the molecular states, a significant magnetoresistance can also be observed.

Topical Talk TT 35.5 Thu 12:20 H 0104

Spin-current manipulation of atomic-scale magnets using SP-STM — •Stefan Krause — Institute of Applied Physics, University of Hamburg, Germany

A prerequisite on the way to advanced applications in spintronics is the detailed understanding of current-induced magnetization switching (CIMS). Here, the spin-transfer torque generated by a spin current forces a magnet to reverse its magnetization. Spin-polarized scanning tunneling microscopy (SP-STM) provides an ideal representation of a tunneling magneto-resistance device, with vacuum serving as the tunnel barrier between a biased magnetic tip and a magnetic sample.

In our experiments the ultimate lateral resolution of SP-STM is used for a very local observation and manipulation of individual Fe/W(110) nanoislands in the superparamagnetic regime. Performing a current-dependent lifetime analysis of the magnetic states, three fundamental contributions to CIMS are clearly separated and quantified: spin-transfer torque, Joule heating and Oersted field [1,2].

Lowering the temperature leads to a stabilization of the nanomagnets. In this regime the high spin-polarized tunnel current solely triggers magnetization reversal, and the threshold is determined by ramping the tunnel current. For fast reversal, short high-current pulses are applied, thereby demonstrating the capability of SP-STM for the reliable manipulation of magnetism on the atomic scale[3].

[1] S. Krause *et al.*, Science **317**, 1537 (2007).
[2] S. Krause *et al.*, Phys. Rev. Lett. **107**, 186601 (2011).
[3] G. Herzog *et al.*, Appl. Phys. Lett. **96**, 102505 (2010).

TT 36: Superconductivity: Cryodetectors

Time: Thursday 9:30–12:15 Location: H 2053

TT 36.1 Thu 9:30 H 2053

Superconductor-Insulator-Superconductor Mixer Devices for 1.1 THz — •Stefan Selig, Marc Peter Westig, Karl Jacobs, and Cornelia Honingh — I. Physikalisches Institut, Universität zu Köln

Superconducting frequency mixers are a crucial component of high spectral resolution heterodyne receivers for radio astronomy. Superconductor-Insulator-Superconductor (SIS) mixers are the established highest sensitivity choice in the submillimeter wavelength range. There is great interest in using SIS-mixers also for THz-frequencies since they offer a higher intermediate frequency bandwidth and potentially higher sensitivity and stability than superconducting hot electron bolometer mixers which are currently used in this regime.

A possible junction design for 1.1 THz would consist of a niobium-based SIS-junction embedded in NbTiN top and bottom wiring layers. It has been shown that such a junction exhibits strong DC heating effects due to quasiparticle trapping, the absence of diffusion cooling, and a slow electron-phonon interaction time. The heating substantially reduces the mixer performance. We investigate the possibility of adding a gold layer between the junction's Nb top electrode and the NbTiN top wiring in order to increase the heat transport coefficient. This and some additional challenges concerning the fabrication of these devices will be discussed in this talk.

TT 36.2 Thu 9:45 H 2053

Rückgeführte Referenzmessung von Magnetfeldfluktuationsthermometer — •Marco Schmidt[1], Jörn Beyer[1], Jost Engert[1], Sassan AliValiollahi[2] und Henry-Jobes Barthelmess[2] — [1]Physikalisch-Technische Bundesanstalt, 10587 Berlin, Abbestr. 2-12 — [2]Magnicon GmbH, 22397 Hamburg, Lemsahler Landstr. 171

Das Magnetfeldfluktuationsthermometer (MFFT) ist ein SQUID-basiertes, hochlineares Rauschthermometer für den Temperaturbereich von 1 mK bis 4 K. Das MFFT misst magnetisches Flussdichterauschen, das über einem Kupferkörper, dem eigentlichen Temperatursensor, von der thermisch angeregten Bewegung der Elektronen im Metall verursacht wird. Die Temperaturbestimmung erfolgt durch Analyse des Flussdichte-Rauschspektrums mit einem nichtlinearen Approximationsverfahren. Das MFFT ist ein einfach zu verwendendes Thermometer. Seine Anwendung erfordert jedoch eine einmalige Referenzmessung an einer bekannten Temperatur, die bisher vom Anwender durchzuführen ist. Mit dem Ziel, die Nutzung des MFFTs zu vereinfachen und seine Akzeptanz zu erweitern, wurde ein Tieftemperaturmessplatz für MFFT-Referenzmessungen aufgebaut. Supraleitenden Referenzpunkte (Cd, Zn, Al) deren Übergangstemperaturen auf die Temperaturskala PLTS-2000 rückgeführt sind, werden für die Realisierung der Referenztemperaturen verwendet. Mit dem neuen Messaufbau werden metrologisch-genaue MFFT-Referenzmessungen durchgeführt. Diese Messungen ermöglichen die Ermittlung der MFFT-

Gesamtmessunsicherheit konform zum Guide to the expression of uncertainty in measurement (GUM).

TT 36.3 Thu 10:00 H 2053

Thin NbN film structures on SOI for SNSPD — •Konstantin Il'in[1], Stephan Kurz[1], Dagmar Henrich[1], Matthias Hofherr[1], Michael Siegel[1], Alexei Semenov[2], and Heinz-Wilhelm Huebers[2] — [1]IMS, KIT, Karlsruhe, Germany — [2]DLR, Berlin, Germany

Superconducting Nanowire Single-Photon Detectors (SNSPD) made from ultra-thin NbN films on sapphire demonstrate almost 100% intrinsic detection efficiency (DE). However the system DE values is less than 10% mostly limited by a very low absorptance of NbN films thinner than 5 nm. Integration of SNSPD in Si photonic circuit is a promising way to overcome this problem. We present results on optimization of technology of thin NbN film nanostructures on SOI (Silicon on Insulator) substrate used in Si photonics technology. Superconducting and normal state properties of these structures important for SNSPD development will be presented and discussed.

TT 36.4 Thu 10:15 H 2053

Influence of geometry on the critical current of superconducting nanowire single-photon detectors — •Dagmar Henrich[1], Patrick Reichensperger[1], Matthias Hofherr[1], Konstantin Il'in[1], Michael Siegel[1], Alexei Semenov[2], Heinz-Wilhelm Hübers[2,3], and Denis Vodolazov[4] — [1]IMS, Karlsruhe Institut für Technologie, Karlsruhe, Germany — [2]DLR, Berlin, Germany — [3]IOAP, Technische Universität Berlin, Berlin, Germany — [4]Nizhni Novgorod State University, Nizhni Novgorod, Russia

Superconducting Nanowire Single Photon Detectors (SNSPD) are made from thin superconducting films which are patterned into very narrow meander shaped lines. The current density distribution inside the nanowire, predicted by theory, shows an accumulation at the inner edges of such turns, which limits the total device critical current. Since the sensitivity of the SNSPDs as well as the spectral detection efficiency are strongly dependent on the factor of the local bias current to the critical current, the designs must be optimized to homogenize the current distribution. We experimentally investigate the influence of the angle and radius of curves on the critical current of nanowires. The samples are 300 nm wide nanowires made from ultra-thin NbN films deposited by DC reactive magnetron sputtering on 750°C heated sapphire substrates. Based on the results, we propose a design of an optimized detector layout for SNSPDs with homogeneous local detection efficiency.

TT 36.5 Thu 10:30 H 2053

Hot Spots and THz waves in single crystal $Bi_2Sr_2CaCu_2O_8$ mesas — •Boris Gross[1], Stefan Guenon[1], Matthias Gruenzweig[1], Jie Yuan[2], Mengyue Li[3], Zenguo Jiang[3], Yangyin Zhong[3], Akira Iishi[2], Peiheng Wu[3], Takeshi Hatano[2], Roman Mints[4], Dieter Koelle[1], Huabing Wang[2], and Reinhold Kleiner[1] — [1]PIT II, Universität Tübingen, Germany — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Research Institute of Superconductor Electronics, Nanjing University, China — [4]Faculty of Exact Science, Tel Aviv University, Ramat Aviv, Israel

Josephson Junctions offer a natural way to convert a dc voltage into high-frequency electromagnetic (e.m.) radiation. Intrinsic Josephson junctions (IJJs) in $Bi_2Sr_2CaCu_2O_8$ (BSCCO) are very promising candidates to be used as devices in the THz regime, allowing frequencies up to 10 THz. Stacks of many hundred IJJs can be fabricated easily. Research on BSCCO THz generators stagnated in the past due to perhaps modest success in creating operating devices. In 2007 Ozyuzer et al. detected coherent radiation up to 0.85 THz from large, rectangular mesa structures on BSCCO single crystals, reviving the research in this field. More than 500 junctions in the stack oscillated in phase, leading to a power of up to 0.5 μW. The mesas are believed to work as a cavity for electromagnetic standing waves, synchronizing the junctions in the stack. We report on the investigation of heat distribution, e.m. standing waves and THz e.m. wave generation in BSCCO mesas, using a combination of transport measurements, direct e.m. wave detection and Low Temperature Scanning Laser Microscopy.

15 min. break.

TT 36.6 Thu 11:00 H 2053

Progress in the development of non-hysteretic rf-SQUIDs for a multiplexed MMC readout — •Sebastian Kempf, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg.

Recently it was shown that the performance of single channel Metallic Magnetic Calorimeters (MMCs) meets the requirements of many applications like, for example, high resolution x-ray spectroscopy. Presently, a number of cryogenic multiplexing schemes are investigated to increase the channel count of MMC detector arrays significantly. A quite promising approach employs a so-called microwave SQUID multiplexer. Here, non-hysteretic unshunted rf-SQUIDs transduce the detector signals into a frequency shift of related superconducting microwave resonators with unique resonance frequencies. By injecting a microwave frequency comb and monitoring either phase or amplitude of each resonator, it is thus possible to infer the initial detector signals.

Based on experimental results obtained with our first prototype SQUID multiplexer and numerical simulations we optimized our current multiplexer design concerning rf-SQUID layout, SQUID-to-resonator coupling and fabrication of the Nb/Al-AlOx/Nb Josephson junctions. We discuss advantages of the modified fabrication process, differences between both multiplexer designs, the expected performance improvements and present first measurements of this second generation SQUID multiplexer.

TT 36.7 Thu 11:15 H 2053

Metallic Magnetic Calorimeters for High-Resolution X-ray Spectroscopy in Atomic Physics — •S. Schäfer, C. Pies, S. Kempf, J.-P. P, S. Uhl, S. Heuser, T. Wolf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff Institut für Physik, INF 227, 69120 Heidelberg

Highly-charged heavy ions are model systems for the investigation of quantum electrodynamical effects in strong electromagnetic fields.

We are developing x-ray detectors based on 1x8 arrays of Metallic Magnetic Calorimeters (MMCs) optimized for the spectroscopy of highly-charged ions at GSI/FAIR and the EBIT facility at the MPI for nuclear Physics in Heidelberg. One of the detector arrays (maXs-20) is designed to provide an energy resolution below 3 eV (FWHM) and sufficient stopping power for x-rays in the energy range up to 20 keV. The second device (maXs-200) is optimized for the detection of x-rays up to 200 keV and should yield an energy resolution below 30 eV (FWHM).

We present detector designs, outline the micro-fabrication process and discuss the results of characterization measurements with ^{55}Fe and ^{241}Am calibration sources including energy resolution, signal rise time and cross-talk between adjacent detectors of both arrays.

TT 36.8 Thu 11:30 H 2053

Neutron Scattering Facility for the Measurement of Light Quenching Factors of Low-Temperature Dark Matter Detectors — •Christian Ciemniak[1], Franz von Feilitzsch[1], Josef Jochum[2], Jean-Côme Lanfranchi[1], Walter Potzel[1], Raimund Strauss[1], and Stephan Wawoczny[1] — [1]Technische Universität München — [2]Eberhard-Karls-Universität Tübingen

Most direct dark matter search experiments aim at the detection of WIMPs (Weakly Interacting Massive Particles). To cover a large mass range, scintillating multi-material single crystals (e.g. $CaWO_4$, NaI, TeO_2) are of special interest. Operated as low-temperature detectors, each particle interaction produces a scintillation light and a phonon signal simultaneously in these crystals. Since the ratio of the two quantities depends on the type of particle interaction, it is possible to discriminate the electron and different types of nuclear recoils. The signal region for each type of interaction is quantified by the quenching factor (QF). At the Maier-Leibnitz Laboratorium in Garching, a dedicated neutron scattering facility has been set up to characterize scintillating multi-material target crystals and measure the bulk QFs of the different nuclei. A detector operated at mK temperatures is irradiated by mono-energetic neutrons ($\approx$ 11MeV). Both the phonon and the scintillation light signals are read out. The neutron's time of flight measurement at fixed scattering angle allows to identify the recoiling nucleus and to determine its QF.

TT 36.9 Thu 11:45 H 2053

Results of Light Quenching Factor Measurements of $CaWO_4$ at mK Temperatures for the Dark Matter Experiments CRESST and EURECA — •Raimund Strauss[1], Christian Ciemniak[1], Franz v. Feilitzsch[1], Josef Jochum[2], J.-C. Lanfranchi[1], Walter Potzel[1], and Stephan Wawoczny[1] — [1]Physik-Department E15, Technische Universität München, D-85747

Garching, Germany — [2]Eberhard-Karls-Universität Tübingen, D-72076 Tübingen, Germany

The CRESST and the future EURECA experiments aim at the direct detection of Cold Dark Matter (DM) with scintillating $CaWO_4$ crystals operated as cryogenic detectors at mK temperatures. DM particles such as the highly motivated Weakly Interacting Massive Particles (WIMPs) are expected to coherently scatter off nuclei and the corresponding nuclear recoils can be measured by the induced heat (phonon channel) and the corresponding scintillation light. Light Quenching Factors (QFs) quantify the individual reduction of the relative light yield for O, Ca and W recoils compared to electron recoils. The QFs of $CaWO_4$ are of utmost importance for the DM analysis as they allow a discrimination of backgrounds and - if a positive signal is observed - a WIMP mass-spectroscopy. Recently an extensive facility for the measurement of light QFs at mK temperatures via neutron scattering (time-of-flight) has been set up and successfully commissioned at the Maier-Leibnitz Laboratorium (MLL) in Garching. We present here first results for the QFs of $CaWO_4$ crystals at low temperatures.

TT 36.10 Thu 12:00 H 2053

Optimization of Cryogenic Light Detectors for the CRESST Experiment — •Anja Tanzke — MPI for Physics, Munich, Germany

The CRESST experiment aims to directly detect Dark Matter in the form of WIMPs. These hypothetical particles are expected to weakly interact via elastic scattering. The deposited energy is measured by the amplitude of the temperature pulse registered with a superconducting transition edge sensor on the scintillating target crystal. Additionally, the particle dependent scintillation light of the target crystal is detected by a cryogenic light detector. The performance of this detector is investigated and optimizations will be presented.

TT 37: Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 2

Time: Thursday 9:30–13:00 Location: H 3005

TT 37.1 Thu 9:30 H 3005

Superposition of BEC and a first-order phase transition in a repulsive Bose gas — •Michael Maennel[1], Klaus Morawetz[1,2], and Pavel Lipavsky[3,4] — [1]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany — [2]International Institute of Physics, Universidade Federal do Rio grande do Norte, 59.072-970 Natal-RN, Brazil — [3]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

We investigate a Bose gas with finite-range interaction using a scheme to eliminate self-interaction in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature, without the use of anomalous functions. In the vicinity of the onset of Bose-Einstein condensation (BEC) chemical potential and pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore for sufficiently strong interaction the equation of state becomes multivalued near the BEC transition. For a Hatree-Fock or Hartree-Fock-Bogoliubov approximation such a multivalued region can be avoided by a Maxwell construction. However, for the T-matrix approximation there remains a multivalued region even after a Maxwell construction.

TT 37.2 Thu 9:45 H 3005

Dissipative and Finite Temperature Dynamics using Vidals Superoperator Renormalization — •Lars Bonnes and Andreas Läuchli — Institut für Theoretische Physik, Universität Innsbruck, Österreich

The study of dynamical properties of quantum systems has gained new momentum through the progress made in the preparation of and control of low dimensional quantum system in ultra cold atomic and molecular gases. Matrix product state bases methods such as the density matrix renormalization group have proven invaluable for the numerical study of the ground-state properties as well as the (non- equilibrium) dynamics of one dimensional systems. Using the superoperator renormalization algorithm by Zwolak and Vidal [**PRL** 93, 207205 (2004)], one has access to the full dynamics of a density matrix such that one can incorporate not only non-zero temperatures but also dissipative dynamics given by a Lindblad equation.

We present results on finite-temperature quench dynamics as well as the dissipative dynamics of a Bose- Hubbard model using an efficient quantum number enabled implemention. We then address question of ballistic versus diffusive spreading of correlations and the entanglement properties of the finite-temperature states.

TT 37.3 Thu 10:00 H 3005

Interacting Bosonic Quantum Ratchets — •Karen Rodriguez and Achim Rosch — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

We study the Hamiltonian quantum ratchet dynamics of cold Bosons loaded on optical lattices. Under the influence of time-periodic space-dependent hopping and local potential, the relevant symmetries are broken leading the system to develop unidirectional transport in long term evolutions. By means of the Floquet theory and the Gutwiller wave function, we analyze the transport problem and the crucial role of the interactions on the ratchet average dc-current.

TT 37.4 Thu 10:15 H 3005

Floquet states of many-body quantum systems — •Sergey Denisov, Armin Seibert, Alexey Vladimir Ponomarev, and Peter Hänggi — Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg

Periodic driving of a quantum many-body system could provide an access to a multitude of new-non-equilibrium states, essentially different from those a system exhibits at equilibrium. However, the field of ac-driven many-body quantum systems is a little-explored area, mainly for two reasons. First, until recently there were enough exciting problems to study at the equilibrium corner. Second, even under equilibrium conditions, a typical many-body system is a hard nut to crack due to the exponential growth of the number of system states with the number of quantum entities it contains. We discuss the possible directions to take in order to get insight into the evolution of ac-driven many-body quantum systems, outline the obstacles and possible means to overcome them. Our approach is based on the Floquet operator formalism and density-matrix renormalization group (DMRG) methods.

TT 37.5 Thu 10:30 H 3005

Doublon dynamics in the one dimensional extended Hubbard model — •Felix Hofmann and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Germany

The existence of repulsively bound states within the Hubbard model has been known since the early work of Hubbard. Here, their time evolution is calculated numerically exact in few-particle subspaces using the Lanczos method and will give insight into their propagation und stability properties. In general, nonvanishing couplings of the extended model, describing dipolar cold gases, cause a renormalization of the hopping parameter. An internal vibrational degree of freedom is accessible in the case of equal couplings and allows for a free propagation of repulsively bound pairs. In an effective description they will be subjected to a nearest-neighbor interaction, which will not give rise to a quantum-droplet phase unlike in the bosonic case [1]. In agreement with Fermi's golden rule, a power law decay will take place on short time scales until the probability for finding a repulsively bound state in the system approaches a constant value. Already moderate coupling strengths will lead to a high stability which even increases in the presence of more particles in the system, which is also confirmed by calculations for the half-filled system [2]. This establishes the possibilty of the experimental observation of repulsively bound pairs.

[1] D. Petrosyan et al., Phys. Rev. A 76, 033606 (2007).
[2] K. A. Al-Hassanieh et al., Phys. Rev. Lett. 100, 166403 (2008).

TT 37.6 Thu 10:45 H 3005

Noise properties of periodic driven quantum systems —

•Vicente Leyton[1], Vittorio Peano[2], and Michael Thorwart[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

The Lax formula for two-time correlations combined with the Floquet formalism is used for the study of the noise properties of periodically driven nonlinear oscillators in contact with a dissipative environment. In particular, we consider the case of the quantum Duffing oscillator, where its non-equidistant energy spectrum leads to multiphoton transitions induced by the external driving at external frequencies close to the fundamental oscillator frequency. We consider the regime of weak coupling, in which the contact with the environment induces dissipative ransitions between nearest neighbour levels only. In addition to the dissipative dynamics, when the driving is at resonance with some multiphoton transition, Rabi oscillations between the states involved in the multiphoton transition are induced. We study the fluctuations of the number of photons pumped into the system when the multiphoton Rabi dynamics is faster than dissipative processes. We find a rich structure in the noise power spectrum including side-peaks associated to the multiphoton transitions. Moreover, we can extract information on the dissipative rate for resonant dynamical tunnelling in the dynamically induced bistable quasienergy landscape. The procedure presented here is extendible to other nonlinear systems like the driven Jaynes-Cummings model.

TT 37.7 Thu 11:00 H 3005

Localized phase structures growing out of quantum fluctuations in two tunnel-coupled atomic condensates — •Clemens Neuenhahn[1], Anatoli Polkovnikov[2], and Florian Marquardt[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute for Theoretical Physics II, Staudtstr. 7, 91058 Erlangen, Germany — [2]Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA

We investigate the relative phase between two weakly interacting 1D condensates of bosonic atoms after suddenly switching on the tunnel-coupling. The following phase dynamics is governed by the quantum sine-Gordon equation. In the semiclassical limit of weak interactions, we observe the parametric amplification of zero-point quantum fluctuations leading to the formation of breathers with a finite lifetime. The typical lifetime and density of the these 'quasibreathers' are derived employing exact solutions of the classical sine-Gordon equation. Both quantities (density and lifetime) depend crucially on the initial, overall relative phase between the condensates, which is considered as a tunable parameter.

15 min. break.

TT 37.8 Thu 11:30 H 3005

Damping of Bloch Oscillations in the Hubbard Model — •Martin Eckstein[1] and Philipp Werner[2] — [1]Max Planck Research Department for Structural Dynamics, University of Hamburg, Centre for Free Electron Laser Science, Hamburg, Germany — [2]Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

Using nonequilibrium dynamical mean-field theory (DMFT), we study the isolated Hubbard model in a static electric field in the limit of weak interactions. Linear response behavior is established at long times, but only if the interaction exceeds a critical value, below which the system exhibits an ac-type response with Bloch oscillations [1]. The transition from ac to dc response is defined in terms of the universal long-time behavior of the system, which does not depend on the initial condition. In order to understand whether these phenomena can be observed in experiments with ultracold gases, one has to estimate the importance of the inhomogeneous confining trap. This is done within a realspace DMFT approach.

[1] M. Eckstein and Ph. Werner, Phys. Rev. Lett. 107, 186406 (2011).

TT 37.9 Thu 11:45 H 3005

New approach to many-body non equilibrium dynamics: functional renormalization group master equation — •Johannes Hick[1], Thomas Kloss[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Goethe Universität Frankfurt am Main, Germany — [2]Laboratoire de Physique et Modélisation des Milieux Condensé, CNRS and Université Joseph Fourier, Grenoble, France

We use a functional renormalization group (FRG) approach to study the non-equilibrium time evolution of non-interacting bosons which are coupled to a phonon bath. We show that with a suitable cutoff procedure the resulting FRG flow equation for the distribution function resembles a master equation whose scale-dependent transition rates are determined by a system of FRG flow equations. We compare numerical results of this FRG master equation approach with perturbative results based on a conventional Boltzmann equation.

TT 37.10 Thu 12:00 H 3005

Polaron to molecule transition in strongly interacting Fermi gases — •Tilman Enss and Richard Schmidt — TU München, Germany

A light impurity in a Fermi sea undergoes a transition from a polaron to a molecular bound state for increasing interaction. We develop a new method to compute the spectral functions of the polaron and molecule in a unified framework based on the functional renormalization group with full self-energy feedback. We discuss the energy spectra and decay widths of the attractive and repulsive polaron branches as well as the molecular bound state. The decay follows a characteristic power-law scaling near the transition, showing that the transition is of first order.

TT 37.11 Thu 12:15 H 3005

Relaxation of fermionic quantum systems after an interaction quench — •Simone A. Hamerla and Götz S. Uhrig — TU Dortmund, Theoretische Physik I, 44221 Dortmund, Germany

An impressive progress on experimental side has led to great interest in non-equilibrium dynamics. Thus we investigate the behavior of fermionic systems after a quench, i.e., a sudden change in the intrinsic parameters. We focus on interaction quenches and study the momentum distribution of 1D and 2D Hubbard models, where the interaction between particles is suddenly turned on.

In our approach we find surprising correspondence between results for the 1D model and the $D = \infty$ DMFT results in the case of large interaction strengths.

The technique used is a semi-analytic approach based on the Heisenberg equations of motion [1]. We aim at a description of the behavior in the prethermalization regime, i.e., on short and intermediate time scales. Besides the momentum distribution the method allows for a discussion of other observables for various dopings.

[1] G.S. Uhrig Phys. Rev. A 80, 061602(R)

TT 37.12 Thu 12:30 H 3005

Bosonic spectral functions in the dynamical mean-field theory calculated with a strong-coupling impurity solver — •Anna Kauch[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoza 69, PL-00-681 Warszawa, Poland

With the use of a strong-coupling solver for the bosonic dynamical mean-field theory (B-DMFT)[1] we investigate the evolution of spectral functions across the phase transition from the Mott-insulating to the superfluid phase in the Bose-Hubbard model. The B-DMFT provides a comprehensive and thermodynamically consistent description of correlated lattice bosons. Within the B-DMFT normal and Bose-Einstein condensed bosons are treated on equal footing. In the B-DMFT the bosonic lattice problem is replaced by a single site coupled to two bosonic baths corresponding to normal and condensed bosons, respectively. This yields a set of equations which have to be solved self-consistently. The use of a strong-coupling solver allows us to compute the spectral functions in different transition scenarios (density driven vs. interaction driven transition).

[1] K. Byczuk and D. Vollhardt, Phys. Rev. B 77, 235106 (2008)

TT 37.13 Thu 12:45 H 3005

Non-adiabatic ramps in quantum many-particle systems — •Masud Haque — Max Planck Institute for Physics of Complex Systems

A change of system parameter can be neither truly instantaneous nor truly adiabatic in real life. For several quantum many-particle systems, I will consider non-equilibrium dynamics induced by finite-rate ramps. The ramp rate extrapolates between an instantaneous quench and an adiabatic sweep. I will characterize the deviation from adiabaticity through the excess energy or "heating" of the system.

For cold-atom systems in a harmonic trapping potential, I will show that the non-adiabatic heating in finite-time ramps has universal features common to a wide range of systems.

TT 38: Correlated Electrons: Spin Systems and Itinerant Magnets 1

Time: Thursday 9:30–13:00 Location: H 3010

TT 38.1 Thu 9:30 H 3010

Disentanglement of static and dynamic magnetism in itinerant AFe$_4X_2$ systems studied by Muon Spin Relaxation and Mössbauer Spectroscopy — •Til Goltz[1], Nandang Mufti[2], Christoph Geibel[2], Johannes Spehling[1], Hubertus Luetkens[3], and Hans-Henning Klauss[1] — [1]Institute of Solid State Physics, TU Dresden, Germany — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland

The AFe$_4X_2$ (A=Y, Lu, Zr; X=Ge, Si) family of transition metal tetrels has shown to be a promising candidate for studying the change of the electronic ground state under chemical substitution [1]. Within the ZrFe$_4$Si$_2$-type structure (P4$_2$/mnm), the iron atoms are arranged in chains of edge-linked tetrahedra [2]. Their structure is prone for reduced dimensionality or frustration and is thus expected to lead to emergent phenomena near a quantum critical point.
In this talk, we give an overview of our recent experimental findings from Muon Spin Relaxation and Mössbauer Spectroscopy experiments for a variety of AFe$_4X_2$. We focus on the ZrFe$_4$Si$_2$ compound, where we observe electronic spin fluctuations already at 100 K whereas long-range magnetic order sets in only below 10 K.
[1] N. Mufti, T.G. et al., DPG Spring Meeting 2011 (TT 49.11)
[2] O.Ya. Oleksyn et al., Proc. 10th Int. Conf. Solid Compounds of Transition Elements, Münster, 1991

TT 38.2 Thu 9:45 H 3010

Non-magnetic impurities in a classical spin liquid — •Arnab Sen[1], Kedar Damle[2], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Tata Institute of Fundamental Research, Mumbai, India

Impurities can potentially reveal the underlying correlations in spin liquid states that appear deceptively featureless in their ground state properties. We consider the archetypal frustrated antiferromagnet $SrCr_{9p}Ga_{12-9p}O_{19}$ (SCGO) in which Ga ions act as non-magnetic impurities in the magnetic lattice composed of Cr^{3+} S=3/2 spins for disordered $p < 1$ samples. We show that a spin in direct proximity to a pair of vacancies is cloaked by a spatially extended spin texture that encodes the correlations of the parent spin liquid. In this spin liquid regime, our analytic theory predicts that the combined object has a magnetic response identical to a classical spin of length S/2=3/4, which dominates over the small intrinsic susceptibility of the pure system. We calculate the full texture on the lattice in the spin liquid regime and check that it agrees well with Monte-Carlo (MC) simulations. This texture leaves an unmistakable imprint on the measured ^{71}Ga NMR lineshapes, which we compute using MC simulations and compare with experimental data. These spin-textures have long range interactions with each other in the spin liquid regime. We show how these interactions can be understood in a simple manner from our analytic theory, and support the predictions using numerical simulations.

TT 38.3 Thu 10:00 H 3010

Magnetic excitations in disordered striped antiferromagnetic insulators — •Eric Andrade and Matthias Vojta — Technische Universität Dresden

The compounds of the $La_{2-x}Sr_xCoO_4$ series are isostructural to the 214 family of cuprate superconductors, but nevertheless remain insulating over a wide range of doping. Recently, it was observed that the $x = 1/3$ compound displays a peculiar type of magnetism, with short-ranged static antiferromagnetic order and an hour-glass-like magnetic excitation spectrum, which can be directly associated with the presence of stripe order. Here we argue that inhomogeneities, coming from deviations of perfectly ordered stripes, are of central importance and, by calculating the magnetic excitation spectrum, we show that a scenario of disordered charge stripes (formed by Co^{2+} and Co^{3+} ions) is consistent with the experimental data.

TT 38.4 Thu 10:15 H 3010

Orbital and magnetic excitations in the weakly coupled spin chain system $CaCu_2O_3$ — •Valentina Bisogni[1], Krzysztof Wohlfeld[1], Roberto Kraus[1], Jan Trinckauf[1], Claude Monney[2], Satoshi Nishimoto[1], Ke Jin Zhou[2], Vladimir Strocov[2], Bernd Büchner[1], Jeroen van den Brink[1], Thorsten Schmitt[2], and Jochen Geck[1] — [1]IFW Dresden, Dresden, Germany — [2]Paul Scherrer Institut, Villigen PSI, Switzerland

Recently, resonant inelastic X-ray scattering (RIXS) on the 1D spin chain system Sr_2CuO_3 has revealed an unprecedented and strong dispersion of d-d excitations. This result has been interpreted as the spin and orbital separation from the elementary electron in a 1D S=1/2 system. In this talk we report on Cu L$_3$ RIXS in quasi 1D $CaCu_2O_3$ consisting of two coupled spin chains. Due to its buckled geometry, the inter-chain interaction of this system is one order of magnitude smaller than the in-chain interaction. Therefore, $CaCu_2O_3$ is an ideal model system to study the effect of a weak inter-chain interaction on both the low (spin excitation) and the high (d-d excitations) energy scale. Although the dispersion of the spinon continuum can largely be accounted for by neglecting the presence of the inter-chain interaction, surprisingly the absence of a strong dispersion in the d-d excitations emerges from the raw data. A deep analysis of these results shows indeed that the various orbital channels feel different dimensionalities, 1D or 2D. The important role played by inter-chain interactions for the magnetic and orbital excitations in this class of compounds will be discussed in this context.

TT 38.5 Thu 10:30 H 3010

Pulse field ultrasonic experiments in the quasi-2d antiferromagnet Cs_2CuBr_4 — •Bernd Wolf, Pham Thanh Cong, Natalia Krüger, Franz Ritter, Wolf Assmus, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

The insulator Cs_2CuBr_4 is a frustrated quasi-twodimensional triangular lattice (bc plane) spin-1/2 Heisenberg antiferromagnet (HAFM) with a weak interlayer coupling. The long-range antiferromagnetic order ($T_N = 1.4$ K at B = 0) can be suppressed to $T_N = 0$ in a magnetic field $B_c \sim 31$ T (B//a). For temperatures $T > T_N$ the magnetic properties of the material are dominated by quasi-2d spin fluctuations, which are also present in the ordered magnetic state. Here we present pulsed field measurements up to 50 T of the longitudinal elastic constants c_{11} for 1.2 K $< T <$ 4.2 K. A large softening, caused by the coupling of the quasi-2d spin fluctuations, is observed for magnetic fields smaller than B_c, which is more pronounced for lower temperatures. As expected, in the fully polarized state, the c_{11} mode is field independent for all temperatures. In addition, we compare the magnetoelastic properties of Cs_2CuBr_4 with those of the isostructural quasi-2D HAFM Cs_2CuCl_4.

TT 38.6 Thu 10:45 H 3010

Pulse field ultrasonic experiments in the quasi-2d antiferromagnet Cs_2CuBr_4 — •Bernd Wolf, Pham Thanh Cong, Natalia Krüger, Franz Ritter, Wolf Assmus, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

The insulator Cs_2CuBr_4 is a frustrated quasi-twodimensional triangular lattice (bc plane) spin-1/2 Heisenberg antiferromagnet (HAFM) with a weak interlayer coupling. The long-range antiferromagnetic order ($T_N = 1.4$ K at B = 0) can be suppressed to $T_N = 0$ in a magnetic field B_c 31 T (B//a). For temperatures $T > T_N$ the magnetic properties of the material are dominated by quasi-2d spin fluctuations, which are also present in the ordered magnetic state. Here we present pulsed field measurements up to 50 T of the longitudinal elastic constants c_{11} for 1.2 K $< T <$ 4.2 K. A large softening, caused by the coupling of the quasi-2d spin fluctuations, is observed for magnetic fields smaller than B_c, which is more pronounced for lower temperatures. As expected, in the fully polarized state, the c_{11} mode is field independent for all temperatures. In addition, we compare the magnetoelastic properties of Cs_2CuBr_4 with those of the isostructural quasi-2D HAFM Cs_2CuCl_4.

TT 38.7 Thu 11:00 H 3010

Low temperature thermal and electrical transport properties of $ZrZn_2$ in high magnetic field — •Yang Zou[1], Michael Sutherland[1], Stephen Hayden[2], Daniel Rothfuss[3], Andreas Fleischmann[3], Christian Enss[3], and F. Malte Grosche[1] — [1]University of Cambridge, UK — [2]University of Bristol, UK — [3]Universität Heidelberg, Germany

Metals close to a ferromagnetic quantum critical point offer a comparatively clear and well-defined environment to investigate the breakdown of Landau's Fermi liquid theory. The low temperature band ferromag-

net $ZrZn_2$ violates the predictions of Fermi liquid theory over a wide temperature range at low temperatures. Transport and heat capacity measurements suggest the presence of a marginal Fermi-liquid, predicted to occur close to a ferromagnetic quantum critical point by spin fluctuation theory [1]. In order to investigate the nature of the Fermi-liquid breakdown in this material, we have implemented electrical and thermal conductivity measurements down to temperatures of 100 mK and in high magnetic field. In zero field our measurements confirm the finding reported in [2] that, to leading order in temperature T, the electrical and effective thermal resistivities at low temperature take a $T^{5/3}$ and T form, respectively. These are the signatures of the marginal Fermi-liquid. At very low temperatures and in finite magnetic field we find that the electrical resistivity assumes quadratic temperature dependence, consistent with a return to conventional Fermi-liquid behaviour.

[1] Sutherland et al. ArXiv:1110.5240v1 [cond-mat.str-el].
[2] Smith et al. Nature **455** 7217 (2008).

15 min. break.

Invited Talk TT 38.8 Thu 11:30 H 3010

Emergent electrodynamics of skyrmions in chiral magnets — •Christian Pfleiderer — Technische Universität München, D-85748 Garching, Germany

Small angle neutron scattering and measurements of a topological Hall signal identify the formation of skyrmion lattices in the non-centrosymmetric B20 compounds MnSi, $Mn_{1-x}Fe_xSi$, $Mn_{1-x}Co_xSi$ and the strongly doped semiconductor $Fe_{1-x}Co_xSi$. This observation has been confirmed by Lorentz force microscopy in thin samples of $Fe_{1-x}Co_xSi$, FeGe and, most recently, MnSi, where even individual skyrmions have been spotted. Because the skyrmion lattices are exceptionally weakly pinned to the crystal lattice, extreme care has to be exercised when studying the precise intrinsic morphology of related spin textures in bulk samples. As a particularly striking property each skyrmion supports precisely one quantum of emergent magnetic flux. This permits a highly efficient coupling between skyrmions and conduction electrons which results in spin torque effects at ultra-low current densities as seen in small angle neutron scattering and the emergent electric field when the skyrmions move.

Work in collaboration with: T. Adams, A. Bauer, B. Binz, P. Böni, G. Brandl, R. A. Duine, K. Everschor, C. Franz, M. Garst, R. Georgii, S. Gottlieb-Schönmeyer, M. Halder, W. Heusler, M. Janoschek, F. Jonietz, T. Keller, K. Mittermüller, S. Mühlbauer, W. Münzer, A. Neubauer, P.G. Niklowitz, R. Ritz, A. Rosch, C. Schnarr, T. Schulz, A. Tischendorf and M. Wagner

TT 38.9 Thu 12:00 H 3010

Fluctuation-driven first order transition in the chiral magnets — •M. Garst[1], M. Janoschek[2,3,4], P. Krautscheid[1], A. Bauer[3], C. Pfleiderer[3], P. Böni[3], and R. Georgii[3,5] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln — [2]Department of Physics, University of California, San Diego, La Jolla, CA 92093-0354, USA — [3]Physik Department E21, Technische Universität München, D-85748 Garching — [4]Laboratory for Neutron Scattering, Paul-Scherrer Institut & ETH Zürich, CH-5232 Villigen, PSI, Switzerland — [5]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, D-85748 Garching

Chiral magnets such as MnSi, $Fe_{1-x}Co_xSi$, MnGe or FeGe possess a weak Dzyaloshinskii-Moriya spin-orbit interaction that leads to a twist of the magnetization on long length scales resulting in chiral magnetic textures. We discuss theoretically and experimentally how this chiral spin-orbit interaction is reflected in the spin dynamics close to the magnetic transition at T_c in MnSi and related compounds. As the transition is approached chiral fluctuations become soft resulting in neutron scattering intensity concentrated on a sphere in reciprocal space. At a characteristic Ginzburg temperature $T^* > T_c$ these fluctuations start to interact strongly resulting in pronounced renormalization effects, causing a turning point in the susceptibility $\partial_T^2 \chi(T) = 0$ and an invariant point in the specific heat $\partial_H C(H) = 0$, also known as Vollhardt invariance. Perhaps even more importantly, these chiral critical fluctuations drive the magnetic transition at T_c first order consistent with a Brazovskii theory for chiral magnetic fluctuations.

TT 38.10 Thu 12:15 H 3010

On the magnetic phase diagram of B20 compounds inferred from magnetization and ac susceptibility — •Andreas Bauer and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

We report comprehensive, simultaneous measurements of the magnetisation, M, and the ac susceptibility, χ_{ac}, across the magnetic phase diagram of optically float-zoned high-quality single crystals of MnSi, where we explore the importance of the excitation frequency, excitation amplitude, sample shape, and crystallographic orientation. We show that the temperature dependence of the magnetisation of MnSi reported by Kadowaki et al. [1] is connected with a single skyrmion phase. Moreover, our data establishes consistently for all major crystallographic directions a well defined, slightly broadened first order transition at the helical to conical phase boundary, as well as for the skyrmion lattice phase. The same general features are also observed for typical temperature and field scans in $Mn_{1-x}Fe_xSi$ and $Fe_{1-x}Co_xSi$. Taken together, our results question the phase diagram of FeGe reported by Wilhelm et al., which was purely inferred from the ac susceptibility at 1 kHz of a vapour grown single crystal with ill-defined sample shape for a single field direction [2].

[1] K. Kadowaki et al., J. Phys. Soc. Japan, **51**, 2433 (1982)
[2] H. Wilhelm et al., PRL **107**, 127203 (2011)

TT 38.11 Thu 12:30 H 3010

Relevance of magnetic anisotropies for the skyrmion lattice in MnSi — •Tim Adams[1], Andreas Bauer[1], Marco Halder[1], Robert Georgii[1,2], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), D-85748 Garching, Germany

We used high-precision small angle neutron scattering and magnetisation measurements to determine the strength of the magnetic anisotropies in MnSi. To minimise the effects of uncontrolled demagnetising fields a spherical sample was studied. The strength of the leading order quartic anisotropy terms, which by symmetry arguments cannot couple to the skyrmion lattice, are thereby inferred from variations of the transition field to the conical state. This is followed by anisotropy terms beyond fourth order, which are inferred from the orientation of the skyrmion lattice in the plane perpendicular to the applied field and tiny systematic tilts out of this plane. Taken together our data allows us to discuss the relevance of magnetic anisotropies for the morphology and stabilityof the skyrmion lattice in bulk samples of MnSi and related systems.

TT 38.12 Thu 12:45 H 3010

Uniaxial pressure studies of helimagnetic order and the skyrmion lattice phase in MnSi — •Alfonso Chacón Roldán[1], Andreas Bauer[1], Tim Adams[1], Georg Brandl[1,2], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), D-85748 Garching, Germany

We report small angle neutron scattering and ac susceptibility measurements of the uniaxial pressure dependence of the helimagnetic order and the skyrmion lattice phase in MnSi. For our studies a bespoke sample stick with a He-activated bellow system has been built that permits simultaneous neutron scattering and susceptibility measurements. We find that both the helimagnetic order as well as the skyrmion lattice phase are very sensitive to the application of uniaxial stress. Besides a reorientation of the skyrmion lattice the most prominent effect is either a pronounced suppression or an enhancement of the skyrmion lattice phase depending on the field and stress direction. We discuss our results in the context of the mechanism that stabilises the skyrmion lattice phase.

TT 39: Transport: Graphene 1 (jointly with MA, HL, DY, DS, O)

Time: Thursday 9:30–13:00 Location: BH 334

TT 39.1 Thu 9:30 BH 334

Spin relaxation in graphene induced by adatoms — •Jan Bundesmann and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

By means of a recursive Green's function method we study diffusive spin-dependent transport through graphene and graphene nanostructures. Diffusion in graphene mainly originates from charges trapped in the substrate. In addition we assume the presence of adsorbed atoms or molecules. These are the origin of a locally fluctuating spin-orbit coupling. While both intrinsic spin-orbit interaction and spin-orbit coupling induced by electric fields or curvature are rather weak (typically $\mathcal{O}(\mu eV)$), underneath adatoms these values can reach the height of meV. Our results show that adatoms clearly reduce the spin relaxation time in graphene. The ones we obtain are on the order of magnitude as the ones found in experiments ($\mathcal{O}(ns)$).

Depending on the type of adatom, the effect on intrinsic and extrinsic spin-orbit interaction is of different strength. We study how this influences the relaxation of in-plane or out-of-plane polarized spins.

Lastly we plan to address the questions if adatoms tend to relax spins via the Elliot-Yafet or rather via the Dyakonov-Perel mechanism.

TT 39.2 Thu 9:45 BH 334

Emergent Gauge Fields in Bilayer Graphene — •Roland Winkler[1,2,3] and Ulrich Zülicke[4] — [1]University of Basque Country and IKERBASQUE Foundation, Bilbao, Spain — [2]Northern Illinois University, DeKalb, Illinois 60115, USA — [3]Argonne National Laboratory, Argonne, Illinois 60439, USA — [4]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington 6140, New Zealand

We present a detailed study of the electronic properties of bilayer graphene. Group theory is used to derive an invariant expansion of the Hamiltonian for electron states near the **K** point taking into account the effect of electric and magnetic fields, strain and spin-orbit coupling. We obtain several new gauge fields for band electrons in bilayer graphene, resulting in novel orbital and spin-related effects.

RW is supported by IKERBASQUE Foundation, Bilbao, Spain. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357. UZ is supported by MacDiarmid Institute for Advanced Materials and Nanotechnology.

TT 39.3 Thu 10:00 BH 334

Single-parameter pumping in graphene — •Sigmund Kohler[1], Pablo San-Jose[2], Elsa Prada[1], and Henning Schomerus[3] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain — [2]Instituto de la Estructura de la Materia, CSIC, 28006 Madrid, Spain — [3]Department of Physics, Lancaster University, Lancaster, LA1 4YB, United Kingdom

The ratchet or pump effect, which is the induction of a dc current by an ac force in the absence of any net bias, represents one of the most intriguing phenomena in non-equilibrium transport. For graphene, one expects that its gapless and chiral nature negatively affects pumping, because it hinders the confinement of electrons. Despite this expectation, a pump mechanism that is particularly efficient in graphene exists [1]: It is based on barriers in which the, say, left half is modulated by an ac gate voltage. Then electrons entering the barrier in evanescent modes from that side may be excited to propagating modes. Evanescent mode entering from the right, by contrast, decay before reaching the driving region. This mechanism is rather efficient in graphene, because all evanescent modes within a certain energy range contribute. The corresponding mechanism in a two-dimensional electron gas works only with modes that fulfill certain resonance conditions, which leads to a much smaller pump current.

[1] P. San-Jose, E. Prada, S. Kohler, and H. Schomerus, Phys. Rev. B **80**, 155408 (2011)

TT 39.4 Thu 10:15 BH 334

Self-consistent theory of the second-harmonic generation in graphene — •Sergey Mikhailov — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

A self-consistent-field theory of the second-order nonlinear electromagnetic response of graphene is developed. The second-order polarizability and the corresponding second-order self-consistent dielectric response function of graphene are calculated for the first time. The second harmonic generation in graphene is shown to be about two orders of magnitude stronger than in typical semiconductor structures. Under the conditions of 2D plasmon resonances the second harmonic radiation intensity is further increased by several orders of magnitude.

TT 39.5 Thu 10:30 BH 334

The Hubbard model on the bilayer honeycomb lattice with Bernal stacking — •Thomas C. Lang[1], Stefan Übelacker[1], Zi Yang Meng[2], Michael Scherer[1], Carsten Honerkamp[1], Alejandro Muramatsu[3], Fakher F. Assaad[4], and Stefan Wessel[1] — [1]RWTH Aachen, Aachen, Germany — [2]Louisiana State University, Baton Rouge, USA — [3]Universität Stuttgart, Stuttgart, Germany — [4]Universität Würzburg, Würzburg, Germany

Using a combination of quantum Monte Carlo, the functional renormalization group and mean-field theory we study the Hubbard model on the bilayer honeycomb as a model for interacting electrons on bilayer graphene. The free bands consisting of two Fermi points with quadratic dispersions lead to a finite density of states, which triggers the antiferromagnetic instability and spontaneously breaks sublattice and spin rotational symmetry once a local Coulomb repulsion is introduced. We show that the antiferromagnetic instability is insensitive to the inclusion of extended Coulomb interactions and discuss effects on the sublattice magnetization and of finite size systems in numerical approaches.

TT 39.6 Thu 10:45 BH 334

Coulomb drag in graphene via kinetic equation approach — •Michael Schuett[1], Pavel M. Ostrovsky[1,2], Igor V. Gornyi[1,3], Mikhail Titov[4], Boris N. Narozhny[5], and Alexander D. Mirlin[1,5,6] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [3]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia. — [4]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK — [5]Institut für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [6]Petersburg Nuclear Physics Institute, 188350 St. Petersburg, Russia.

We calculate the Coulomb drag resistivity at finite temperature for two graphene monolayers within the kinetic equation approach. The emphasis is put on the case of fast electron-electron collisions compared to disorder induced scattering. We obtain the asymptotic behavior of the Coulomb drag resistivity ρ_D both for small chemical potentials (μ_1, μ_2) in the two layers as well as chemical potentials larger than temperature. When only one layer is at the Dirac point the Coulomb drag resistivity is zero. However when approaching the Dirac point of both layers simultaneously, the Coulomb drag resistivity does not vanish as long as $\mu_1 \propto \mu_2 \to 0$. For any finite disorder strength or alternating current Coulomb drag resistivity obeys again $\rho_D(\mu_1 = 0, \mu_2 = 0) = 0$, as expected from the particle hole symmetry argument. When both layers have large chemical potentials we recover the Fermi liquid behavior.

TT 39.7 Thu 11:00 BH 334

Manifestation of electron-electron interaction in the magnetoresistance of graphene — •Johannes Jobst[1], Daniel Waldmann[1], Igor V. Gornyi[2,3], Alexander D. Mirlin[2,4,5], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]Inst. für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [5]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We investigate the magnetotransport in large area graphene Hall bars epitaxially grown on silicon carbide. In the intermediate field regime between weak localization and Landau quantization the observed temperature-dependent parabolic magnetoresistivity is a manifestation of electron-electron interaction. We can consistently describe the data with a model for diffusive (magneto)transport that covers the crossover to the ballistic regime. We find a temperature-driven

crossover related to the reduction of the multiplet modes contributing to electron-electron interaction from 7 to 3 due to intervalley scattering. In addition we find a field-driven crossover from purely diffusive to partially ballistic behavior.

15 min. break.

TT 39.8 Thu 11:30 BH 334

Orbital Magnetism in graphene bulk and nanostructures — •Lisa Hesse, Jürgen Wurm, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

We study the magnetic response of finite and bulk graphene structures due to orbital motion of the charge carriers. Besides a semiclassical approach we use exact quantum mechanical calculus within the Dirac formalism to derive different analytic expressions for the magnetic susceptibility of extended systems at various field regimes. This allows us to study on the one hand edge effects which are accessible through our semiclassical treatment but also to gain profound knowledge of the importance of bulk effects in finite systems. In order to provide an independent confirmation of the theory we also perform numerical calculations on graphene nanostructures based on a tight-binding approximation.

TT 39.9 Thu 11:45 BH 334

Klein paradox for arbitrary spatio-temporal scalar potential barrier and Josephson-like current in graphene — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [2]Institut für Physik Universität Augsburg, D-86135 Augsburg, Germany

We derive the exact time evolution according to the Dirac-Weyl equation, describing a mono-layer of graphene, in the presence of a scalar potential $U(x,t)$ of arbitrary spatial and temporal dependence at normal incidence, $p_y = 0$. This solution shows that the Klein paradox (the absence of backscattering) persists even for arbitrary temporal modulations of the barrier. Moreover, we identify an unusual oscillating current j_y running along the barrier, despite of the vanishing momentum in y-direction. This current exhibits resemblence to the Josephson current in superconductors, including the occurance of Shapiro steps and its sine-like dependence on the phase difference of wave functions.

TT 39.10 Thu 12:00 BH 334

Relaxation in graphene quantum dots — •Christoph Neumann[1], Christian Volk[1,2], Sebastian Kazarski[1], Stefan Fringes[1], Stephan Engels[1,2], Bernat Terres[1,2], Jan Dauber[1,2], Stefan Trellenkamp[2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene quantum dots (QDs) have received increasing attention over the last years as interesting candidates for the future implementation of spin qbits. Compared to GaAs-based QDs, their smaller hyperfine and spin-orbit coupling promises more favorable spin coherence times. However, while the preparation, manipulation, and read-out of single spins has been demonstrated in GaAs structures, research on graphene QDs is still at an early stage. Although Coulomb blockade phenomena and excited state spectroscopy is already well established, experimental signatures allowing the identification of relaxation times have been hard to trace. Here we report on pulse gating experiments on graphene quantum devices. We will present measurements of the relaxation rates in single-layer graphene QDs. The investigated devices consist of an island with a diameter of 120 nm, 4 lateral graphene gates and 2 charge detectors. From so-called diamond measurements we extract a charging energy of 11 meV and excited state level spacings of 2-4 meV. The gates enable us to tune the tunnelling rates from the GHz down to the low MHz regime. Finally low-bias pulse gate measurements allow us to extract relaxation rates on the order of 50 ns.

TT 39.11 Thu 12:15 BH 334

Minimal tight-binding model for transport in graphene heterojunctions — •Ming-Hao Liu, Jan Bundesmann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

A real-space Green's function formalism based on a minimal tight-binding model is adopted to efficiently simulate ballistic transport in graphene heterojunctions. The basic idea is to make use of the Bloch theorem along the transverse dimension of the bulk graphene, which greatly reduces the computation load and hence allows experimental sizes in the longitudinal dimension. Numerically, we will show (i) consistency with the existing results based on the effective Dirac theory for chiral tunneling through *pnp* junctions in monolayer graphene (MLG) and bilayer graphene, (ii) good agreement with recent ballistic experiments on *pnp* junctions in MLG, and (iii) new predictions for spin-dependent tunneling through *pn* junctions in MLG in the presence of the Rashba spin-orbit coupling.

TT 39.12 Thu 12:30 BH 334

Quantum Hall effect in graphene with superconducting electrodes — •Markus Weiss, Peter Rickhaus, and Christian Schönenberger — Departement Physik, Universität Basel, Klingelbergstrasse 82, CH-4056 Basel

We report on the realization of an integer quantum Hall system with superconducting electrodes. Graphene was contacted to niobium electrodes that show a critical field of about 4 tesla, where electronic transport passes mainly through quantum Hall edge-states and bulk transport is largely suppressed. We find a magnetic field range of more than one tesla where well developed quantum Hall plateaus coexist with superconductivity in the leads. In high magnetic fields with the electrodes in the normal state we observe plateaus at G=νe^2/h for ν=2, 4, and 10. Reducing the magnetic field to below the upper critical field of the electrodes, the conductance on the plateaus shows a sudden increase. Whereas the conductance on the ν=2 plateau increases only by 10%, the increase on the ν=6 and ν=10 plateau is considerably larger with 60% and 80%, respectively. We attribute this conductance enhancement to multiple Andreev reflection processes along the graphene-superconductor interface, that lead to the formation of Andreev edge-states. The observed conductance enhancement of the ν=6 and 10 plateaus is consistent with a doubling of the conductance contribution of the second and third edge-states. We attribute the small conductance increase on the ν=2 plateau to the special nature of the zero energy Landau level, that makes the corresponding edge-state sensitive to the structure of the graphene edge.

TT 39.13 Thu 12:45 BH 334

Klein paradox for arbitrary spatio-temporal scalar potential barrier and Josephson-like current in graphene — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [2]Institut für Physik Universität Augsburg, D-86135 Augsburg, Germany

We derive the exact time evolution according to the Dirac-Weyl equation, describing a mono-layer of graphene, in the presence of a scalar potential $U(x,t)$ of arbitrary spatial and temporal dependence at normal incidence, $p_y = 0$. This solution shows that the Klein paradox (the absence of backscattering) persists even for arbitrary temporal modulations of the barrier. Moreover, we identify an unusual oscillating current j_y running along the barrier, despite of the vanishing momentum in y-direction. This current exhibits resemblence to the Josephson current in superconductors, including the occurance of Shapiro steps and its sine-like dependence on the phase difference of wave functions. [1] S.E. Savel'ev, W. Häusler, and P. Hänggi, ArXiv: 1107.4983 .

TT 40: Correlated Electrons: Low-dimensional Systems - Materials 3

Time: Thursday 15:00–18:15 Location: H 0104

TT 40.1 Thu 15:00 H 0104

Large quantum fluctuations in the strongly coupled spin-$\frac{1}{2}$ chains of green dioptase: a magic message from birds and trees — Oleg Janson, Alexander Tsirlin, Miriam Schmitt, and •Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

We present a microscopic magnetic model for the natural mineral (green) dioptase $Cu_6Si_6O_{18}{\cdot}6H_2O$. Based on full-potential DFT calculations, we find two relevant exchange couplings in this compound: an antiferromagnetic coupling J_c, forming spiral chains along the hexagonal axis, and a ferromagnetic interchain coupling J_d within the structural Cu_2O_6 dimers. To corroborate the proposed spin model, we perform quantum Monte-Carlo simulations for the dioptase spin lattice. The evaluated ground-state (the propagation vector and the sublattice magnetization) and thermodynamic properties $[\chi(T)]$ are in remarkably good agreement with the experimental data. The refined model parameters are $J_c = 78\,\mathrm{K}$ and $J_d = -37\,\mathrm{K}$ with $J_d/J_c \simeq -0.5$ [1]. Despite the lack of frustration and the 3D nature of the spin lattice, the low coordination number of 3 suffices to cause strong quantum fluctuations, as evidenced by the experiments. Alterations of the J_c–J_d model in closely related compounds will be briefly discussed.

[1] O. Janson, A. A. Tsirlin, M. Schmitt, and H. Rosner, Phys. Rev. B 82, 014424 (2010); arXiv:1004.3765.

TT 40.2 Thu 15:15 H 0104

DFT-based microscopic modeling for the spin-$\frac{1}{2}$ kagome systemherbertsmithite γ-$Cu_3Zn(OH)_6Cl_2$ — •Oleg Janson and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

Herbertsmithite γ-$Cu_3Zn(OH)_6Cl_2$ is a real material realization of the $S = 1/2$ kagome Heisenberg model. Extensive experimental characterization of this compound evidences the absence of long-range magnetic ordering down to 70 mK despite a leading exchange coupling of 190 K [1]. To account for the experimental data, a sizable structural Cu–Zn disorder was suggested. Very recent single crystal experiments revealed that these defects are confined to the interplane sites, while the magnetic kagome layers are almost defect-free [2].

Following the DFT-based study of the closely related compounds kapellasite α-$Cu_3Zn(OH)_6Cl_2$ and haydeeite α-$Cu_3Mg(OH)_6Cl_2$ [3], we apply our computational approach to the more complex case of herbertsmithite. Taking the idealized structure as a starting point, we investigate the influence of the Cu–Zn disorder onto the magnetic coupling regime. The numerical results are compared to the recent single-crystal experiments.

[1] J. S. Helton *et al.*, Phys. Rev. Lett. **98**, 107204 (2007).
[2] T. Imai *et al.*, Phys. Rev. B **84**, 020411(R) (2011).
[3] O. Janson, J. Richter, and H. Rosner, Phys. Rev. Lett. **101**, 106403 (2008); J. Phys.: Conf. Ser. **145**, 012008 (2009).

TT 40.3 Thu 15:30 H 0104

$Ca_2Y_2Cu_5O_{10}$: the first authentic frustrated quasi-1D ferromagnet and a particular rehabilitation of spin wave theory based analysis — •Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Satoshi Nishimoto[1], Jiri Malek[1,3], Jeroen van den Brink[1], Miriam Schmitt[4], Helge Rosner[4], Masaaki Matsuda[5], Kunihiko Oka[6], Hirotaka Yamaguchi[6], and Toshimitsu Ito[6] — [1]IFW-Dresden, ITF, D01171 Dresden, Germany — [2]Inst. f. Problems of Material Sciences, NASU, Kiev, Ukraine — [3]Inst. of Physics, ASCR, Prague, Czech Republic — [4]MPI-CPFS, Dresden, Germany — [5]Quantum Cond. Division, Oak Ridge National Lab., Oak Ridge, USA — [6]AIST, Tsukuba, Ibaraki, Japan

We reexamine the magnetic excitations (ME) for $Ca_2Y_2Cu_5O_{10}$ with edge-shared CuO_2 chains (ESC). For this aim we report inelastic neutron scattering data and present the ME dispersion along $\mathbf{Q} = (H, 0, 1.5)$, unaffected by the main interchain couplings. This allows a precise extraction of the inchain couplings (IC) $J_1 \approx -170\,\mathrm{K}$, $J_2 \approx 32\,\mathrm{K}$. Their ratio $\alpha = |J_2/J_1| \approx 0.19$ indicates an exceptional position in the ESC family: close to the critical point (CP) of the J_1-J_2 spin model $\alpha_c = 1/4$, but on the *ferromagnetic* (FM) side of its phase diagram. The obtained J's agree with the results obtained for a realistic 5-band extended Hubbard *pd* model and L(S)DA+U calculations. We predict Zhang-Rice singlet features in RIXS, EELS and optics visible at 300 K for sizable frustration only. This is the signature of a frustrated FM near a CP. The weak IC determine the predicted saturation field of 65 T and J_1 gives the width of the ME dispersion.

TT 40.4 Thu 15:45 H 0104

NMR measurements on T'-La_2CuO_4, a parent compound of electron-doped cuprate superconductors — •Katharina Weber[1], Marco Günther[1], Hubertus Luetkens[2], Gwendolyne Pascua[2], Roland Hord[3], Barbara Albert[3], Lambert Alff[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon Spin Spectroscopy, PSI — [3]Eduard-Zintl-Institut, TU Darmstadt — [4]Institute of Materials Science, TU Darmstadt

The study of La_2CuO_4 in the metastable T' phase is important for the understanding of the cuprate superconductors, for it allows a direct comparison to its counterpart T-La_2CuO_4, a parent compound of hole-doped cuprates. We present our mircoscopic study of the antiferromagnetically ordered phase of T'-La_2CuO_4. Pulsed ^{139}La-NMR was used to obtain spectra and relaxation rates in a temperature range from 10 to 240 K in an external field of about 5 T. The comparison of the spectra to a simulation allows us to determine the hyperfine field on the La site. The NMR measurements reveal static magnetic order below $T_N = 207$ K in contrast to previous moun spin rotation experiments on the same sample, indicating static order below 115 K [1]. However the NMR spin-lattice relaxation rates imply a change of spin dynamics at 120 K.

[1] R. Hord, H. Luetkens, G. Pascua, A. Buckow, K. Hofmann, Y. Krockenberger, J. Kurian, H. Maeter, H.-H. Klauss, V. Pomjakushin, A. Suter, B. Albert, and L. Alff, Phys. Rev. B 82, 180508(R) (2010).

TT 40.5 Thu 16:00 H 0104

High temperature magnetic heat transport of low-dimensional quantum antiferromagnets — •Oleg Mityashkin[1], Ashwin Mohan[1], Nikolai Hlubek[1], Mahmoud Abdel-Hafiez[1], Christian Hess[1], Bernd Büchner[1], Surjeet Singh[2], Romuald Saint-Martin[3], and Alexandre Revcolevschi[3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Indian Institute of Science Education and Research (IISER), NCL Innovation Park, Pune, India — [3]Laboratoire de Physico-Chimie de L'Etat Solide, Universite Paris-Sud, 91405 Orsay, France

We have investigated the magnetic heat transport of several cuprate materials realizing low dimensional $S = 1/2$ quantum antiferromagnets, in the temperature range [7, 650] K. The results at low temperatures have been obtained using a four-point steady state method, whereas for high temperatures a dynamical laser flash analysis has been employed. In particular, we have studied the spin chain material $SrCuO_2$ and the 2D AFM square lattice La_2CuO_4. We observe a strong suppression of the magnetic heat conductivity with increasing temperature. We analyze and discuss the behavior of the heat conductivity by considering several scattering processes, in particular defect scattering and phonon scattering. Surprisingly, the results for these compounds obtained with the dynamical laser flash method vary with sample thickness. We associate this with a fundamental problem of this measurement technique.

TT 40.6 Thu 16:15 H 0104

Single Crystal Growth and Physical properties of $La_8Cu_7O_{19}$ — •Ashwin Mohan[1], Surjeet Singh[2], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Indian Institute of Science Education and Research (IISER), NCL Innovation Park, Pune, India.

The cuprate $La_8Cu_7O_{19}$ is an example of a low dimensional system having five-leg ladders in its spin structure. It is an interesting candidate to explore the whole range of phenomena occurring in such low dimensional systems and to investigate the resemblance of these odd leg ladders to one dimensional spin chains by probing spin excitations. Here, we present the single crystal growth of this compound and discuss first experimental data of basic physical properties of our crystal.

15 min. break.

TT 40.7 Thu 16:45 H 0104

Exotic Magnetization Plateaux in a Quasi-2D Shastry-Sutherland System — •Gregor Raphael Foltin[1], Salvatore Manmana[2], Frédéric Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl Theoretische Physik 1, Technische Universität Dortmund , D-44221 Dortmund , Germany — [2]JILA , University of Colorado at Boulder, Colorado 80302 U.S.A. — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne , Switzerland

We report our findings for a quasi-2D approximation to the Shastry-Sutherland lattice which we refer to as a 4-leg Shastry-Sutherland tube. This system consists of mutually orthogonal $S = 1/2$ Heisenberg dimers which are coupled via an inter-dimer coupling J'. Using pCUTs and the DMRG, we identify as a function of J' and the magnetic field a series of magnetization plateaux. Here we focus on the ones at 1/8 and 1/4. In contrast to previous findings for coupled dimer systems, quantum fluctuations induced by correlated hopping terms influence significantly the nature of these Mott insulating states. We characterize the state at 1/4 to be a semi-classical one, and the one at 1/8 to possess a stripe structure caused by an interplay of the peculiar geometry and the inter-dimer couplings. This particular finding suggests the system to be in an insulating state in the longitudinal, but a maximally entangled state in the transverse direction. We discuss possible relations of our findings to the full 2D system, which is the underlying model for the description of the quantum magnetic material $SrCu(BO_3)_2$.

TT 40.8 Thu 17:00 H 0104

Pressure evolution of the Shastry-Sutherland magnet $SrCu_2(BO_3)_2$ — •Alexander Tsirlin and Helge Rosner — Max-Planck Institute CPfS, Dresden, Germany

We investigate the evolution of crystal structure and individual magnetic couplings in the spin-$\frac{1}{2}$ Shastry-Sutherland magnet $SrCu_2(BO_3)_2$ under hydrostatic pressure. Our results based on *ab initio* electronic structure calculations suggest the highly anisotropic compressibility of the structure that strongly shrinks along the interlayer c direction, while only weakly changing in the ab plane. This leads to a moderate change in the intralayer exchange couplings J and J' within the Cu_2O_6 dimers and between the dimers, respectively. Above 4.5 GPa, $SrCu_2(BO_3)_2$ transforms into a monoclinic phase that has been scarcely characterized experimentally. We propose an improved structural model of this phase, and identify its spin system as an anisotropic Shastry-Sutherland lattice featuring inequivalent inter-dimer couplings J_1' and J_2'. Our results compare well to the available experimental data, and call for a further investigation of the spin-lattice coupling phenomena in $SrCu_2(BO_3)_2$.

TT 40.9 Thu 17:15 H 0104

Microscopic mechanism for the 1/8 magnetization plateau in $SrCu_2(BO_3)_2$ — •Mike Nemec, Gregor Raphael Foltin, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Tu Dortmund, Germany

The frustrated quantum magnet $SrCu_2(BO_3)_2$ shows a remarkably rich phase diagram in an external magnetic field which is not fully understood theoretically so far. The experimental results show a sequence of magnetization plateaux where the most prominent magnetization plateau is the one at 1/8. Theoretically, one expects that this frustrated quantum magnet should be well described by the Shastry-Sutherland model but recent calculations did not find the same sequence of magnetization plateaux as in experiments. In particular, no 1/8 plateau is found in theory. Here we study the effects of additional magnetic coupling terms like a finite Dzyaloshinskii-Moriya interaction. Most interestingly, the quantum fluctuations induced by such additional magnetic couplings lead very naturally to a stabilization of the 1/8 plateau for realistic values of the magnetic exchange constants.

TT 40.10 Thu 17:30 H 0104

Effect of bond disorder on weakly-coupled spin-1/2 antiferromagnetic Heisenberg chains — •Matthias Thede[1,2], Fan Xiao[3], Elvezio Morenzoni[1], Christopher Landee[3], and Andrey Zheludev[2] — [1]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland — [2]Paul Scherrer Institut, Villigen-PSI, Switzerland — [3]Department of Physics and Carlson School of Chemistry, Clark University, USA.

We study the effect of chemical disorder on magnetic ordering in the quasi-one-dimensional antiferromagnets $Cu(py)_2(Cl_{1-x}Br_x)_2$. The two end compounds are S = $\frac{1}{2}$ linear-chain systems with J = 2.3 meV and J = 4.5 meV, for x = 0 and x = 1, respectively. Weak inter-chain interactions lead to long range order at T_N = 1.1 K and T_N = 0.7 K, respectively. Partial substituting Br for Cl randomizes the bond strength in the spin chains. We probe magnetic and thermodynamic properties of $Cu(py)_2(Cl_{1-x}Br_x)_2$ with susceptibility, specific heat and MuSR measurements. For all samples, the temperature dependence of the magnetic susceptibility follows expectations for a S=$\frac{1}{2}$ Heisenberg chain. Specific heat data reveals more interesting behavior. While at the Cl end a very slow decrease of T_N with x is observed, on the Br side, suppression of T_N relative to x=1 is much more rapid. This disparity in the behavior samples is consistent with MuSR measurements. For the two end-compounds and $Cu(py)_2(Cl_{0.95}Br_{0.05})_2$, there is a clear evidence of static magnetic behavior below T_N. However, $Cu(py)_2(Cl_{0.94}Br_{0.06})_2$ show totally different muon spectra, indicating a strong in homogeneity of the static magnetization.

TT 40.11 Thu 17:45 H 0104

Field driven ordering in a frustrated spin ladder with bond randomness — •Erik Wulf[1], Sebastian Mühlbauer[1], Tatiana Yankova[1,2], and Andrey Zheludev[1] — [1]Neutron Scattering and Magnetism Group, Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland — [2]Chemistry Department, M. V. Lomonosov Moscow State University, Moscow, Russia

We studied the influence of bond randomness on field driven magnon ordering in a frustrated 4-leg ladder. Weak interladder interactions and strong coupling along the ladder legs characterize the almost perfect 1D behavior of $H_8C_4SO_2 \cdot Cu_2Cl_4$. By overcoming the critical field of H_c=3.7T the gap between singlet ground state and excited triplet state is closed. The material undergoes a phase transition from spin liquid to long-range spiral order. Chemical substitution of the nonmagnetic Cl^- ions by Br^- ions causes bond disorder in $H_8C_4SO_2 \cdot Cu_2(Cl_{1-x}Br_x)_4$. The effect on the phase transition was characterized by measurements of the magnetization and the specific heat [1]. It was shown that already low Br^- concentrations of x=1% replace the phase transition by a crossover. While the specific heat data of the pure material exhibit a sharp λ-anomaly the data measured at x $\geq$ 1% show a broad peak. The same behavior is observed in the susceptibility data. In contrast to the transition the critical field itself is almost unaffected.

This work is partially supported by the Swiss National Science Foundation under project 6 of the Materials with Novel Electronic Properties program.

[1] E. Wulf, S. Mühlbauer, T. Yankova and A. Zheludev, Phys. Rev. B **85**, 174414 (2011).

TT 40.12 Thu 18:00 H 0104

ESR studies of the quasi-2D frustrated Cs_2CuBr_4 — •S.A. Zvyagin[1], D. Kamensky[1], J. Wosnitza[1], M. Ikeda[2], T. Fujita[2], M. Hagiwara[2], O.A. Starykh[3], R. Hu[4,5], H. Ryu[4], and C. Petrovic[4] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]KYOKUGEN, Osaka University, Toyonaka, Osaka 560-8531, Japan — [3]Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — [4]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA — [5]University of Maryland, Center for Nanophysics and Advanced Materials, College Pk, MD 20742 USA

We report low-temperature electron spin resonance (ESR) studies of single-crystalline samples of Cs_2CuBr_4, a spin-1/2 antiferromagnet with a triangular spin-lattice structure. A remarkable angular dependence of the resonance field, including the splitting of the ESR line for some orientations of the magnetic field, and the presence of a gap in the ESR excitation spectrum at temperatures above the Neel temperature, T_N = 1.3 K, have been revealed. Our observations suggest that uniform Dzyaloshinskii-Moriya interaction affects the low-energy excitation spectrum in this frustrated compound. The results are compared with that obtained recently for the isostructural material Cs_2CuCl_4 [1].

The work was supported in part by DFG and EuroMagNET II (EU Contract No. 228043).

[1] Povarov et al., Phys. Rev. Lett. 107, 037204 (2011)

TT 41: Focused Session: Cryogenic Detectors

Time: Thursday 15:00–17:30 Location: H 2053

Invited Talk TT 41.1 Thu 15:00 H 2053

Performance and Understanding of Transition-Edge Sensor Microcalorimeters — •Simon Bandler — NASA/Goddard Space Flight Center, Greenbelt, MD, USA — University of Maryland College Park, College Park, MD, USA

Microcalorimeters and bolometers incorporating Transition-Edge Sensor (TES) thermometers are achieving record-setting performance for a wide range of measurements ranging from microwave power to MeV-scale particles. TES thermometers consist of superconducting thin films electrically biased in the resistive transition. In this presentation I will describe recent results from a variety of different microcalorimeters designed for X-ray spectroscopic measurements in astrophysics and solar physics. These devices combine excellent energy sensitivity and high efficiency, can be fabricated in large numbers using lithographic techniques, and can be read out in large numbers using SQUID amplifiers. Despite the record-setting performance and growing utilization of the technology, a theoretical model of the physics governing TES devices' superconducting phase transition has until recently proven elusive. Our group at NASA has shown that TESs exhibit weak-link behavior, where, unlike previous models, the average strength of the order parameter varies over the TES. We find our TES measurements have a natural explanation in terms of a spatially varying order parameter. Implications of weak link behavior for microcalorimeter array design, performance and read-out are discussed.

Invited Talk TT 41.2 Thu 15:30 H 2053

Kinetic Inductance Detectors — •Jochem Baselmans — SRON Utrecht, The Netherlands

Microwave Kinetic Inductance Detectors, MKIDs, combine device simplicity, intrinsic multiplexing capability and a good sensitivity for radiation detection from the UV to the sub-mm part of the electromagnetic spectrum and for high energy particle detection. As a consequence MKIDs are now being developed in a plethora of varieties and for many different applications. Especially at Far Infra-Red-wavelengths band MKIDs offer the possibility to increase the size of detector arrays enormously, which if realized will undoubtedly revolutionize far-infrared astronomy. Arrays for the FIR currently reach photon noise limited performance and a high level of technological maturity, illustrated by the successful demonstration of increasingly large arrays at several ground based observatories such as the CSO, IRAM and APEX. I will address the fundamental limit in device performance, which is due to excess quasiparticle excitations at low bath temperatures $< T_c/10$ and possible mitigation strategies. I will also discuss recent progress in detector multiplexing: Using a single coax cable and one cryogenic microwave amplifier we can read out hundreds of pixels with photon noise limited performance.

15 min. break

Topical Talk TT 41.3 Thu 16:15 H 2053

Magnetic calorimeters for x-ray and particle detection — •Andreas Fleischmann — Universität Heidelberg, INF 227, 69120 Heidelberg,

Metallic magnetic calorimeters (MMC) are calorimetric particle detectors, typically operated at temperatures below 100 mK, that make use of a paramagnetic temperature sensor to transform the temperature rise upon the absorption of a particle in the detector into a measurable magnetic flux change in a dc-SQUID. During the last years a growing number of groups has started to develop MMC for a wide variety of applications, ranging from alpha-, beta- and gamma-spectrometry over the spatially resolved detection of accelerated molecule fragments to arrays of high resolution x-ray detectors. For soft x-rays an energy resolution of 2.0 eV (FWHM) has been demonstrated and we expect that this can be pushed below 1 eV in near future. We give an introduction to the physics of MMCs including the typically observed noise contributions and their impact on the energy resolution. We discuss general design considerations, the micro-fabrication of MMCs and the performance of micro-fabricated devices for a couple of applications.

Topical Talk TT 41.4 Thu 16:40 H 2053

Readout of TESs and MCCs with SQUID current sensors — •Jörn Beyer — Physikalisch-Technsiche Bundesanstalt Berlin

Transition-Edge Sensors (TESs) and Magnetically Coupled Calorimeters (MCCs) are two categories of low-temperature, low-impedance radiation detectors, that have the potential to significantly improve a variety of photon-sensing applications. For example, TES and MCC detectors and systems are under development to detect single THz photons, to enable the measurement of photon number states at telecom wavelengths with very high quantum efficiency or for high-resolution x ray and gamma ray spectrometers. Owing to their excellent sensitivity and dynamic performance as well as their compatibility with the low operating temperatures, current sensors based upon Superconducting Quantum Interference Devices (SQUIDs) are ubiquitously used to read out TESs and MCCs. The required SQUID performance in terms of input referred current noise, dynamic range, bandwidth, acceptable power dissipation and potential back-action can vary substantially for different TES or MCC detectors. Consequently, suitable SQUID current sensors need to be adapted to the readout configuration at hand. Ground- and satellite-based astronomy instruments that use thousands of TES pixels set particularly stringent requirements on the detector readout and require SQUID-based multiplexers. This contribution will review concepts and performance of state-of-the-art SQUID current sensors for single TES and MCC readout as well as SQUID multiplexing techniques.

Topical Talk TT 41.5 Thu 17:05 H 2053

Direct Dark Matter Search with the CRESST II Detector — •Jean-Côme Lanfranchi — Physik-Department E15, TU München, James-Franck-Strasse, 85748 Garching — Exzellenzcluster Universe, Boltzmannstrasse 2, 85748 Garching

CRESST (Cryogenic Rare Event Search with Superconducting Thermometers) is an experiment aimed at the direct detection of Dark Matter. The experiment uses scintillating $CaWO_4$ single crystals operated at mK-temperatures to measure the recoil energy deposited by elastic WIMP (Weakly Interacting Massive Particle) nucleon scattering. By recording phonons as well as the associated scintillation light generated by an energy deposition in the crystal, CRESST is able to achieve a unique background suppression on an event-by-event level. In a two-year measuring campaign CRESST II has gathered $\sim$ 730 kg days of data. In the analyzed data set an excess of events in the region of interest was observed and is at present difficult to explain with contributions from common backgrounds such as alpha-, beta-, gamma-radiation or neutrons. In a maximum likelihood analysis it could be demonstrated that these backgrounds alone are not sufficient to account for the number of events observed. However, the addition of a signal induced by a relatively light WIMP (10-30 GeV) could explain the observed discrepancy on a $\geq 4.2\ \sigma$ level. The associated parameters for such a Dark Matter particle will be discussed. The talk will conclude with an outlook on future efforts to pin down the nature of the observed events and on the low-temperature detector developments required to further reduce background.

TT 42: Superconductivity: Fabrication, Properties, Electronic Structure

Time: Thursday 15:00–18:00 Location: H 3005

TT 42.1 Thu 15:00 H 3005

Angular-dependent specific heat of the fully organic superconductor β''-$(ET)_2SF_5CH_2CF_2SO_3$ - evidence for an FFLO phase — •Rico Beyer[1], J.A. Schlueter[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor (HLD), Forschungszentrum Dresden- Rossendorf (FZD), Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, USA

Since 1964 predicted, there is no clear-cut experimental proof of the

existence of a field-induced superconducting state with finite center of mass momentum ($\mathbf{q} \neq 0$) [1]. In 2007, Lortz *et al.* reported thermodynamic evidence for a FFLO state in κ-$(ET)_2Cu(NCS)_2$ [2], where ET stands for bisethylenedithio-tetrathiafulvalene. They found an emerging sharp double-peak structure in the specific heat, indicating first-order phase transitions at high magnetic fields applied parallel to the superconducting ET layers. Expecting similar novel results for β''-$(ET)_2SF_5CH_2CF_2SO_3$, we performed high-resolution specific-heat measurements for different orientations with very fine steps around perfect parallel alignment. In conclusion, we found an upturn in the field-temperature phase diagram of the superconducting phase beyond the Pauli-Clogston limit and we could observe a double-peak structure above 9,4 Tesla but only by tilting the field 0,2 degree out of the ET sheets. Part of this work has been supported by EuroMagNET, EU contract 228043.

[1] P. Fulde and R.A. Ferrel, Phys. Rev. **135**, A550 (1964); A.I. Larkin and Y.N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964)
[2] R. Lortz *et al.*, Phys. Rev. Lett. **99**, 187002 (2007)

TT 42.2 Thu 15:15 H 3005

Low-temperature transport in ultra-thin tungsten films — •Olivio Chiatti[1,2], Christopher Nash[2], and Paul Warburton[2] — [1]Neue Materialien, Institut f. Physik, Humboldt-Univ. zu Berlin, D-10099 Berlin — [2]London Centre for Nanotechnology, University College London, 17-19 Gordon Street, London, WC1H 0AH, UK

Tungsten-containing films, fabricated by focused-ion-beam-induced chemical vapour deposition, are known to have an enhanced superconducting transition temperature compared to bulk tungsten [1], and have been investigated previously for film thickness down to 25 nm [2]. In this work, by using ion-beam doses below 50 pC/μm^2 on a substrate of amorphous silicon, we have grown continuous films with thickness below 20 nm. The electron transport properties were investigated at temperatures down to 350 mK and in magnetic fields up to 3 T, parallel and perpendicular to the films. The films in this work are closer to the limit of two-dimensional systems and are superconducting at low temperatures. Magnetoresistance measurements yield upper critical fields of the order of 1 T, and the resulting coherence length is smaller than the film thickness.

[1] Sadki et al., Appl. Phys. Lett. **85**, 6206 (2004)
[2] Li et al., J. Appl. Phys. **104**, 093913 (2008); Li et al., IEEE Trans. Appl. Superc. **19**, 2819 (2009)

TT 42.3 Thu 15:30 H 3005

Vibrational and Thermal Properties of ZnX (X=S, Se, Te): Density Functional Theory versus Experiment — •Reinhard K. Kremer[1], Manuel Cardona[1], Robert Lauck[1], Gisela Siegle[1], Aldo H. Romero[2], and Alexander Schindler[3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Departamento de Materiales, Unidad Querétaro, CINVESTAV, Querétaro 76230, Mexico — [3]NETZSCH-Gerätebau GmbH, Wittelsbacherstrasse 42, D-95100 Selb, Germany

We calculated the phonon dispersion relations of ZnX (X=S, Se, Te) employing up-to-date *ab initio* codes. The dispersion relations have been used to evaluate the temperature dependence of the respective specific heats of crystals with varied isotopic compositions. These results are compared with measurements performed on crystals down to 2 K. The calculated and measured data are generally in excellent agreement. Trends in the phonon dispersion relations and the corresponding densities of states for the zinc chalcogenide series of zincblende type materials are discussed.

TT 42.4 Thu 15:45 H 3005

Ultrafast Phonon Hardening in Copper after Femtosecond Laser Excitation — •Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University Kassel, Heinrich-Plett-Str. 40, Kassel, Germany

When a femtosecond laser pulse interacts with a material it produces hot electrons, which can lead to changes in the interatomic potential. As a consequence, the lattice becomes unstable and forces appear on the atoms, driving many interesting ultrafast structural phenomena involving lattice vibrations. In this work we compute the dynamical matrix of copper before and after femtosecond laser excitation. For all phonon modes we find hardening as a function of the electronic temperature in the laser-excited state, which is opposite to the behavior of most materials, which soften when electrons are excited. We use this finding to study the possibility to squeeze the lattice vibrations in copper at low temperatures below the zero point motion.

TT 42.5 Thu 16:00 H 3005

A combined experimental and theoretical de Haas-van Alphen study on $PrPt_4Ge_{12}$ — V. Petzold[1], •B. Bergk[2,3], R. Gumeniuk[1], O. Ignatchik[2], A. Polyakov[2], K. Götze[2], A. Leithe-Jasper[1], W. Schnelle[1], M. Nicklas[1], J. Wosnitza[2], J. Grin[1], and H. Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden – Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [3]Technische Universität Dresden, Institute of Materials Science, D-01069 Dresden, Germany

The skutterudite $PrPt_4Ge_{12}$ superconducts at a surprisingly high temperature of $T_c \approx 8$ K [1]. Furthermore, a remarkably strong coupling [1], a gap function with point-like nodes [2], the exclusion of heavy fermions as an explanation [2], or the breaking of time-reversal symmetry [3] could not yet be arranged in a unified picture.

In this study, we combine band structure calculations and experiments to elucidate the electronic structure of $PrPt_4Ge_{12}$. We treat the strongly correlated 4f electrons of Pr in various approximations. Their reliability is tested by comparing with de Haas-van Alphen (dHvA) measurements on $PrPt_4Ge_{12}$ single crystals.

With the dHvA data-based strategy, introduced in [4], we estimate which parts of the complex Fermi surface are affected by the strong coupling established in the literature [1] .

[1] Gumeniuk et al., PRL **100** (2008) 017002,
[2] Maisuradze et al., PRL **103** (2009) 147002,
[3] Maisuradze et al., PRB **82** (2010) 024524,
[4] Bergk et al., PRL **100** (2008) 257004

TT 42.6 Thu 16:15 H 3005

Electronic structure of doped hydrocarbon superconductors — •Friedrich Roth[1], Benjamin Mahns[1], Matteo Gatti[2], Pierluigi Cudazzo[2], Bernd Büchner[1], Angel Rubio[2], and Martin Knupfer[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastián, Spain

We performed electron energy-loss spectroscopy studies in transmission in order to get a deeper insight into the electronic structure of the potassium intercalated recently discovered aromatic hydrocarbon superconductors, such as picene or coronene. A comparison of the loss function of the undoped and doped compound shows the appearance of a new peak in the case of picene and several new peaks in the case of coronene in the optical gap. For picene we find a remarkable negative plasmon dispersion and a dramatic increase for the value of the background dielectric constant upon doping.

15 min. break.

TT 42.7 Thu 16:45 H 3005

Density functional theory study of alkali doped picene — •Milan Tomić, Hunpyo Lee, Roser Valentí, and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität, Frankfurt am Main, Germany

We have employed density functional theory methods to determine the equilibrium structures of $A_x$picene where A = Na, K, Rb, Cs and x = 1, 2, 3. We have also considered x=4 case in the light of possibility of mixed phase existence. We have found that alkali doping with one, two and three alkali ions per picene molecule leads to subsequent filling of the LUMO and LUMO+1derived bands of picne, leading to quarter, half and three quarter filled systems. We have analysed the electronic structures using tight binding methods to derive the kinetic energy part of the underlying Hubbard Hamiltonian. As the interaction strength U on the picene molecules is expected to be large compared to the bandwidth, we have also employed manybody methods on the resulting Hamiltonian. We have also compared our results to photoemission experiments.

TT 42.8 Thu 17:00 H 3005

Non-metallicity in potassium-doped picene films — •Andreas Ruff[1], Milan Tomic[2], Hunpyo Lee[2], Harald O. Jeschke[2], Roser Valentí[2], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

We have performed a comparative study of the electronic structure of the potassium-doped organic semiconductor picene ($K_x$picene) using

photoemission and density-functional calculations.

Theoretically we have investigated compounds of $K_x$picene with integer $x = 1, 2, 3$ to clarify the atomic positions of the alkali metal dopants and the resulting bandstructure. Experimentally, we recorded a series of photoemission spectra with doping concentrations in the range of $x = 0...3$. While the *ab initio* electronic structure calculations reveal metallic behavior for K_1picene and K_3picene and semiconducting properties for K_2picene, the system remains insulating for all doping concentrations x from the spectroscopic view.

We discuss this discrepancy in terms of possible strong electron correlation effects and/or phonons as well as the occurrence of chemical phase separation in our samples.

TT 42.9 Thu 17:15 H 3005

Energy-Gap Dynamics of a Superconductor NbN Studied by Time-Resolved Terahertz Spectroscopy — •Matthias Beck[1], Paul Leiderer[1], Viktor V. Kabanov[2], Gregory Gol'tsman[3], Manfred Helm[4], and Jure Demsar[1,2] — [1]Dept. of Physics and Center for Appl. Photonics, Univ. of Konstanz — [2]Zukunftskolleg, Univ. of Konstanz, — [3]Moscow State Ped. Univ., Moscow — [4]Helmholtz-Zentr., Dresden-Rossendorf

Using time-resolved terahertz (THz) spectroscopy we performed direct studies of the photoinduced suppression and recovery of the SC gap in a conventional SC NbN. Both processes are found to be strongly temperature and excitation density dependent. The analysis of the data with the established phenomenological Rothwarf-Taylor model enabled us to determine the important microscopic constants: the Cooper pair-breaking rate via phonon absorption and the bare quasiparticle recombination rate. From the latter we were able to extract the dimensionless electron-phonon coupling constant, $\lambda = 1.1 \pm 0.1$, in excellent agreement with theoretical estimates. The technique also allowed us to determine the absorbed energy required to suppress SC, which in NbN equals the thermodynamic condensation energy (in cuprates the two differ by an order of magnitude). Finally, we present the first studies of dynamics following resonant excitation with intense narrow band THz pulses tuned to above and below the superconducting gap. These suggest an additional process, particularly pronounced near T_c, that could be attributed to amplification of SC via effective quasiparticle cooling.

TT 42.10 Thu 17:30 H 3005

Correlation Effects in the Double Photoemission of Pb(111) — •Robert Wallauer, Stefan Voss, Achim Czasch, Lutz Foucar, Till Jahnke, Horst Schmidt-Böcking, and Reinhard Dörner — Institut für Kernphysik, Universität Frankfurt

The investigation of two electrons emitted by a single photon is particulary sensitive to correlation effects, since their coincident emission is forbidden in the absence of any interaction between them. In order to study this process, we setup an experiment in which we measure two electrons in coincidence and can calculate their complete momentum.

We measured a Pb single crystal in superconducting and normal state at Photon energies between 20 and 40 eV. The emission of Cooperpairs has been predicted for this process. Despite of highly improved pulse analysis tools, it could not be identified so far. For photon energies above 25 eV the DPE current is dominated by Auger-processes involving the 5d(5/2) and 5d(3/2) core levels. Both, Auger- and Photoelectron are detected in coincidence and the interaction between them can be studied energy- and angular-resolved.

TT 42.11 Thu 17:45 H 3005

Incorporation of self-organised gold nano crystals in $YBa_2Cu_3O_{7-\delta}$ thin films: Modification of superconducting properties — •Christian Katzer[1], Peter Michalowski[1], Markus Westerhausen[1], Stefanie Koch[1], Frank Schmidl[1], Sebastian Treiber[2], Joachim Albrecht[3], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena, Deutschland — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Deutschland — [3]Hochschule Aalen, Beethovenstraße 1, 73430 Aalen, Deutschland

Using pulsed laser deposition we are able to fabricate and examine Yttrium-Barium-Copper-Oxide (YBCO) thin films of high quality. A particular point of interest thereby is the influence of a pre-deposited gold layer with a well-defined film thickness. During the growth of the YBCO thin film the intermediate gold layer self assembles into crystalline nano particles, which modify the growth conditions and hence the physical properties of the growing YBCO. We report on the modification of structural and superconducting properties of our YBCO thin films (such as rocking curve widths, critical temperature T_c and critical current density j_c) comparing conventional to Au added YBCO. The temperature dependence of the critical current density thereby was determined using transport measurements as well as magneto-optical measurements [1]. Furthermore investigations of the flux noise of our gold modified YBCO films will be presented.

[1] C. Katzer et al., Europhys. Lett. **95** (2011), 68005

TT 43: Correlated Electrons: Metal-Insulator Transition 2

Time: Thursday 15:00–17:45 Location: H 3010

TT 43.1 Thu 15:00 H 3010

Correlation effects in ruthenates: LDA+DMFT study — •Evgeny Gorelov and Eva Pavarini — IAS-3, Forschungszentrum Jülich, 52425 Jülich

The ruthenates of the Ruddlesden-Popper family $A_{n+1}Ru_nO_{3n+1}$ where $A = (Sr, Ca)$ are unique among transition-metal oxides, because the change of cation A and/or in the number n of RuO_2 layers leads to a variety of collective phenomena, ranging from multi-band Mott transitions to ferro- and meta-magnetism. To understand these systems, it is necessary to disentangle the effects of Coulomb repulsion in the $4d^4$ Ru shell from those of lattice distortions and chemistry. By using the LDA+DMFT approach, we show how such disentanglement explains the nature of the metal-insulator transition in single-layered Ca ruthenates [1] and the evolution of electronic structure in n-layered Sr ruthenates [2]. We use LDA+DMFT scheme based on the N-th Order Muffin-Tin Orbital approach and the weak-coupling CT-quantum Monte Carlo method as impurity solver. This method allows us to take into account the full rotationally-invariant Coulomb interaction, as well as full on-site self-energy matrix in orbital space with spin-orbit coupling. We discuss changes in effective mass and orbital polarization as a result of spin-flip processes and spin-orbit interaction.

[1] E. Gorelov et al., Phys. Rev. Lett. **104**, 226401 (2010).
[2] M. Malvestuto et al., Phys. Rev. B **83**, 165121 (2011).

TT 43.2 Thu 15:15 H 3010

Modeling the disordering of the cooperative Jahn-Teller distortion in $KCuF_3$ — •Joaquin Gabriel Miranda[1], Erik Koch[1], and Eva Pavarini[2] — [1]German Research School for Simulations Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich — [2]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich

We study the melting of the cooperative Jahn-Teller distortion. To properly describe this order-disorder transition we have to work with large real-space cells. For this we use a combination of first-principle calculations (LDA+U) and Monte Carlo (MC) simulation. First we determine the potential energy surface for displacements of the fluorine ions. Subtracting the long-ranged Coulomb terms lead to a short-ranged parametrization of the dynamical matrix for pairs of fluorine displacements. We then use the parametrized LDA+U energies as the input for Monte Carlo simulations of extended supercells to study the spacial range of the lattice ordering as a function of temperature.

TT 43.3 Thu 15:30 H 3010

Response of acoustic phonons to charge and orbital order in $LaSr_2Mn_2O_7$ — •Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[2], Ray Osborn[2], Hong Zheng[2], John F. Mitchell[2], Ying Chen[3,4], Songxue Chi[3,4], Jeffrey W. Lynn[3], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne IL, USA — [3]NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg MD, USA — [4]Department of Materials Science and Engineering, University of Maryland, USA — [5]Department of Physics, University of Colorado, USA

The acoustic phonons in the 50% doped bilayer manganite $LaSr_2Mn_2O_7$ exhibiting CE type charge order were investigated using inelastic neutron scattering. At the onset of charge ordering, we observe an abrupt increase(decrease) of the energies(linewidths) of the transverse acoustic phonon along (110), which crosses the CE ordering wavevector. This effect is, however, not localized at the CE ordering wave vector, but is observed over an extended range of momentum transfers, for which the phonon energy is lower than 15 meV. These observations indicate a reduced electron-phonon coupling due to a partial removal of the Fermi surface and provide direct evidence for a link between electron-phonon coupling and charge order in manganites. However, the observed response is not consistent with a standard charge-density-wave mechanism, clearly showing that the transition is unconventional.

TT 43.4 Thu 15:45 H 3010

Hour-glass dispersion in overdoped single-layered manganites — •H. Ulbrich[1], P. Steffens[2], D. Lamago[3], Y. Sidis[3], and M. Braden[1] — [1]University of Cologne — [2]ILL, Grenoble, France — [3]LLB Saclay, France

The mechanism of the high-T_c superconductivity in the cuprates is still an unsolved problem in modern solid state physics. Stripe ordering may play an important role in the physics of high-T_c superconductors. Experimentally, observations of the spin-wave dispersion which forms a shape like an hour-glass have been taken as proof for stripe scenarios in the cuprates [1]. Stripe ordering can be observed in several transition-metal compounds. In manganites, additionally the e_g-orbitals on Mn^{3+} ions play a crucial role. A pattern for the ordering schema in overdoped manganites (x> $\frac{1}{2}$) has just been established [2]. We studied the single-layered systems $Re_{1-x}A_{1+x}MnO_4$ (Re=Pr,Nd; A=Ca,Sr) with x=$\frac{2}{3}$. The position of the magnetic superstructure reflections of Mn^{4+} exhibits a fourfold pattern. Inelastic neutron data around the incommensurate magnetic satellites reveal an hour-glass like spin-wave dispersion, comparable to the cuprates and recently in cobaltates [1,3]. However, our dispersion in the $Pr_{0.33}Ca_{1.67}MnO_4$ compound, which exhibits a large correlation length of the magnetic order, showing a branch dispersing outward from the incommensurate zone-center. Upon heating, the correlation length decreases and concomitantly, the dispersion develops in a full hour-glass shape.

[1] J.M. Tranquada et al., Nature, 429, 534 (2004).
[2] H. Ulbrich et al., Phys. Rev. Lett. 106, 157201 (2011).
[3] A.T. Boothroyd et al., Nature 471, 341 (2011).

TT 43.5 Thu 16:00 H 3010

Signature of antiferromagnetic long range order in the optical spectrum of strongly correlated electron systems — •Ciro Taranto[1], Giorgio Sangiovanni[1], Antoine Georges[2,3,4], Massimo Capone[5], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France — [4]DPMC, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève, Suisse — [5]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, 34136 Trieste, Italy

We show how the onset of a non-slater antiferromagnetic ordering in a correlated material can be detected by optical spectroscopy. Using dynamical mean-field theory we identify [1] two distinct features: The antiferromagnetic ordering is associated with an enhanced spectral weight above the optical gap, and well separated spin-polaron peaks emerge in the optical spectrum. Both features are indeed observed in $LaSrMnO_4$[2].

[1]C. Taranto, G. Sangiovanni, A. Georges, M. Capone, K. Held and A. Toschi, *in preparation.*
[2]A. Gössling, M. W. Haverkort, M. Benomar, Hua Wu, D. Senff, T. Möller, M. Braden, J. A. Mydosh and M. Grüninger, Phys. Rev. B **77** , 035109 (2008).

15 min. break.

TT 43.6 Thu 16:30 H 3010

Orbital-order melting in rare-earth manganites — •Andreas Flesch[1], Guoren Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany

The mechanism of orbital ordering in rare-earth manganites, in particular in $LaMnO_3$, has been debated since long. For $LaMnO_3$, it was recently shown that the purely electronic super-exchange mechanism alone cannot explain the persistence of Jahn-Teller distortions in nanoclusters at high temperature [1]. However, its role in the orbital order-to-disorder transition (orbital-order melting) remains unclear. In this talk, we present order parameter (orbital polarization) and total energy calculations based on the LDA+DMFT approach for the series of rare-earth manganites. By comparing our results to experiments, we show that super-exchange plays a minor role in the orbital-order melting transition observed in rare-earth manganites [2].

[1] E. Pavarini and E. Koch, PRL **104**, 086402 (2010)
[2] A. Flesch, G. Zhang, E. Koch, and E. Pavarini, arXiv:1106.2439

TT 43.7 Thu 16:45 H 3010

Ultrafast strain engineering in complex oxide heterostructures — •Paul Popovich[1], Andrea Caviglia[1], Raoul Scherwitzl[3], Wanzheng Hu[1], Hubertus Bromberger[1], Rashmi Singla[1], Matteo Mitrano[1], Matthias C. Hoffmann[1], Stefan Kaiser[1], Pavlo Zubko[3], Sergio Gariglio[3], Jean-Marc Triscone[3], Michael Först[1], and Andrea Cavalleri[1,2] — [1]Max-Planck Research Group for Structural Dynamics - Center for Free Electron Laser Science, University of Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, UK — [3]Departement de Physique de la Matiere Condensee, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneve 4, Switzerland

The mechanical coupling between the substrate and the thin film is expected to be effective on the ultrafast timescale, and could be exploited for the dynamic control of materials properties. Here, we demonstrate that a large-amplitude mid-infrared field, made resonant with a stretching mode of the substrate, can switch the electronic properties of a thin film across an interface. Exploiting dynamic strain propagation between different components of a heterostructure, insulating antiferromagnetic $NdNiO_3$ is driven through a prompt, five-order-of-magnitude increase of the electrical conductivity, with resonant frequency and susceptibility that is controlled by choice of the substrate material. Vibrational phase control, extended here to a wide class of heterostructures and interfaces, may be conducive to new strategies for electronic phase control at THz repetition rates.

TT 43.8 Thu 17:00 H 3010

Coherent phonons: an all-optic probe of ultrafast structural phase transitions — •Laura Foglia[1], Simon Wall[1], Daniel Wegkamp[1], Kannatassen Appavoo[2], Joyeeta Nag[2], Richard F. Haglund[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber-Institut der MPG, Dep. of Phys. Chem., Berlin, Germany — [2]Dep. of Physics and Astronomy, Vanderbilt University, Nashville, USA

The ionic equilibrium position in a crystal and its vibrational response to an external perturbation are determined by the lattice potential, resulting from the interaction of cores and electrons. During a structural phase transition, the lattice potential symmetry changes, modifying both ionic positions and phonon spectrum. If the transition is driven out of equilibrium, the potential may change on a different time scale than the ionic positions. We exploit the generation of coherent phonons by a laser pulse as an all-optical probe of the lattice potential symmetry with fs time resolution, and apply this technique to the study of the photoinduced phase transition in VO_2. Coherent phonons are observed as a modulation of the broadband transient reflectivity for fluences below the transition threshold $\Phi_c = 6.2 \mathrm{mJ/cm^2}$. This modulation, due to the four lowest Raman active modes of the monoclinic VO_2 phase, disappears above Φ_c. By measuring the coherent response of the excited state in a three pulse experiment, we show that the change of the potential symmetry occurs on a sub-phonon-period time scale, much faster than the lattice rearrangement. We conclude that, in this non-equilibrium regime, the photoinduced phase transition is directly driven by electron-induced changes of the lattice potential.

TT 43.9 Thu 17:15 H 3010

An efficient treatment of the high-frequency tail of the self-energy function and its relevance for multi-orbital models — •Gang Li and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

An efficient and stable method is presented to determine the one-particle Green's function in the hybridization-expansion continuous-time (CT-HYB) Quantum Monte Carlo method, within the framework

of dynamical mean-field theory. The high-frequency tail of the impurity self-energy is replaced by a noise-free function determined by a dual-expansion around the atomic limit. This scheme essentially does not depend on the explicit form of the interaction term and does not introduce additional numerical cost to the runtime simulation. As an application, a 2-orbital Anderson impurity model with a general onsite interaction form is studied. The phase diagram is extracted as a function of the Coulomb interactions for a varity of Hund's coupling strengths.

TT 43.10 Thu 17:30 H 3010

Effective models for spin liquid phases in Hubbard models — Hong Yu Yang[1], Fabrizio Albuquerque[2], Sylvain Capponi[2], Andreas Läuchli[3], and •Kai Phillip Schmidt[4] — [1]Institut de théorie des phénomènes physiques, EPF Lausanne, 1015 Lausanne, Switzerland — [2]Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, 31062 Toulouse Cedex 04, France — [3]Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria — [4]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is one of the most studied microscopic models in condensed matter physics. It describes on a very simple level the interplay between the kinetics and the Coulomb interaction of electrons in solid state systems. Generically, one expects at half filling a metallic phase for large kinetics while a Mott insulator is present for large interactions. In recent years more and more evidences have been found that especially on frustrated lattices there is the possibility of exotic and insulating intermediate phases without long-range order. It is therefore an obviously relevant question what kind of effective low-energy theory describes such Mott phases and how to derive them. This is particular complicated when the spin liquid is located close to the metal-insulator transition as for the recently discovered spin liquid of the Hubbard model on the honeycomb lattice. In this talk we discuss these issues for the Mott phase of the Hubbard model on the triangular and on the honeycomb lattice.

TT 44: Transport: Nanoelectronics III - Molecular Electronics 2

Time: Thursday 15:00–17:15 Location: BH 334

TT 44.1 Thu 15:00 BH 334

Charge transport in single molecule junctions with graphene leads — •Ivan Pshenichnyuk, Susanne Leitherer, Pedro B. Coto, and Michael Thoss — Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

High electron mobility, mechanical rigidity and optical transparency make graphene a promising candidate as material for electrodes in nanoelectronic devices. In this work, we investigate charge transport in single molecule junctions with graphene leads. The methodology used is based on a combination of first-principles electronic structure calculations to characterize the molecule-graphene junctions and the Landauer transport formalism. Considering different examples for molecular bridges between graphene electrodes, in particular pentacene-based molecules as well as polyyne chains, we analyze the transmission probability and the current-voltage characteristics.

TT 44.2 Thu 15:15 BH 334

Thermopower of biphenyl-based single-molecule junctions — •Marius Bürkle[1], Linda A. Zotti[2], Janne K. Viljas[3], Thomas Wandlowski[4], Marcel Mayor[5], Gerd Schön[1], and Fabian Pauly[1] — [1]Institut für Theoretische Festkörperphysik and DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [3]Low Temperature Laboratory, Aalto University, Aalto, Finland — [4]Department of Chemistry and Biochemistry, University of Bern, Bern, Switzerland — [5]Department of Chemistry, University of Basel, Basel, Switzerland

Employing ab initio electronic structure calculations combined with non-equilibrium Green's function techniques we study the dependence of the thermopower on the degree of π-conjugation in biphenyl-based single molecule gold junctions. We control the degree of π-conjugation by changing the torsion angle φ between the two phenyl rings by means of alkyl side chains connected to the molecules. We find that the absolute value of the thermopower decreases weakly as $\cos^2\varphi$. We show that the observed $\cos^2\varphi$ dependence is robust with respect to different anchoring groups and binding positions. The anchoring group determines the sign of the thermopower. Sulfur and amine give rise to $Q > 0$ and cyano to $Q < 0$ respectively. Different binding positions on the contrary lead to variations of the absolute values of the thermopower. The observed ab initio results are found to be described well by means of a π-electron tight binding model.

TT 44.3 Thu 15:30 BH 334

Spin transport and tunable Gilbert damping in a single-molecule magnet — •Milena Filipovic[1], Federica Haupt[2], Cecilia Holmqvist[1], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, D-52056 Aachen, Germany

We study spin transport through a molecular level coupled to two leads and a single-molecule magnet in a magnetic field. The molecular spin is treated as a classical variable and, due to the external magnetic field, precesses around the field axis. Expressions for charge and spin currents are derived by means of the Keldysh nonequilibrium Green's function technique in linear response. The exchange coupling between the electronic spins and the magnetization dynamics of the molecule creates inelastic tunneling processes which contribute to the spin currents. The inelastic spin currents, in turn, generate a spin transfer torque [1,2] acting on the molecular spin. This back-action includes one component that gives a contribution to the Gilbert damping and one component that changes the precession frequency. The Gilbert damping coefficient, α, can be controlled by changing the bias and gate voltages, and has a non-monotonic dependence on the tunneling rates. We compare our results to the Gilbert damping coefficient calculated in Ref. [3] in the small precession frequency regime $\hbar\omega \ll k_B T$.

[1] Y. Tserkovnyak et al., Rev. Mod. Phys. 77, 1375 (2005).
[2] C. Holmqvist et al., Phys. Rev. B 83, 104521 (2011).
[3] N. Bode et al., arXiv:1110.4270v1 (2011).

TT 44.4 Thu 15:45 BH 334

THz torsional vibrations in biphenyl-based molecular junctions: transient oscillations and resonance — •Matthias Hinreiner[1], Dmitry Ryndyk[1], Denis Usvyat[2], Thomas Merz[2], Martin Schütz[2], and Klaus Richter[1] — [1]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [2]Institute for Physical and Theoretical Chemistry, University of Regensburg, Regensburg, Germany

We investigate the torsional vibrations in biphenyl-based molecular junctions and transport properties in presence of an external THz field.

Ab-initio calculations with external electric fields show that the torsional angle ϕ of 4,4'-dithiol-biphenyl demonstrates only very tiny response. However, if functional groups are added to the molecule to induce a dipole moment in each of the rings, an external field can change ϕ. Two examples of such molecules are 3,3'-diflouride-4,4'-dithiol-biphenyl and 2,2'-dithiol-5,5'-bipyridine. As the conductivity of biphenyl-based molecules is proportional to $cos^2(\phi)$, we show that the current through these molecules drops if the external THz field frequency gets in resonance to the torsional vibration mode.

15 min. break.

TT 44.5 Thu 16:15 BH 334

Electron transport through helical, biimidazole-based structures — •Thomas Brumme, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany

Molecular electronics and spintronics provide a promising strategy to overcome limitations of semiconductor-based technologies by implementing electronic functionalities at the molecular scale. However, in order to create single molecule spintronics devices one needs to understand the spin-dependent transport through the molecular system, its dependence on different molecular properties and possible mechanisms to change the magnetization of the molecule. Molecular systems

with screw symmetry like DNA are especially interesting for spintronics applications since the transport through these systems can be spin selective [1]. We investigate the eletronic structure of a molecular helix formed by silver atoms and biimidazole units ($[Ag(NO_3)(H_2\text{biim})]_n$, [2, 3]). First-principles calculations reveal that several molecular orbitals possess screw symmetry and are completely delocalized along the helix. Based on this results we explore the possibility of spin-selective electron transport through this molecular helix.

[1] B. Göhler et al., Science **331**, 894 (2011)
[2] C.A. Hester et al., Polyhedron **16**, 2893 (1997)
[3] M. Sowwan et al., Journal of Nanomaterials **2010** (2010)

TT 44.6 Thu 16:30 BH 334

Spin selective transport through helical molecular systems — •Rafael Gutierrez[1], Elena Diaz[2], Ron Naaman[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany — [2]GISC, Departamento de Fisica de Materiales, Universidad Complutense, E-28040 Madrid, Spain — [3]Department of Chemical Physics, Weizmann Institute, 76100 Rehovot, Israel

Highly spin selective transport of electrons through a helically shaped electrostatic potential is demonstrated in the frame of a minimal model approach. The effect is significant even in the case of weak spin-orbit coupling. Two main factors determine the selectivity, an unconventional Rashba-like spin-orbit interaction, reflecting the helical symmetry of the system, and a weakly dispersive electronic band of the helical system. The weak electronic coupling, associated with the small dispersion, leads to a low mobility of the charges in the system and allows even weak spin-orbit interactions to be effective. The results are expected to be generic for chiral molecular systems displaying low spin-orbit coupling and low conductivity.

TT 44.7 Thu 16:45 BH 334

Quantum Interference Effects in Single-Molecule Junctions — •Stefan Ballmann[1], Rainer Härtle[2], Pedro Brana-Coto[2], Michael Thoss[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany — [2]Institut für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Germany

We analyze quantum interference effects in single-molecule junctions both experimentally and theoretically by means of the mechanically controlled break junction technique, density-functional theory and a non-equilibrium Green's function approach. Interference occurs as a suppression of the current level, when quasi-degenerate electronic states contribute to transport. Such levels are quite common in many molecules used for single-molecule junctions. However, such destructive interference can be lifted by coupling the electron system to vibrations, resulting in an enhancement of the current [1]. We demonstrate that this effect is dominant in single-molecule junctions by analyzing temperature dependent IV characteristics.

[1] R. Härtle, M. Butzin, O. Rubio-Pons, M. Thoss, Phys. Rev. Lett. 107, 046802 (2011).

TT 44.8 Thu 17:00 BH 334

STM transport theory for π-conjugated molecules on thin insulating films — •Sandra Sobczyk, Andrea Donarini, and Milena Grifoni — Institute of Theoretical Physics, University of Regensburg, Germany

In seminal experiments, scanning tunneling microscopy (STM) has been performed on molecules on insulating films having a thickness of only few atomic layers. The layer is in turn grown on top of a metallic surface. At the same time the electrons can still tunnel through the insulating films, facilitating spectroscopy and imaging with low-temperature STM.

We present an STM theory that is sufficiently general to be applied to any STM device consisting of a π-conjugated molecule weakly coupled to the substrate and the tip. We show that the strongly asymmetric coupling to the leads, that is provided by the geometry of the substrate and the tip, leads to qualitatively different, energy dependent transfer rates. We apply the theory to a benzene molecule and we demonstrate that the mentioned differences in the rates yield two different types of current suppression, one caused by Coulomb interaction and one by interference effects due to involved orbitally degenerate states. We also simulate constant height current maps and identify the characteristic topographic fingerprints of the two forementioned blocking mechanisms.

TT 45: Correlated Electrons: Poster Session

We recommend to hang up the posters already during the morning sessions.

Time: Thursday 15:00–19:00 Location: Poster B

TT 45.1 Thu 15:00 Poster B

High-field magnetotransport study of $YbRh_2Si_2$ — •Naren HR[1], Sven Friedemann[2], Cornelius Krellner[1], Christoph Geibel[1], Frank Steglich[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 OHE, United Kingdom

Heavy fermion behavior is expected to be suppressed at magnetic fields high enough such that the Zeeman and the Kondo energy scales become comparable. In the prototypical heavy fermion compound $YbRh_2Si_2$, this scale is estimated to be around 10 T where anomalies have been observed in several thermodynamic quantities [1]. With a focus on this issue we present high-field (upto 15 T) magnetoresistance and Hall effect measurements on $YbRh_2Si_2$ down to 50 mK. We study the temperature evolution of the anomalies observed in our magnetotransport measurements. These features can be favourably compared to those seen in thermopower data [2]. Our measurements shed light on whether the localisation of *f*-electrons at such fields is accompanied by topological transformations of the Fermi surface as speculated in the iso-structural heavy fermion metamagnet $CeRu_2Si_2$ [3,4].

[1] P Gegenwart et al, New. J. Phys. **8**, 171 (2006)
[2] R Daou et al, *this conference*
[3] H Pfau et al, arXiv:1110.1160v1 (2011)
[4] R Daou et al, Phys. Rev. Lett., **96**, 026401 (2006)

TT 45.2 Thu 15:00 Poster B

Magnetic properties of $Yb(Rh_{1-x}Co_x)_2Si_2$ with $x = 0.58$ — •A. Haase[1], O. Stockert[1], C. Klingner[1], C. Krellner[1], S. Matas[2], M. Brando[1], C. Geibel[1], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

The heavy-fermion compound $YbRh_2Si_2$ is an ideal model system to study quantum criticality. Due to its very low antiferromagnetic ordering temperature $T_N \approx 70\,\text{mK}$ and the small ordered magnetic moment, the magnetic structure of $YbRh_2Si_2$ is still unknown. Isoelectronic doping with Co leads to an increase of the ordering temperature T_N and of the ordered magnetic moment. The $(x\text{-}T)$-phase diagram of $Yb(Rh_{1-x}Co_x)_2Si_2$ shows a marked dip in the ordering temperature T_N near a Co concentration of about 50%. This may indicate a change of magnetic structure. For $x > 0.58$ the magnetic structure is incommensurate below T_N with a propagation vector $\tau_1 = (0.25\,0.08\,1)$ followed by a change to a commensurate structure at a lower T_L with $\tau_2 = (0.25\,0.25\,1)$. For $x = 0.58$ only the commensurate magnetic order was found below $T \approx 750\,\text{mK}$ up to now. For lower Co-concentrations the magnetic structure is still unknown. To study the change of magnetic structure in more detail, we performed magnetisation, heat capacity and resistivity measurements on $Yb(Rh_{0.42}Co_{0.58})_2Si_2$, which is near the minimum in the $(x\text{-}T)$-phase diagram. While in zero magnetic field heat capacity and resistivity measurements reveal only one phase transition at $T_N \approx 800\,\text{mK}$, a second transition was detected in the magnetisation at $T = 650\,\text{mK}$ and $B < 0.2\,\text{T}$.

TT 45.3 Thu 15:00 Poster B

Thermoelectric transport in $Ce_{1-x}La_xNi_2Ge_2$ — •Ulrike Stockert[1], Adam P. Pikul[2], Nubia Caroca-Canales[1], Stefanie Hartmann[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institute of Low Temperature and Structure Research, Polish Academy of Sci-

ences, Wrocław, Poland

Investigations of the thermoelectric power S provide a sensitive probe of low energy excitations in metallic systems. In Ce-based heavy-fermion systems, Kondo interaction and crystal electric field (CEF) excitations usually give rise to large positive anomalies in $S(T)$.

We performed thermopower and resistivity measurements on the diluted heavy fermion system $Ce_{1-x}La_xNi_2Ge_2$ between 2 K and 300 K. In this temperature range the Kondo interaction as well as CEF excitations of the Ce^{3+} moments play a major role in the transport and scattering processes of the system. Our thermopower measurements reveal a reduction of the Kondo energy scale from about 30 K to 2 K with decreasing Ce concentration x, while the CEF levels remain almost unchanged. Simultaneously, the crossover from coherent to impurity scattering is observed in the resistivity $\rho(T)$. Interestingly, $\rho(T)$ varies smoothly upon Ce-La substitution, while $S(T)$ changes rather abruptly for high Ce concentrations $x \geq 0.9$. We discuss our findings in comparison to recent specific heat measurements on the system.

TT 45.4 Thu 15:00 Poster B

The hidden order transition in URu_2Si_2 investigated by high-resolution angle-resolved photoemission spectroscopy — •Jan Trinckauf[1], Daniel Shai[2], John Harter[2], Torben Hänke[1], Graeme Luke[3], Kyle Shen[2], and Jochen Geck[1] — [1]IFW Dresden, Germany — [2]Cornell University, Ithaca, USA — [3]McMaster University, Hamilton, Canada

We present a study of the hidden order transition in URu_2Si_2 by means of high-resolution angle-resolved photoemission spectroscopy (ARPES). In particular, we find a strong excitation energy dependence of a flat quasi particle band that is associated with and strongly affected by the hidden order transition[1,2]. We compare our ARPES data to density functional theory (DFT) calculations in the local density approximation (LDA)+U to simulate various degrees of 5f localization.

[1] Santander-Syrio et al., Nat. Phys. 2009
[2] Yoshida et al., Phys. Rev. B 2010

TT 45.5 Thu 15:00 Poster B

Quantum Criticality in $Ta(Fe_{1-x}V_x)_2$ Probed by ^{51}V NMR and Magnetization — •Panchanana Khuntia, Michael Baenitz, Manuel Brando, Alexander Kerkau, Guido Kreiner, and Frank Steglich — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Itinerant $3d$ weak ferromagnets like e.g. $NbFe_2$ or MnSi are tunable towards a (quantum) critical regime by doping, external pressure or magnetic field. The vicinity of a QCP leads to non Fermi liquid (NFL) behavior manifested by scaling laws in bulk properties like magnetization $M(T)$, resistivity $\rho(T)$ and specific heat $C(T)$. In NMR, NFL phenomena are associated with non-Korringa like features in spin lattice relaxation rate $(1/T_1)$ for $T \to 0$. We focus on NMR investigations on polycrystalline $Ta(Fe_{1-x}V_x)_2$ ($x = 0.02, 0.05, 0.2,\ 0.3$) samples. For $x = 0.02$, the magnetic properties are reminiscent of itinerant FM at the verge of a FM instability with enhanced $M(T \to 0)$ indicating FM fluctuations. ^{51}V NMR spectra are broadened inhomogeneously at low temperatures with considerable shift which reflects the hyperfine coupling of itinerant $3d$ moments with the ^{51}V nuclei.$^{51}(1/T_1T)$ violates the Korringa law and exhibits a $T^{-0.8}$ dependence for small fields which is a signature of critical fluctuations. The value of the Korringa product(<1) indicates FM correlations between itinerant moments. Further doping the system undergoes AFM ordering up to $x = 0.3$, where a simple paramagnetic behavior is observed. $Ta(Fe_{1-x}V_x)_2$ is of special interest because FM critical fluctuations evolve in the proximity of an AFM state by nominal V doping.

TT 45.6 Thu 15:00 Poster B

Inelastic Neutron Scattering on the heavy-fermion compound $YbNi_4P_2$ — •Zita Huesges[1], Oliver Stockert[1], Cornelius Krellner[1], Micheal Koza[2], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France

It was recently discovered that the strongly correlated electron compound $YbNi_4P_2$ is one of the few heavy-fermion systems exhibiting a ferromagnetic phase transition at very low temperature (T_C=0.17 K) because of strong Kondo screening. It is thus a very promising candidate to study a Kondo system close to ferromagnetic quantum criticality. While nickel is nonmagnetic in $YbNi_4P_2$, the ytterbium moments are located on chains along the c-direction of the tetragonal unit cell so that the magnetic interaction is mainly one-dimensional. Together with geometrical frustration in the ab-plane , $YbNi_4P_2$ is therefore prone to enhanced quantum fluctuations.

Here, we present time-of-flight neutron spectroscopy measurements on polycrystalline $YbNi_4P_2$ to study the magnetic excitations. This gives insight into the particular magnetic interactions, such as the crystalline electric field and the Kondo fluctuations.

TT 45.7 Thu 15:00 Poster B

Annealing effects in the antiferroquadrupolar compound $U(Pd_{1-x}Pt_x)_3$ — •Dirk Schulze Grachtrup[1], Kerstin Westkämper[1], Markus Schäpers[1,2], Matthias Bleckmann[1,3], Stefan Süllow[1], and Keith A. McEwen[4] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden, Germany — [3]Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe, Erding, Germany — [4]University College London, London, United Kingdom

The double hexagonal compound UPd_3 undergoes several successive phase transitions to antiferroquadrupolar (AFQ) ordered phases below 8 K. Measurements of UPd_3 in magnetic fields reveal a complex response of these AFQ phases to the applied field, leading to a rich magnetic phase diagam [1-3].

Doping of UPd_3 with Pt leads to a rapid suppression of the ordered phases in $U(Pd_{1-x}Pt_x)_3$. Recent studies of single crystalline $U(Pd_{1-x}Pt_x)_3$ in the regime $x \leq 0.01$ revealed a strong reduction of the ordering temperatures with doping. At $x = 0.005$ ordering temperatures are reduced to about one half compared to those of pure UPd_3. For $x = 0.01$ the AFQ order is almost completely suppressed. Here, we present the effects of annealing on specific heat and resitivity of single crystalline samples of $U(Pd_{1-x}Pt_x)_3$.

[1] Y. Tokiwa *et al.*, J. Phys. Soc. Jpn. **70** (2001) 1731
[2] D. F. McMorrow *et al.*, Phys. Rev. Lett. **87** (2001) 057201
[3] H. C. Walker *et al.*, Phys. Rev. Lett. **97** (2006) 137203

TT 45.8 Thu 15:00 Poster B

Field-induced Quantum Critical Point in the heavy-fermion superconductor Ce_2PdIn_8 — •Jinkui Dong[1,2], Yoshi Tokiwa[1], Philipp Gegenwart[1], Shiyan Li[2], Daniel Gnida[3], and Dariusz Kaczorowski[3] — [1]I. Physikalisches Institut, Georg-August-Universität Goettingen, 37077 Goettingen, Germany — [2]Department of Physics, State Key Laboratory of Surface Physics, and Laboratory of Advanced Materials, Fudan University, Shanghai 200433, China — [3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wroclaw, Poland

The in-plane resistivity ρ, specific heat C and thermal conductivity κ of the heavy-fermion superconductor Ce_2PdIn_8 single crystals were measured down to 50 mK. A field-induced quantum critical point, occurring at the upper critical field H_{c2}, is demonstrated from the $\rho(T) \sim T$ near H_{c2} and $\rho(T) \sim T^2$ when further increasing the field. In specific heat measurements, the normal-state electronic specific-heat coefficient displays logarithmically divergent behavior, comparable to $CeCoIn_5$ and in agreement with 2D quantum criticality of spin-density-wave type. The large residual linear term κ_0/T at zero field and the rapid increase of κ(H)/T at low field give evidence for nodal superconductivity in Ce_2PdIn_8. The jump of κ(H)/T near H_{c2} suggests a first-order-like phase transition at low temperature. These results mimic the features of the famous $CeCoIn_5$ superconductor, implying that Ce_2PdIn_8 may be another interesting compound to investigate for the interplay between magnetism and superconductivity.

TT 45.9 Thu 15:00 Poster B

Theory of the Spin Exciton Formation inside the Hidden Order Phase of CeB_6 — •Alireza Akbari and Peter Thalmeier — Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

The heavy fermion metal CeB_6 exhibits hidden order of antiferroquadrupolar (AFQ) type below $T_Q = 3.2$K and subsequent antiferromagnetic (AFM) order at $T_N = 2.3$K. It was interpreted as ordering of the quadrupole and dipole moments of a Γ_8 quartet of localised Ce $4f^1$ electrons. This established picture has been profoundly shaken by recent inelastic neutron scattering [1] that found the evolution of a feedback spin exciton resonance within the hidden order phase at the AFQ wave vector appears and is stabilized by the AFM order. We develop an alternative theory based on a fourfold degenerate Anderson lattice model, including both order parameters as particle-hole condensates of itinerant heavy quasiparticles. This explains in a natural

way the appearance of the spin exciton resonance and the momentum dependence of its spectral weight, in particular around the AFQ vector and its rapid disappearance in the disordered phase. Analogies to the feedback effect in unconventional superconductors and Kondo semiconductors are pointed out.
[1] G. Friemel et al., arXiv:1111.4151.

TT 45.10 Thu 15:00 Poster B

Continuous unitary transformation of the single impurity Anderson model — •Jörn Krones and Götz S. Uhrig — TU Dortmund, Theoretische Physik I, 44221 Dortmund, Germany

Quantum impurity systems, such as the considered single impurity Anderson model (SIAM) have been of significant interest throughout the last decades. An efficient way to deal with the exponentially varying energy scales in such models is the numerical renormalization group (NRG). The free orbital regime (FO) at high energies crosses over to the local moment regime (LM) as energies are decreased with a final crossover to the strong coupling regime (SC) at very small energies. The two crossovers are determined by characteristic energies. The crossover from FO to LM is determined by the coulomb interaction U while the crossover from LM to SC is determined by the exponentially small Kondo temperature T_k. Perturbation theory provides a good description for energies $E \gtrsim T_\mathrm{k}$ but breaks down for $E \approx T_\mathrm{k}$.
It is our aim to use non-perturbative continuous unitary transformations as a new approach to investigate the full energy regime from the conduction electron bandwidth D down to exponentially small energies $E \ll T_\mathrm{k}$. We want to construct an effective Hamiltonian in form of a linear chain similar to Wilson's treatment, labeled by single particle energies and interaction terms.

TT 45.11 Thu 15:00 Poster B

Mean-Field Theory of the Time-Dependent Kondo Effect — •Mohammad Sayad and Michael Potthoff — I. Institut für Theoretische Physik, University of Hamburg, Germany

We propose a generalization of the hybridization mean-field theory [1,2] to Kondo systems far from thermal equilibrium. This time-dependent mean-field approach is used to study the formation or breaking of a Kondo singlet on the time axis. To this end we consider a Kondo impurity on a one-dimensional tight-binding chain as well as on two- and three-dimensional clusters after a sudden change of the exchange-coupling strength. We present results for the ground-state and the finite-temperature equilibrium phase diagram of the Kondo Hamiltonian and for the non-equilibrium final-state dynamics after a quench through the phase boundary and discuss the time-dependent competition of the Kondo effect with the RKKY interaction for systems with two magnetic impurities.
[1] C. Lacroix and M. Cyrot, Phys. Rev. B 20, 1969 (1979)
[2] D. Newns and N. Read, Advances in Physics 36, 799 (1987).

TT 45.12 Thu 15:00 Poster B

Kondo Resonance for Orbitally Degenerate Systems — •Arthur Huber, Aljoscha B. J. Wilhelm, Michael Karolak, Tim O. Wehling, and Alexander I. Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

The Kondo effect is usually connected with the interaction between a localized spin moment and itinerant electrons. However, it is also possible that another internal degree of freedom associated with a degeneracy gives rise to a Kondo effect. One example is the so-called orbital Kondo effect [1], where the pseudospin arising from an orbital degeneracy is screened by the conduction electrons. To acquire a better understanding of this specific Kondo effect, we investigate a general two-band Anderson impurity model within continuous time quantum Monte Carlo simulations [2]. To this end we calculate the static charge susceptibility. Furthermore we investigate, the effects of an external "pseudomagnetic" field in detail.
[1] O.Y. Kolesnychenko *et al.*, Nature (London) **415**, 507 (2002).
[2] E. Gull *et al.*, Rev. Mod. Phys. **83**, 349404 (2011).

TT 45.13 Thu 15:00 Poster B

Numerical renormalization group calculation of total energies and specific heats of quantum impurity models — •Lukas Merker and Theo Costi — Peter Grünberg Institut (PGI-2) and Institute for Advanced Simulation (IAS-3), Forschungszentrum Jülich, 52425 Jülich, Germany

The calculation of thermodynamic properties of quantum impurity models within the numerical renormalization group method proceeds via the impurity contribution to the thermodynamic potential $\Omega_\mathrm{imp} = \Omega_\mathrm{total} - \Omega_0$, where Ω_total, and Ω_0 are the thermodynamic potentials in the presence and absence of the impurity, respectively. Here, we propose a method to obtain specific heats of quantum impurity models via a direct calculation of the internal energy requiring only the evaluation of local static correlation functions. We apply this scheme to the Anderson impurity model and show by direct comparison with the exact results from Bethe Ansatz [1] that it recovers accurately both the Kondo induced specific heat peak at low temperatures as well as the charge fluctuation induced peak at higher temperatures [2].
[1] A. M. Tsvelick and P. B. Wiegmann, Phys. Lett. **89**A, 368 (1982)
[2] L. Merker and T. A. Costi, preprint (2011).

TT 45.14 Thu 15:00 Poster B

Mechanism for Giant Thermopower in negative-U Molecular Quantum Dots — •Theo Costi[1], Sabine Andergassen[2], and Veljko Zlatic[3] — [1]Peter Grünberg Institut (PGI-2) and Institute for Advanced Simulation (IAS-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, 59056 Aachen, Germany and JARA-Fundamentals for Information Technology — [3]Institute of Physics, 10001 Zagreb, Croatia

We investigate with the aid of numerical renormalization group techniques the thermoelectric properties of a molecular quantum dot described by the negative-U Anderson model. We show that the charge Kondo effect provides a mechanism for enhanced thermoelectric power via a correlation induced asymmetry in the spectral function close to the Fermi level. We show that this effect results in a dramatic enhancement of the Kondo induced peak in the thermopower of negative-U systems with Seebeck coefficients exceeding $50\mu V/K$ over a wide range of gate voltages [1].
[1] S. Andergassen, T. A. Costi and V. Zlatić, Phys. Rev. B (arXiv:1101.4124)

TT 45.15 Thu 15:00 Poster B

Distance dependence of the spin-spin correlation function of two Kondo impurities coupled to a one-dimensional Hubbard chain — •Alexander Tiegel, Piet Dargel, and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany

The distance dependence of the ground state spin-spin correlation function $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle$ of two spin-1/2 Kondo impurities antiferromagnetically attached to a one-dimensional Hubbard chain is studied at half-filling. The results are obtained via the density-matrix renormalization group (DMRG) method. In the case of weak couplings one finds a RKKY dominated behavior for all accessible distances. A crossover into the Kondo regime occurs with increasing coupling and inter-impurity distances R. It is especially studied to which extent there exists a power-law decrease of the inter-impurity correlation function. In the absence of an on-site repulsion a $1/R^2$ behavior of the correlations is observed for large distances and strong couplings. Furthermore the asymptotic properties of the correlation function are discussed if the Coulomb interaction is taken into account. The results are supported by perturbation theory.

TT 45.16 Thu 15:00 Poster B

Hubbard-Holstein Model with Dispersive Phonons — •Patrick Haase, Sebastian Fuchs, and Thomas Pruschke — Georg-August Universität, Göttingen, Deutschland

We investigate the local density-of-states in a Hubbard-Holstein model with dispersive phonons. We solve the model in the dynamical mean field approximation using a continuous-time quantum Monte Carlo solver. We extract the local density of states from the imaginary time Green's function by means of the Maximum Entropy method.

TT 45.17 Thu 15:00 Poster B

Numerical Renormalization Group for dissipative quantum impurity systems — •Etienne Gärtner, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zuelpicherstr. 77, 50937 Cologne, Germany

The Numerical Renormalization Group (NRG) has been adapted to treat open dissipative quantum systems, but significant challenges remain. Certain models are well-described by this bosonic NRG in certain parameter regimes, but the essential requirement for Hilbert space truncation causes problems in other situations. Here we develop a novel

extension of the regular bosonic NRG, employing an optimized basis to capture the important low-temperature physics in the smallest possible Hilbert space. We test the method with the paradigmatic spin-boson model, and go on to apply the method to a two-bath variant where truncation effects are typically more severe.

TT 45.18 Thu 15:00 Poster B

From periodic to dilute Anderson models: evolution of scales — •Lucas Hollender, Andrew Mitchell, and Ralf Bulla — Institut für theoretische Physik, Köln, Deutschland

The periodic Anderson model shows a characteristic energy scale below which the magnetic moments are coherently screened by conduction electrons. We examine within DMFT the behavior of this coherence scale as the number of magnetic impurities is reduced. First, we consider periodic systems comprising inequivalent impurity sublattices, and find a subtle interplay between sublattice scales. Dilute impurity behavior is then obtained on decoupling sublattices completely. Finally, we develop an inhomogeneous DMFT approach to study the extreme non-periodic limit of a few randomly distributed impurities, where single-impurity physics can dominate. The simplest two-impurity system can also be solved directly with NRG, and provides a benchmark.

TT 45.19 Thu 15:00 Poster B

Non-Fermi liquid physics in two-channel Kondo models — •Andrew Mitchell — Institut für Theoretische Physik, Universität zu Köln, Germany

The two-channel Kondo (2CK) model possesses a non-Fermi liquid (NFL) quantum critical point, arising when two conduction channels compete to Kondo-screen a single spin-$\frac{1}{2}$ impurity. The two-impurity Kondo (2IK) model also has a NFL critical point. We establish an exact connection between the models, showing that the 2IK critical fixed point is identical to that of a 2CK model with potential scattering. Furthermore, we demonstrate that the same critical physics arises in chains of impurities, and the spin-S generalization of the 2IK model. But conductance lineshapes measurable in experiment encode the full RG flow. We study the onset of NFL physics, showing that distinctive signatures arise as a function of device asymmetry; and the ultimate recovery of standard Fermi liquid behavior resulting from symmetry-breaking perturbations.

[1] Mitchell, Sela, Logan, `arXiv:1111.6503v1` (2011)
[2] Mitchell, Logan, Krishnamurthy, Phys. Rev. B **84**, 035119 (2011)
[3] Sela, Mitchell, Fritz, Phys. Rev. Lett. **106**, 147202 (2011)

TT 45.20 Thu 15:00 Poster B

Out-of-equilibrium steady state properties of the Bose-Fermi Kondo model — •Pedro Ribeiro and Stefan Kirchner — Max-Planck-Institute for the Physics of Complex Systems

We study the out-of-equilibrium steady state properties of the Bose Fermi Kondo describing a local magnetic moment coupled to two leads supporting bosonic and fermionic low energy excitations. The model describes a single-electron transistor with ferromagnetic leads where the magnetization of the two leads is taken to be antiparallel and the effective magnetic field seen by the local impurity vanishes. In such setup, a Kondo peak in the differential conductance can be observed in the Coulomb-blockade regime. The Bose Fermi Kondo captures the essential physical picture as the Kondo effect is critically destroyed upon increasing the coupling to the magnons in the leads. We explore the different regimes of this model using a dynamical large-N approach and study the response functions when a finite bias voltage or a temperature gradient is imposed across the leads. We report the existence of an effective temperature $T_{\rm eff}$ and show that the local susceptibility, as a function of $T_{\rm eff}$ follows the equilibrium scaling form. We also address the electric and thermal current response.

TT 45.21 Thu 15:00 Poster B

Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot — •Sebastian Bock[1,2], Denes Sexty[1,2], and Thomas Gasenzer[1,2] — [1]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany — [2]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

We study the Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot. The quantum dot is coupled between two leads forming a chemical-potential gradient and the tunneling to the leads is taken into account exactly. We apply the functional-integral approach based on the Schwinger-Keldysh closed time path integral to derive the Kadanoff-Baym dynamic equations from the two-particle-irreducible (2PI) effective action. The dynamic equations are derived in non-perturbative approximation of the resummation of the bubble chains to all orders. We analyse the dynamical evolution of the two-point correlation function with respect to the Kondo resonance.

TT 45.22 Thu 15:00 Poster B

Low-energy optics of $Sr_{1-x}Ca_xRuO_3$ — Diana Geiger[1], •Marc Scheffler[1], Martin Dressel[1], Melanie Schneider[2], and Philipp Gegenwart[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]I. Physikalisches Institut, Georg-August-Universität, Göttingen, Germany

The pseudo-cubic perovskite ruthenates $SrRuO_3$ and $CaRuO_3$ have recently attracted interest due to their unconventional electronic properties. For both materials, non-Fermi liquid behavior has been reported in previous optical studies at infrared frequencies. In addition to these two pure compounds, the doping series $Sr_{1-x}Ca_xRuO_3$ offers a rich phase diagram: going from the itinerant ferromagnet $SrRuO_3$ to the paramagnet $CaRuO_3$, indications for a quantum phase transition at x ≈ 0.8 have been found.

Using THz spectroscopy at frequencies between 5 cm^{-1} and 45 cm^{-1}, we have studied thin-film samples of the $Sr_{1-x}Ca_xRuO_3$ system, which were prepared by metalorganic aerosol deposition. From transmission and phase measurements we have determined the frequency-dependent conductivity for a set of temperatures between 5 K and 300 K, and we discuss it in the framework of the extended Drude model with frequency-dependent relaxation rate and effective mass. While for pure $SrRuO_3$ as well as for doped systems approaching the quantum phase transition we find conventional metallic Drude behavior, $CaRuO_3$ exhibits highly unusual optical properties which we compare to results of dc measurements on these thin films, which also revealed temperature ranges with non-Fermi liquid behavior.

TT 45.23 Thu 15:00 Poster B

Quantum critical field and pressure tuning in the heavy fermion ferromagnet $CeAgSb_2$ — •Peter Logg[1], Zhou Feng[1], Takao Ebihara[2], Patricia Alireza[1], Swee Goh[1], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, Shizuoka University, Shizuoka 422-8529, Japan

Quantum critical phenomena have over the past decade been investigated primarily in ferromagnetic or nearly ferromagnetic d-electron systems and in antiferromagnetic f-electron systems. Here, we present a series of measurements of the ferromagnetic cerium compound $CeAgSb_2$. $CeAgSb_2$ is a Kondo-lattice compound which at ambient pressure undergoes a ferromagnetic transition at T_c = 9.6 K. Ferromagnetism is rapidly suppressed by applied hydrostatic pressure, and at pressures > 3.5 GPa it is replaced by an unidentified ordered phase, presumably antiferromagnetism. Alternatively, the ferromagnetic phase may be suppressed to 0K by the application of a magnetic tuning field, which is applied perpendicular to the easy-axis of magnetisation.

We investigate both the P-T and H-T phase diagrams of this compound through a series of ac-susceptibility, resistivity and high-pressure magnetisation measurements.

TT 45.24 Thu 15:00 Poster B

Single crystal growth of $Yb(Rh_{1-x}Ni_x)Si_2$: influence of chemical pressure and electron doping — •Elias Blumenröther, Hirale. S Jeevan, Yoshi Tokiwa, Maik Schubert, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany

$YbRh_2Si_2$ is a well-known heavy fermion compound, which has been investigated intensively due to proximity to an antiferromagnetc field induced quantum critical point (QCP). Recent experimental and theoretical investigations propose that this system displays an unconventional QCP driven by localized moments. We report details of the single crystal growth and physical properties of non-isovalent partial substitution of Rh by Ni. We have grown single crystals of $Yb(Rh_{1-x}Ni_x)Si_2$ for x = 0 to 1 using an Indium-flux method in an oxide crucible. The structure of the single crystals and their composition were investigated by Xray-diffraction and microprobe analysis, respectively. We will report resistivity, specific heat and magnetic susceptibility measurements for various doping concentrations. Ni substitution has a twofold effect: chemical pressure and doping with electrons. By

comparison with isovalent Co substitution and Fe-(hole)-doping, conclusions concerning the influence of chemical pressure and the change in carrier concentration are drawn.

This work is supported by the DFG Reserach Unit 960 (Quantum Phase Transitions).

TT 45.25 Thu 15:00 Poster B

Effect of hole doping and chemical pressure in $Yb(Rh_{1-x}Fe_x)_2Si_2$ — •Manuel Mchalwat, Hirale S. Jeevan, Yoshi Tokiwa, Maik Schubert, and Philipp Gegenwart — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The heavy fermion compound $YbRh_2Si_2$ shows a quantum critical point when the temperature of antiferromagnetic ordering is suppressed to zero by an external magnetic field. Besides the energy scale defined by the quantum critical fluctuations of the order parameter one finds an additional scale T^* which also merges into the quantum critical point. This scale is connected to a reconstruction of the fermi surface, but it is argued whether a Kondo breakdown or a Zeeman-driven Lifshitz transition is the origin. In order to test both hypothesis we synthesized single crystals of $Yb(Rh_{1-x}Fe_x)_2Si_2$ to introduce holes into the system. Thus the electronic structure is changed, which should have a strong influence on the Lifshitz transition. The measured low temperature properties are discussed with respect to both scenarios.

The work has been supported by the DFG through FOR 960 (Quantum Phase Transitions).

TT 45.26 Thu 15:00 Poster B

Spin structure of Fe- and Co-substituted MnSi and MnGe — •Sven-Arne Siegfried[1], Dirk Menzel[1], Sergey Grigoriev[2], Vadim Dyadkin[2], Nadezhda Potapova[2], Evgeny Moskvin[2], Anatoly V. Tsvyashchenko[3], Mathias Kraken[1], and Jochen Litterst[1] — [1]IPKM, TU Braunschweig, Germany — [2]PNPI, Gatchina, Russia — [3]IHPP, Troitsk, Russia

The intriguing magnetic and transport properties of the transition metal-monosilicides TM-Si (TM = Mn, Fe, Co) have been studied extensively during the last thirty years, whereas the properties of the TM-monogermanides are much less investigated due to the complexity of the synthesis. Both systems order in a helical spin structure which can be transformed by a magnetic field into a conical and even a parallel configuration. Close to the ordering temperature a skyrmionic A-phase exists. SQUID magnetization and Mössbauer-spectroscopic measurements on $Mn_{1-x}Co_xSi$ and $Mn_{1-x}Fe_xSi$ have been performed to determine the magnetic phase diagrams. For a critical substitution of Co ($x_{Co} \approx 0.08$) and Fe ($x_{Fe} \approx 0.15$) the ferromagnetic order in MnSi is suppressed. The intermixing compound $Mn_{1-x}Fe_xGe$ has been magnetically characterized for the first time. A preliminary magnetic phase diagram for different Fe-concentrations has been created. Small angle neutron scattering has been used to determine the spin structure of this compound. The monogermanides show a remarkably huge increase of the helix period from 3 nm for MnGe up to 70 nm for FeGe compared to 18 nm for MnSi, and the critical fields H_{C1} and H_{C2} increase from MnGe towards FeGe by the factor of 10.

TT 45.27 Thu 15:00 Poster B

Magnetic order and Spin Dynamics in the Heavy Fermion System $YbNi_4P_2$ — •Johannes Spehling[1], Marco Günther[1], Nicholas Yéche[1], Hans-Henning Klauss[1], Hubertus Luetkens[2], Chris Baines[2], Cornelius Krellner[3], Christoph Geibel[3], and Frank Steglich[3] — [1]Institut für Festkörperphysik, TU Dresden,Germany — [2]Laboratory for Muon-Spin Spectroscopy, PaulScherrer Institut, Villigen, Switzerland — [3]Max-Planck-Institutfür Chemische Physik fester Stoffe Dresden, Germany

A longstanding question in the field of quantum criticality relates to the possible existence of a ferromagnetic (FM) quantum critical point (QCP). At a QCP, collective quantum fluctuations tune the system continuously from a magnetically ordered to a non-magnetic ground state. However, so far no $4f$-material with a FM QCP is found. Recently, in the HF metal $YbNi_4P_2$ with a quasi 1D-electronic structure, FM quantum criticality above a low FM transition temperature of $T_C = 170$ mK was suggested. Our zero field muon spin relaxation on $YbNi_4P_2$ proves static magnetic order with a strongly reduced ordered Yb^{3+} moment below T_C. Above T_C, the muon asymmetry function $P(t, B)$ is dominated by quasi homogeneous spin fluctuations and exhibits a time-field scaling relation $P(t, B) = P(t/B^{\gamma})$ indicating cooperative critical spin dynamics. At $T = 190$ mK, slightly above T_C, $\gamma = 0.81(5)$ K suggesting time-scale invariant power-law behavior for the dynamic electronic spin-spin autocorrelation function. The results will be disussed in comparizon with the AFM compound $YbRh_2Si_2$. [1] C. Krellner *et al.*, New J. Phys. **13**, 103014 (2011).

TT 45.28 Thu 15:00 Poster B

Spin-wave excitations in antiferromagnetically ordered $YbCo_2Si_2$ — •O. Stockert[1], A. Haase[1], K. Schmalzl[2], N. Mufti[1], and C. Geibel[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France

Research on quantum phase transitions continue to be in the focus in condensed matter physics, because systems at quantum criticality show quite unusual low temperature properties including unconventional superconductivity in some cases. The heavy-fermion compound $YbRh_2Si_2$ is a model system to study quantum criticality. Isostructural $YbCo_2Si_2$ can be considered as the magnetically well ordered counterpart allowing for the investigation of the spin excitations in the antiferromagnetic state below $T_N \approx 1.7$ K. The system exhibits well-defined spin waves in the two ordered phases with distinct dispersion. Although the dispersion along several principal directions are almost unchanged between the low temperature commensurate and the high temperature incommensurate phase, some marked differences are observed in the vicinity of (0 0 1). The results help to understand the basic magnetic interactions in this heavy-fermion compound.

TT 45.29 Thu 15:00 Poster B

Towards a complete preparation chain of single crystal intermetallic compounds under UHV compatible conditions — Andreas Bauer, •Ralitsa Bozhanova, Christian Franz, Saskia Gottlieb-Schönmeyer, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

High quality single crystals are perhaps the most important technical requirement for major advances in condensed matter physics. To achieve the highest purity it is crucial to avoid contaminations at any of the preparational steps of the crystal growth process. We report the development of an Ar glove-box with a load-lock system that allows to go from the cutting of the starting elements to the initial synthesis of polycrystals with RF heating in a pure Ar environment. This forms the starting point for single crystal growth by means of rod casting and optical float-zoning under UHV compatible conditions [1]. The improvements in sample preparation achieved with our glove-box are illustrated in terms of exploratory studies of selected rare-earth compounds.

[1] A. Neubauer et al., RSI **82**, 013902 (2011)

TT 45.30 Thu 15:00 Poster B

Compressible Quantum Critical Metamagnetistm — •Mario Zacharias[1], Indranil Paul[1], and Markus Garst[2] — [1]Institute for Theoretical Physics, University of Cologne — [2]Institut Neel, CNRS/UJF, Grenoble, France

For materials close to quantum criticality the critical degrees of freedom couple generically to the crystal lattice. In case of perturbative couplings, this results e.g. in a divergent Grüneisen parameter allowing to probe critical fluctuations by measuring elastic properties. We argue however that for quantum critical metamagnetism, as discussed in the context of $Sr_3Ru_2O_7$ and $CeRu_2Si_2$, such a coupling is necessarily non-perturbative resulting in a modification of the critical behavior. In particular, we show that the metamagnetic transition is exactly described by mean-field theory without long-range critical fluctuations.

TT 45.31 Thu 15:00 Poster B

Thermal expansion and magnetostriction of CePdAl single crystals — •Kai Grube[1], Sebastian Zaum[1,2], Veronika Fritsch[2], Sarah Woitschach[3], Oliver Stockert[3], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The heavy-fermion compound CePdAl exhibits long-range antiferromagnetic order below $T_N \approx 2.7$ K. It adopts a hexagonal ZrNiAl-type crystal structure in which the triangular coordination symmetry of the magnetic Ce ions gives rise to geometrical frustration. Neutron diffraction experiments indicate that below T_N only two thirds of the

Cer ions partcipate in the long-range magnetic order [1]. We have performed thermal expansion and magnetostriction measurements in magnetic fields up to $B = 14\,\mathrm{T}$ parallel to the c-axis to clarify whether an anisotropic distortion of the unit cell can lift the frustration of the remaining Ce^{3+} moments. The uniaxial pressure dependence of T_N is discussed along with the B-T phase diagram of CePdAl. In addition, the thermal-expansion measurements will be used to look for signs of non-Fermi-liquid behavior induced by the nearby quantum critical point at the onset of magnetic order.

[1] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996)

TT 45.32 Thu 15:00 Poster B

Magnetic anisotropy of the Kondo lattice $CePd_{1-x}Rh_x$ probed with polarized neutrons — •Philipp Schmakat[1,2], Michael Schulz[2], Vladimir Hutanu[2,3], Manuel Brando[4], Christoph Geibel[4], Micha Deppe[4], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik-Department E21, Technische Universität München — [2]Forschungs-Neutronenquelle FRM II, München — [3]RWTH Aachen, Institut für Kristallographie — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the magnetic anisotropy of the Kondo lattice system $CePd_{1-x}Rh_x$ at low temperatures by using polarized neutrons at the instrument POLI-HEIDI where the polarization analysis device CryoPad has been installed recently. The system $CePd_{1-x}Rh_x$ shows significant anisotropy for low Rh concentrations $x < 0.6$. With increasing Rh concentration a ferromagnetic quantum phase transition takes place and the anisotropy reduces. The curvature of the phase boundary $T_C(x)$ changes sign at Rh concentration $x = 0.65$ and a cluster glass phase emerges. Our data are consistent with previous measurements of the magnetisation. The measured polarization matrices will allow us to quantify the average domain size in each direction of space and give us important hints of magnetic stray fields of the sample induced even in zero external magnetic field.

[1] J.G. Sereni, Phys. Rev. B 75, 024432 (2007).
[2] T. Westerkamp, Phys. Rev. Lett. 102, 206404 (2009).

TT 45.33 Thu 15:00 Poster B

Low-Dimensional Chiral Physics: Magnetic Catalysis — •Daniel David Scherer and Holger Gies — Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Jena (Germany)

Magnetic catalysis describes the enhancement of symmetry breaking quantum fluctuations in chirally symmetric quantum field theories by the coupling of fermionic degrees of freedom to a magnetic background configuration. We use the functional renormalization group to investigate this phenomenon for interacting Dirac fermions moving in 2+1 dimensional space-time and provide for a clear renormalization-group picture.

TT 45.34 Thu 15:00 Poster B

Effects of dissipation on the phase transition of the disordered O(2) quantum rotor model — •Nicolas Lorscheid and Heiko Rieger — Universität des Saarlandes

Properties of Josephson arrays are conventionally described using the $O(2)$ quantum rotor Hamiltonian. The properties of the occuring quantum phase transition suggest, that the model belongs to the Kosterlitz-Thouless universality class. In order to study the effects of dissipation on this transition, the system is coupled to a dissipative bath of harmonic oscillators. We study the model using an efficient numerical implementation of the real space renormalization group approach, which makes it possible to treat large systems.

TT 45.35 Thu 15:00 Poster B

Quantum Criticality in the pseudogap Kondo model: a dynamical large-N study — •Farzaneh Zamani, Pedro Ribeiro, and Stefan Kirchner — Max Planck Institute for the Physics of Complex Systems

In the pseudogap Kondo model, a continuous zero-temperature phase transition separates a Kondo-screened phase from a Kondo-destroyed local moment phase. This model is a prototype system to study critical Kondo destruction which has been observed in various intermetallic rare earth compounds. It is also the effective low-energy model to describe point-defects in graphene and non-magnetic impurities in d-wave superconductors and can be realized in certain quantum dot systems. We address the critical properties of the SU(N)XSU(M) pseudogap Kondo model in a dynamical large-N limit [1,2]. Applying the scaling ansatz of [1,3], we obtain the leading and critical exponents in the quantum coherent regime ($\hbar\omega \ll k_B T$). Solving the large-N equations, we obtain the full scaling functions in both the quantum coherent and relaxational regime ($k_B T \ll \hbar\omega$). The local critical correlators have the form of a local conformally invariant fixed point although the underlying model lacks conformal symmetry in the bulk.

[1] O.Parcollet et al. PRB 58, 3794 (1998)
[2] M. Vojta, PRL 87, 097202 (2001)
[3] L. Zhu et al., PRL 93, 267201 (2004).

TT 45.36 Thu 15:00 Poster B

Finite size scaling of the typical density of states using the kernel polynomial method — •Daniel Jung[1], Gerd Czycholl[2], and Stefan Kettemann[1,3] — [1]School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany — [2]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [3]Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), San 31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea

We study the metal-insulator transition (MIT) in effective tight binding models (ETBM) by looking at the scaling behaviour of the typical density of states (GDOS) which we obtain by taking the geometrical mean of the local density of states (LDOS) of many different lattice sites and realizations of disorder. The LDOS can be performantly calculated by means of the kernel polynomial method (KPM). Right now we focus on applying this method to the "standard" Anderson model of disorder to check our own implementation and methodical approach and to validate preceding results by others.

TT 45.37 Thu 15:00 Poster B

With DFT and Ewald-summation to realistic parameters in molecular crystals — •Michael M. E. Baumgärtel, Andreas Dolfen, and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany

For the study of strongly correlated molecular crystals the determination of realistic model parameters is an open problem. Rather than fitting to experimental data or semi-empirical approaches, we demonstrate how to determine material-specific parameters for an extended Hubbard model ab-initio. The model can be restricted to HOMO and LUMO by renormalization of the screened Hubbard parameters. While intra-molecular screening is treated within density functional theory, we describe inter-molecular screening by a lattice of distributed polarizabilities. However, the long-range dipole-dipole interaction makes this approach computationally difficult. We can, though, obtain rapidly converging dipole-response matrix elements in reciprocal space using Ewald-summation. We demonstrate this method for TTF-TCNQ.

TT 45.38 Thu 15:00 Poster B

The origin of magnetic and orbital order in K_2CuF_4 — •Guoren Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany

In this work, we investigate the origin of magnetic and orbital order in K_2CuF_4. We first construct Wannier functions from the Bloch states obtained by local-density approximation calculations with the full-potential linearized augmented plane-wave method. Then, by perturbative theory, we calculate magnetic couplings which are in good agreement with experimental results both for the ambient and high pressure structures. To investigate the origin of orbital order, we perform calculations with local-density approximation+dynamical mean-field theory method. We discuss the roles of superexchange[1] and the charge-transfer effects[2] on the orbital ordering.

[1] K. I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].
[2] M.V. Mostovoy and D. I. Khomskii, Phys. Rev. Lett. **92**, 167201 (2004).

TT 45.39 Thu 15:00 Poster B

Energy shifts in pump-probe resonant soft x-ray diffraction experiments — •Christian Schüssler-Langeheine[1], Christoph Trabant[1,2], and Niko Pontius[1] — [1]Helmholtz-Zentrum Berlin — [2]II. Physikalisches Institut, Universität zu Köln

Time resolved pump-probe resonant soft x-ray diffraction is a novel

method to study elementary coupling mechanisms in correlated solids or ultrafast magnetism in antiferromagnets. Besides information about the amount of order and its periodicity also spectroscopic information is accessible via the energy dependence of diffraction features in the vicinity of absorption edges. From that the electronic character of a photo-excited state can be determined. For a quantitative analysis of the energy-dependent diffraction data the effect of absorption has to be taken into account. It leads to particularly strong effects, when the pump effect causes a gradient of the density of scatterers in the probed volume. We discuss, how this effect affects the spectral shape in resonant soft x-ray diffraction data.

Supported by the BMBF through contract 05K10PK2

TT 45.40 Thu 15:00 Poster B

X-ray Photon Correlation Spectroscopy Study of Phase Separation in Correlated Oxides — •Marcel Buchholz[1], Bo Shi[2], Christoph Trabant[1,3], Chun-Fu Chang[1,4], Michael Sprung[5], Vasco Tenner[2], Christian Gutt[5], Alexander Komarek[1,4], Enrico Schierle[3], Gerhard Grübel[5], Markus Braden[1], Jeroen B. Goedkoop[2], and Christian Schüssler-Langeheine[3,1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Van der Waals-Zeeman Instituut, Universiteit van Amsterdam — [3]Helmholtz-Zentrum Berlin — [4]MPI Chemische Physik fester Stoffe, Dresden — [5]Deutsches Elektronen-Synchrotron, Hamburg

In systems with complex phase diagrams phase separation and phase coexistence may occur. Such effects lead to an involved relation between local electronic structure and macroscopic properties and may cause a high susceptibility of the latter to external stimuli. Phase separation has in fact been proposed as the mechanism leading to the colossal magnetoresistance effect in manganites. We report results from a study of phase separation effects in correlated oxides with x-ray photon correlation spectroscopy (XPCS). This technique provides a sensitivity to the local structure as well as to the spatial pattern of domains and to their dynamics. We studied the phase separation effect around the metal-to-insulator transition in doped titanates with soft x-ray photons from BESSY II and high energy x-rays from the ESRF and the ultra brilliant x-ray storage ring PETRA III. Supported by the DFG through SFB 608 and the BMBF through contract 05K10PK2.

TT 45.41 Thu 15:00 Poster B

Theoretical investigations on the magnetic properties of strongly correlated transition metal oxides — •J. Minar, S. Mankovsky, S. Bornemann, H. Ebert, and D. Ködderitzsch — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

We present a detailed theoretical investigation on the magnetic properties of the strongly correlated transition metal oxides MnO, FeO, CoO, NiO in their different magnetic structures. The Calculations were performed scalar as well as fully relativistically using the LSDA+U formalism implemented within the full potential Korringa Kohn Rostoker (KKR) Green's function method. We will show results for the spin and orbital magnetic moments, exchange coupling constants as well as the magnetic anisotropy energies in these systems and we will also discuss how these quantities depend on the Hubbard parameter U.

TT 45.42 Thu 15:00 Poster B

Low-temperature high-pressure optical investigation of the Mott-Hubbard insulator TiOCl — •Jihaan Ebad-Allah[1], Matthias Klemm[1], Siegried Horn[1], Michael Sing[2], Ralph Claessen[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (with X=Cl or Br) are Mott-Hubbard insulators with a charge gap of ≈ 2 eV. Our recent pressure-dependent infrared spectroscopic investigations on TiOX at room temperature [1] suggested that the application of external pressure induces an insulator-to-metal transition. As a follow-up, we studied the infrared transmittance and reflectance spectra of TiOCl at temperatures from 300 K down to 50 K and for pressures up to 22 GPa. Above 14 GPa a huge growth of spectral weight is observed in the optical conductivity spectrum. Furthermore, we determined the temperature and pressure dependence of the crystal field splitting via the frequency of the orbital excitation.

[1] C. A. Kuntscher et al., Eur. Phys. J. Special Topics **180**, 29 (2010).

TT 45.43 Thu 15:00 Poster B

Long range order effects in the Mott-Hubbard transition and the Variational Lattice Approach — •Aljoscha Wilhelm[1], Christoph Jung[1], Hartmut Hafermann[2], and Alexander Lichtenstein[1] — [1]I. Institut fur Theoretische Physik, Universitat Hamburg, Jungiusstrae 9 — [2]Centre de Physique Theorique (CPHT), Ecole Polytechnique, 91128 Palaiseau Cedex, France

We introduce an efficient strategy to treat long ranged correlations in fermionic lattices, the so called variational lattice approach (VLA). The VLA combines the recently developed dual fermion approach for k-dependent problems and the exact diagonalization technique. We present first benchmark results. The phase diagram of the half-filled paramagnetic Mott-Hubbard transition is discussed and results are compared to CDMFT and DCA calculations.

TT 45.44 Thu 15:00 Poster B

Continuous-time quantum Monte Carlo investigation of the metallic state near a Mott insulator — •Junya Otsuki[1,2] and Dieter Vollhardt[1] — [1]Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — [2]Department of Physics, Tohoku University, Sendai, Japan

Motivated by a recently developed theory of extremely correlated Fermi liquids [1], we investigate the t-J model close to half-filling using the extended dynamical mean-field theory in the presence of fermionic and bosonic baths. The effective impurity model is solved by the continuous-time quantum Monte Carlo (CT-QMC) method which we extend to include the spin-boson coupling in the $U = \infty$ Anderson model. Results for the coherence temperature and the single-particle spectra close to the half-filling are presented.

[1] B. S. Shastry, Phys. Rev. Lett. **107**, 056403 (2011).

TT 45.45 Thu 15:00 Poster B

Correlation functions of the spin-1/2 Heisenberg chain at finite temperature via functional equations — •Britta Aufgebauer and Andreas Klümper — Bergische Universität Wuppertal

We present results on static finite temperature correlation functions of the Heisenberg chain on arbitrary successive sites in the thermodynamic limit. The density matrix, encoding all information about the correlation functions on a fixed number of successive sites, is obtained in a suitable limit of the six-vertex model density matrix on a rectangular lattice of unbounded width and finite height with toroidal boundary conditions. We consider an inhomogeneous density matrix. The inhomogeneities enable the derivation of a functional equation of difference type, valid for a finite set of parameter values. This equation in conjunction with the asymptotic behaviour determines the inhomogeneous density operator uniquely.

The functional equation is a discrete version of the so-called reduced quantum Knizhnik-Zamolodchikov equation fulfilled by the density operator at zero temperature. Despite the fundamentally different analytical properties of the correlation functions, it follows that the algebraic structure survives the introduction of a non-zero temperature. In particular the physical input for the calculation of correlation functions on arbitrary successive sites is a finite number of one- and two-point functions.

TT 45.46 Thu 15:00 Poster B

A numerical and an analytical approach to Chalker Coddington type network models — •Win Nuding[1], Michael Brockmann[1], Andreas Klümper[1], and Ara Sedrakyan[2] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Yerevan Physics Institute, Theoretical Department, Yerevan 36, Armenia

Chalker Coddington type network models appear in the context of the Quantum Hall Effect and the Spin Quantum Hall Effect. These network models and corresponding quantum spin chains are investigated to explain plateau - plateau transitions. In the case of integrable $sl(2,1)$ invariant $3 \otimes \bar{3} \ldots$ spin chains, Bethe Ansatz equations were formulated and solved numerically for small systems. For large systems such numerical calculations are not possible. Therefore an alternative approach on the basis of non linear integral equations (NLIE) is presented. The NLIE can be solved for very large systems giving the scaling dimension.

In the non integrable case row transfer matrices can be calculated explicitly yielding for example Lyapunov exponents and the decay length. Since recent high precision numerical simulations of the Lyapunov exponent in the Chalker-Coddington model [1,2] show disagreement with experimental data, we started numerical simulations of the localization length on random networks.

[1] K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304(R) (2009)
[2] M. Amado, A. Malyshev, A. Sedrakyan, F.Dominguez-Adame, Phys.Rev.Lett. 107,066402 (2011)

TT 45.47 Thu 15:00 Poster B

Out of equilibrium energy dynamics in low dimensional quantum magnets — •Stephan Langer[1], Markus Heyl[1], Ian McCulloch[2], and Fabian Heidrich-Meisner[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, LMU München, Germany — [2]School of physical Sciences, The University of Queensland, Brisbane, Australia

We investigate the real-time dynamics of the energy density in spin-1/2 XXZ chains using two types of quenches resulting in initial states which feature an inhomogeneous distribution of local energies. The first involves quenching bonds in the center of the chain from antiferromagnetic to ferromagnetic exchange interactions. The second quench involes an inhomogeneous magnetic field, inducing both, an inhomogeneous magnetization profile and local energy density. The simulations are carried out using the adaptive time-dependent density matrix renormalization group algorithm. We analyze the time-dependence of the spatial variance of the bond energies and the local energy currents which both yield necessary criteria for ballistic or diffusive energy dynamics. For both setups, our results are consistent with ballistic behavior, both in the massless and the massive phase. For the massless regime, we compare our numerical results to bosonization and the non-interacting limit finding very good agreement. The velocity of the energy wave-packets can be understood as average velocity of excitations induced by the quench.

TT 45.48 Thu 15:00 Poster B

Effective quantum dimer models for strongly correlated fermion systems — •Dominik Ixert and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is the standard model for the description of strongly correlated electron systems. Here we focus on single-band Hubbard models at zero temperature and at half filling. Recently, more and more evidences have been found for exotic insulating quantum spin liquid phases close to the metal-insulator transition. We are aiming at a microscopic description of these interesting non-magnetic phases in terms of effective quantum dimer models. To this end we apply graph-based continuous unitary transformations (gCUTs). It is expected that this approach works well as long as the charge and the spin gap is finite which is for example the case for the quantum spin liquid on the honeycomb lattice.

TT 45.49 Thu 15:00 Poster B

Properties of the Heisenberg two-leg Ladder using graph-based Continuous Unitary Transformations — •Johannes-Konstantin Splinter, Kris Cöster, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

Continuous Unitary Transformations (CUTs) have established themselves to handle a variety of strongly correlated quantum many-body systems. The major challenge for the use of CUTs is to find a proper truncation scheme for the flow-equations. Here, we apply a recently developped new truncation scheme which is expected to give reliable effective low-energy models for gapped phases of quantum lattice models. The basic idea is to combine graph theory and CUTs. These intrinsically robust graph-based continuous unitary transformations (gCUTs) are used to calculate zero- and one-triplon properties of the antiferromagnetic S=1/2 Heisenberg ladder. In order to optimize the gCUTs, we implement the full symmetry group of the ladder system.

TT 45.50 Thu 15:00 Poster B

Comparison of TEBD and NRG methods for computing the nonequilibrium dynamics of nanosystems coupled to a bosonic bath — •Malcolm Einhellinger[1], Eric Jeckelmann[1], Sabine Tornow[2], and Gertrud Zwicknagl[2] — [1]Leibniz Universität Hannover — [2]TU Braunschweig

We investigate the applicability of the Time-Dependent Renormalization Group (TEBD) Algorithm to low-dimensional quantum systems coupled to a bosonic bath. For that purpose we compare outcomes from TEBD realtime simulations with results from the Time-Dependent Numerical Renomalization Group (TD-NRG) Algorithm which has been shown to work well for those kind of problems. In this regard, we study the transport from a donor to an acceptor structure, connected via a bridge molecule. Coupling donor and acceptor to a bosonic bath damps the normally occuring oscillations in the particle densities and gives new insights in the physics of transport effects through bridge molecules.

TT 45.51 Thu 15:00 Poster B

Projective approach to transport in weakly interacting 1-d fermionic quantum systems — •Christian Bartsch — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig

We investigate transport properties of 1-d fermionic hopping models featuring nearest and next-nearest neighbor hopping, where the fermions are additionally subject to a weak mutual interaction. To this end we employ a pertinent approach which allows for a mapping of the underlying Schrödinger dynamics onto an adequate linear quantum Boltzmann equation. This approach is based on a suitable projection operator method. From this Boltzmann equation we are able to numerically obtain diffusion coefficients for the limit of long times and weak interactions in the case of non-vanishing next-nearest neighbor hopping, whereas the diffusion coefficient diverges without next-nearest neighbor hopping. For the latter case we analytically investigate the decay behavior of the current with the result that parts of the current relax arbitrarily slow which suggests anomalous diffusive transport behavior within the scope of our approach.

TT 45.52 Thu 15:00 Poster B

Possible gapless spin liquid in the Kagome Lattice — •Xue-Feng Zhang and Sebastian Eggert — Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

We studied the Hard-Core Bose-Hubbard Model with nearest neighbor repulsion. In the solid phase, we find a new representation to describe the degeneracy of the ground state. By using the Strong Coupling Expansion and the Quantum Monte Carlo simulation, we got the solid melting critical lines for both positive and negative hopping process. And such phase transitions are induced by the fractional charge excitation.

Considering the superfluid and solid phase respectively break different symmetry, we think such second order melting process would not happen between them and the gapless spin glass intermediate phase may exist there.

TT 45.53 Thu 15:00 Poster B

Supersolid phase transitions for hardcore bosons on a triangular lattice — Xue-Feng Zhang, •Raoul Dillenschneider, and Sebastian Eggert — Physics Dept. and Res. Center OPTIMAS, Univ. of Kaiserslautern, 67663 Kaiserslautern, Germany.

Hard-core bosons on a triangular lattice with nearest neighbor repulsion are a prototypical example for a system with supersolid behavior on a lattice. We show that in this model the physical origin of the supersolid phase can be understood quantitatively and analytically by constructing quasiparticle excitations of defects that are moving on an ordered background.

TT 45.54 Thu 15:00 Poster B

The Density Matrix Renormalization Group for spin-1/2-quantum chains: A demonstration program — •Thomas Köhler, Piet Dargel, and Andreas Honecker — Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

We have implemented a density matrix renormalization group algorithm in the formulation of Matrix-Product-States as Web Applet. This implementation offers direct visualization of the running algorithm including energy, static correlation functions and entropy convergence. It offers the computation of several different Spin-1/2-Hamiltonians and we have explicitly evaluated the Ising-chain in a transversal magnetic field.

TT 45.55 Thu 15:00 Poster B

Lanczos algorithm with Matrix Product States for dynamical correlation functions — •Piet Dargel[1], Anton Wöllert[2], Andreas Honecker[1], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München

The Lanczos algorithm is combined with Matrix Product States to calculate dynamical correlation functions. The use of Matrix Product States allows to handle systems that are larger than those accessible

within the standard Lanczos algorithm, for the price of worse convergence of the spectral poles as compared to the original algorithm. In order to achieve a better convergence of the spectral weights and poles we introduce an ex post reorthogonalization method and also test spectral shifts. We present results for the dynamic spin structure factor of the spin-1/2 antiferromagnetic Heisenberg chain. These results are compared to Bethe ansatz results in the thermodynamic limit.

TT 45.56 Thu 15:00 Poster B

cRPA study of a three band one-dimensional Hubbard model — •Michael Seissinger and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Starting from a three band one-dimensional model, we derive an effective one band low energy model using a functional integral formulation of the cRPA approach. The effective model with retarded interactions can be simulated with continuous time weak coupling QMC methods. Our aim is to monitor the variation of the Luttinger liquid exponent as function of the energy scale of the high energy bands which are integrated out in the cRPA approach.

TT 45.57 Thu 15:00 Poster B

QMC impurity solvers for two-particle Green's functions. — •Pavel Augustinský[1,2] and Jan Kuneš[2] — [1]Universitaet Augsburg — [2]Institute of Physics, Academy of Sciences of the Czech Republic

The fundamental observable for QMC impurity solvers, the one-particle Green's function, does not contain a complete information about the studied system. The two-particle Green's function brings additional insight into electronic correlations, response functions and related quantities absent in the one-particle case. However, measurement of 2P Green's functions involves technical difficulties. We present comparison of the Hirsch-Fye and the continuous-time QMC techniques for 2P Green's functions. Namely, we address performance issues and discuss areas of applicability.

TT 45.58 Thu 15:00 Poster B

Band structure engineering and vacancy induced metallicity at the GaAs-AlAs interface — •Mousumi Upadhyay Kahaly, Safdar Nazir, and Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

We study the epitaxial GaAs-AlAs interface of wide gap materials by means of full-potential density functional theory based calculations. We find an insulating state at the interface and a negligible charge transfer. Optimization of the atomic positions results in very small changes in the chemical bonding. We aim to understand how an anionic defect at and near the interface modifies the electronic structure and therefore the physical properties of the GaAs-AlAs heterostructure. Introduction of As vacancies near the interface induces metallicity, which opens great potential for GaAs-AlAs heterostructures in modern electronics. While GaAs and AlAs are known since long to form high quality epitaxial superlattices, the effect of n-doping on the electronic properties of this heterostructure has been ignored so far. The systems under investigation are suitable for disentangling the complex behavior of metallic interface states.

TT 45.59 Thu 15:00 Poster B

Magnetic excitations in the diamond spin system $Cu_3(CO_3)_2(OH)_2$ probed by ESR — •Dmytro Kamenskyi[1], Mykhaylo Ozerov[1], Frederik Wolff-Fabris[1], Joachim Wosnitza[1], Sonia Francoual[2], Vivien Zapf[3], and Sergei Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]Hamburger Synchrotronstrahlungslabor (HASYLAB), Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — [3]National High Magnetic Field Laboratory - Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We report systematic tunable-frequency electron spin resonance (ESR) studies of the natural mineral azurite $Cu_3(CO_3)_2(OH)_2$. This material has a diamond spin-chain structure and exhibits unusual magnetic properties (including a magnetization plateau). ESR experiments have been done at frequencies from 50 to 1000 GHz in magnetic fields up to 51 T. The observed frequency-field dependence of the magnetic excitations clearly indicates the important role of magnetic frustrations in this material, which can be suppressed by high magnetic fields. Our findings are discussed in connection with results of inelastic neutron-scattering experiments. Work was supported by EuroMagNET II (EU contract No. 228043).

TT 45.60 Thu 15:00 Poster B

NMR on the quasi two-dimensional antiferromagnet $Ba(Ni_{1-x}Mg_x)_2V_2O_8$ — •Dirk Waibel[1], Thomas Wolf[2], Hilbert v. Löhneysen[1,2], and Bernd Pilawa[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

Magnetic-field dependent NMR measurements in the quasi two-dimensional (2D) antiferromagnet (AF) $Ba(Ni_{1-x}Mg_x)_2V_2O_8$ have been performed for $\mathbf{B} \perp \mathbf{c}$ and $\mathbf{B} \parallel \mathbf{c}$ at 2 K and 79 MHz. The spin echo signal of the ^{51}V nuclei in the undoped sample consists of one distinct peak for $\mathbf{B} \parallel \mathbf{c}$ which is split into three lines for $\mathbf{B} \perp \mathbf{c}$. The signals of the ^{51}V nuclei significantly broaden upon doping. Futhermore, the ^{51}V nuclear spin-lattice relaxation rate T_1^{-1} has been measured over a temperature range from 6 K to 300 K at 7 T and 79 MHz revealing a strong increase of the T_1^{-1} rate at $T_N = 47.4$ K. This divergent behavior has been analyzed for $\mathbf{B} \perp \mathbf{c}$ and $\mathbf{B} \parallel \mathbf{c}$ in the context of the 2D topological Berezinskii-Kosterlitz-Thouless (BKT) phase transition. Also, the oscillatory decay of the spin echo due to the quadrupole interaction of the ^{51}V $\left(I = \frac{7}{2}\right)$ nuclei is clearly visible in the temperature range from 50 K to 300 K.

TT 45.61 Thu 15:00 Poster B

Atomically resolved images of lithium purple bronze — •Melanie Klinke[1], Robert Bienert[1], Michael Waelsch[1], Tatjana Podlich[1], Rongying Jin[2], and René Matzdorf[1] — [1]Experimentalphysik II, Universität Kassel, Deutschland — [2]Department of Physics and Astronomy, Lousiana State University, USA

The lithium molybdenum purple bronze $Li_{0.9}Mo_6O_{17}$ is a quasi 1D metal at room temperature showing Luttinger liquid physics. The highly anisotropic conductivity runs along the crystallographic b axis where Mo-O chains, formed by the shared edges of the MoO_6 octahedra, provide the electrical transport. $Li_{0.9}Mo_6O_{17}$ samples were investigated with low-temperature scanning tunneling microscopy and spectroscopy. By cleaving the samples at low temperatures (60 K) we obtained atomically resolved images of the surface. In these images the Mo-O chains are visible, which are covered by layers of MoO_6 octahedra and MoO_4 tetrahedra.

TT 45.62 Thu 15:00 Poster B

Non-linear transport properties of pure, Rb- and W-doped blue bronze $K_{0.3}MoO_3$ — •Ali Khairi Al-Hadeethi[1], Dominik Grund[1], Song Yue[2], Martin Dressel[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The temperature dependence of the dc resistivity and the non-linear transport properties of pure, Rb-doped, and W-doped blue bronze $K_{0.3}MoO_3$ single crystals are presented. These are prototypical charge-density-wave (CDW) compounds. Nonlinear conductivity due to the sliding of the CDW is observed, when the applied electric field exceeds the first threshold field (E_T). Furthermore, above a second threshold field ($E_T{}^* > E_T$) coherent CDW-sliding sets in. For all studied materials E_T and $E_T{}^*$ increase monotonically with decreasing temperature . This finding is discussed in terms of the incommensurate-commensurate transition of the CDW and within the frame of the Fukuyama-Lee-Rice model.

TT 45.63 Thu 15:00 Poster B

Thermal conductivity of the $S = 1/2$ two-leg spin-ladder compound bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY) — •Gerhard Kolland[1], Johannes Engelmayer[1], Mark M. Turnbull[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Carlson School of Chemistry and Department of Physics, Clark University, Worcester, Massachusetts, USA

Bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY) is a model material for a Heisenberg $S = 1/2$ two-leg spin-ladder with antiferromagnetic couplings $J_{\mathrm{rung}} \simeq 4.3\,\mathrm{K}$ (along the rungs of the spin-ladder) and $J_{\mathrm{leg}} \simeq 8.4\,\mathrm{K}$ (along the legs) in the strong-leg regime, i.e. $J_{\mathrm{leg}} > J_{\mathrm{rung}}$. In zero magnetic field, the spin ladder has a finite excitation gap, which is closed at a lower critical field $B_{C1} \simeq 3\,\mathrm{T}$, where the system enters a gapless Luttinger-liquid (LL) phase. At the

saturation field $B_{C2} \simeq 30\,\mathrm{T}$ the system leaves the LL phase and a gap opens. We present measurements of the magnetic-field dependent thermal conductivity κ. The field was applied along the b direction. To investigate a magnetic contribution to κ, we measured the thermal conductivity parallel $\kappa_{||}$ and perpendicular $\kappa_{\perp}$ to the ladder direction. At higher temperatures around 2 K, the magnetic-field influence is rather similar for both directions. We observe a broad minimum around 5 T, which sharpens and approaches B_{C1} with decreasing temperature. In addition, the magnetic-field dependent thermal conductivity gets anisotropic. Below 1 K, $\kappa_{||}$ is strongly enhanced, whereas $\kappa_{\perp}$ stays almost constant. *Supported by the DFG through SFB 608.*

TT 45.64 Thu 15:00 Poster B

Magnetic ordering transitions of the effective XY-spin-$\frac{1}{2}$ compound Cs_2CoCl_4 in transverse magnetic fields — •Oliver Breunig[1], Eran Sela[2], Benjamin Buldmann[2], Markus Garst[2], Petra Becker[3], Ladislav Bohatý[3], Christian Dax[1], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 is a model system for studying the magnetism of one-dimensional spin chains. It contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The groundstate doublet is separated from the first excited doublet state by approximately 15 K, such that at temperatures between 0.3 and 4 K the compound is well described by the one-dimensional XXZ model. Decreasing temperature further, magnetic order arises at field-dependent temperatures $T_C(H)$. According to [1] spins are confined to the bc-plane in the ordered phase. Measuring thermal expansion with a magnetic field applied along the crystallographic b-axis, we observe a series of magnetic transitions within the ordered state. We discuss thermodynamic properties of the magnetically ordered state.

This work was supported by the DFG through SFB 608.

[1] M. Kenzelmann et al., Phys. Rev. B **65** (2002).

TT 45.65 Thu 15:00 Poster B

Phase diagram of the Ising chain compound Nb_2O_6 in transverse magnetic field — •Simon Scharffe, Oliver Breunig, Johanna Frielingsdorf, Martin Valldor, Michael Seher, and Thomas Lorenz — II. Physikalisches Insitut, Universität zu Köln

$CoNb_2O_6$ is a model system to investigate a quantum phase transition in magnetic fields. The structure consists of layers of CoO_6 octahedrons separated by non-magnetic NbO_6 layers. Within each layer the Co^{2+}spins are linked through superexchange and form 1D ferromagnetic zigzag chains along the c axis. Due to crystal field effects (compression of the CoO_6 octahedrons) an easy-axis anisotropy of the Co^{2+}moments is present, which leads to an effective spin-1/2 system described by the Ising model. The easy axis is in the a c plane, and alternates by $\pm$ 31° with respect to the c axis for neighboring chains. Due to small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$ the system shows long-range antiferromagnetic order, which is insommensurate below T_{N1}=2.9K and becomes commensurate at T_{N2}=1.9K. A magnetic field parallel to the b axis is normal to the easy axis and allows to study the quantum phase transition of an Ising-spin chain in tranverse field. The system is driven to its quantum critical point between a quasi 1D ferromagnet to a quantum paramagnet. Only few studies of the transverse field case are available so far. We present measurements of specific heat and magnetization in a temperature range from about 0.3 to up to 10 K and discuss the phase diagram.

This work was supported by the DFG through SFB 608.

TT 45.66 Thu 15:00 Poster B

Quasi one-dimensional spin chain materials $AM_2V_2O_8$ — •Michael Seher, Sandra Niesen, Gerhard Kolland, Oliver Heyer, Simon Scharffe, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

Compounds with the general formula $AM_2V_2O_8$ with an alkaline-earth on the A-site and a transition-metal on the M-site show a lot of interesting properties. This class of compounds is mainly isostructural with tetragonal symmetry and provides spin chain structures. The magnetic properties are vitally influenced by the chosen transition metal with its partially filled 3d shell. Thus, these compounds are suitable to study spin systems from $S = 1/2$ to 5/2 and spin quantum number anisotropy can be studied from Ising- to Heisenberg behavior. Here, we present a detailed study on the magnetic phase diagram of the effective $S = 1/2$ Ising system $BaCo_2V_2O_8$. Moreover, we have grown large single crystals of the nearly isotropic Heisenberg systems $BaMn_2V_2O_8$ and the new compound $SrMn_2V_2O_8$. At higher temperatures both compounds behave like 1D magnetic systems. But due to finite interchain couplings both systems show long-range antiferromagnetic order with T_N = 37 K (A= Ba) [1] and T_N = 43 K (A= Sr) [2].

This work is supported by the DFG through SFB 608.

[1] Z. He *et al.* Solid State Comm. **141** (2007) 22
[2] S.K. Niesen *et al.* J. Mag. Mag. Mat. **323** (2011) 2575

TT 45.67 Thu 15:00 Poster B

NMR evidence for peculiar spin gaps in a doped S=1/2 Heisenberg spin chain — •Yannic Utz[1], Christian Rudisch[1], Franziska Hammerath[1], Hans-Joachim Grafe[1], Ashwin Mohan[1], Surjeet Singh[2], Romuald Saint-Martin[3], Alexandre Revcolevschi[3], Patrick Ribeiro[1], Christian Hess[1], Anja Wolter[1], Vladislav Kataev[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]Indian Institute of Science Education and Research, Pune, India — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris-Sud, Orsay, France

We present ^{63}Cu Nuclear Magnetic Resonance (NMR) measurements on undoped, Ca-doped and Ni-doped $SrCuO_2$ single crystals. $SrCuO_2$ is a good realization of a one-dimensional S=1/2 Heisenberg spin chain. This is manifested by the theoretically-expected temperature-independent NMR spin-lattice relaxation rate T_1^{-1}. In $Sr_{0.9}Ca_{0.1}CuO_2$ an exponential decrease of T_1^{-1} below 90 K evidences the opening of a gap in the spin excitation spectrum, which amounts to $\Delta = 50\,\mathrm{K}$ [1]. DMRG calculations are presented to discuss the origin of this spin gap. New results on $SrCu_{0.99}Ni_{0.01}O_2$ also indicate the presence of a spin gap, which is twice as large as in $Sr_{0.9}Ca_{0.1}CuO_2$, despite the minor doping level of Ni compared to Ca. We discuss different possible impacts of Ca (S=0) and Ni (S=1) doping on structural and magnetic properties of the parent compound.

[1] F. Hammerath et al., Phys. Rev. Lett. **107**, 017203 (2011).

TT 45.68 Thu 15:00 Poster B

Thin film growth and characterization of the neutral-ionic phase transition system tetrathiafulvalene-p-chloranil — •Achim Rippert, Milan Rudloff, Kai Ackermann, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

Tetrathiafulvalene-p-chloranil (TTF-QCl4) thin films have been prepared by physical vapor deposition of the pre-reacted source material on different substrate materials. We studied the growth characteristics and electronic transport properties with a view to the influence of substrate-induced effects, such as clamping and strain, on the electronic properties of the layers. TTF-QCl4 is a mixed-stack organic charge transfer compound that shows a temperature-driven paraelectric-to-ferroelectric phase transition associated with a charge of the charge transfer degree at 81 K. This phase transition brings about a distinct change of the electrical conductivity, an anomaly of the frequency dependent dielectric function, as well as a color change of the material. Via partial Br-Cl-substitution the phase transition can be shifted to 0 K resulting in a quantum critical state. Our research aims for taking advantage of thin-film specific control mechanisms, such as induced biaxial strain and electrostatic field effects, and thus providing a new perspective on the neutral-ionic phase transition in the one-dimensional, mixed-stack organic charge transfer compounds.

TT 45.69 Thu 15:00 Poster B

ESR studies of the quasi-2D antiferromagnet $Cu(Pz)_2(ClO_4)_2$ — •M. Ozerov[1], J. Wosnitza[1], E. Čižmár[2], F. Xiao[3], M.M. Turnbull[3], C. P. Landee[4], and S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD),Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]Centre of Low Temperature Physics, P.J. Šafárik University, SK-041 54 Košice, Slovakia — [3]Carlson School of Chemistry and Biochemistry, Clark University, Worcester, Massachusetts 01610, USA — [4]Department of Physics, Clark University, Worcester, Massachusetts 01610, USA

We report systematic high-field electron spin resonance (ESR) studies of the quasi-two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet $Cu(pz)_2(ClO_4)_2$ (pz denotes pyrazine or $C_4H_4N_2$). The linewidth and resonance-field temperature dependences of the ESR absorptions in this compound were investigated in the frequency range from 85 to 416 GHz in magnetic fields up to 16 T. A pronounced ESR linewidth

anomaly was revealed in the vicinity of T_N. This anomaly reflects enhanced critical fluctuations in this compound at the 3D ordering. The experiment revealed a significant change in the linewidth behavior for magnetic fields above 7 T, whose origin will be discussed.

The work was supported in part by DFG and EuroMagNET II (EU Contract No. 228043).

TT 45.70 Thu 15:00 Poster B

$Cs_2CuCl_{4-x}Br_x$: perspectives of experimentally tunable frustration in a triangular lattice — •Kateryna Foyevtsova, Ingo Opahle, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 with an underlying triangular lattice demonstrate rich magnetic phase diagrams, where one finds a spin-liquid phase for Cs_2CuCl_4 and quantum fluctuation stabilized magnetization plateaux for Cs_2CuBr_4. The magnetism of Cs_2CuCl_4 and Cs_2CuBr_4 might be understood in terms of the triangular Heisenberg model with different degrees of frustration: $J'/J \sim 0.3$ for Cs_2CuCl_4 and $J'/J \sim 0.7$ for Cs_2CuBr_4. Recently, mixed systems $Cs_2CuCl_{4-x}Br_x$ have been synthesized for a dense mesh of x values from 0 to 4, which suggests that it might be possible to tune the J'/J ratio by varying x. We apply the density functional theory to study the crystal and electronic structures of some members of the $Cs_2CuCl_{4-x}Br_x$ series. In particular, we are interested in the microscopic equilibrium distribution of the substituted halogen atoms which affects the spin exchange couplings J and J'. We also discuss the two structural phases – orthorhombic and tetragonal – that might emerge during crystal growth, depending on the growth conditions.

TT 45.71 Thu 15:00 Poster B

Searching for the Power-Law Conductivity Inside the Mott Gap in κ-$(ET)_2Cu_2(CN)_3$ — •Sebastian Elsässer[1], John A. Schlueter[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Argonne Nat. Lab., U.S.A.

The organic charge-transfer salt κ-$(ET)_2Cu_2(CN)_3$, which is a Mott insulator, has recently gained interest as possible realisation of the spin-liquid state in two dimensions. This phenomenon is due to spin frustration in the nearly isotropic triangular lattice where spin fluctuations are enhanced and do not order even at the lowest temperatures despite comparable strong antiferromagnetic interactions [1]. Also, spin-liquids support exotic excitations like spinons. Although spinons do not carry charge and thus can not interact with the electromagnetic field directly, they couple to the induced gauge field, leading to a contribution to optical conductivity inside the charge gap. For low frequencies a power-law conductivity $\sigma_1 \propto \omega^{3.33}$ for $\hbar\omega > k_BT$ and $\sigma_1 \propto \omega^2$ for $\hbar\omega < k_BT$ is predicted [2]. To verify this on a quantitative basis, we performed polarisation dependent optical investigations ranging from 23 - 8000 cm^{-1} at temperatures from 300 K - 12.6 K. We find that a power-law is applicable over a wide range inside the Mott gap, however, the exponent clearly deviates from the proposed values as it is actually much lower. The temperature-dependent crossover could not be observed as well. Upon cooling, a saturation of the power-law is observed.

[1] Y. Shimizu *et al.*, Phys. Rev. Lett. **91**, 107001 (2003)
[2] T.-K. Ng and P. A. Lee, Phys. Rev. Lett. **99**, 156402 (2007)

TT 45.72 Thu 15:00 Poster B

Pressure-dependent resistivity measurements on the novel charge-transfer salt (BEDT-TTF)$_2$Cu$_2$Br$_3$ — •Sebastian Köhler[1], Ulrich Tutsch[1], Friedhelm Isselbächer[1], Michael Lang[1], Frauke Schödel[2], Hans-Wolfram Lerner[2], and Matthias Wagner[2] — [1]Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TRR49, D-60438 Frankfurt (M) — [2]Institut für Anorganische Chemie, Goethe-Universität Frankfurt (M), D-60438 Frankfurt (M)

During the course of optimizing parameters for the synthesis of the known charge-transfer salt (BEDT-TTF)$_2$Cu[N(CN)$_2$]Br, a novel salt, (BEDT-TTF)$_2$Cu$_2$Br$_3$ has been obtained [1]. It is known that other compounds from this family of materials exhibit a variety of electronic properties such as (Mott-)insulating, semiconducting, metallic or even superconducting behaviour, accessible by either chemical or hydrostatic pressure. Resistivity measurements have been performed at ambient pressure on single crystals of (BEDT-TTF)$_2$Cu$_2$Br$_3$ in a temperature range from 300 K down to 10 K, yielding a semiconductor-like behaviour with a small gap of about 30 meV. Our aim is to study the possibility of closing the semiconducting gap by applying hydrostatic pressure and thereby to induce metallic or even superconducting behaviour. We present measurements of the resistance under hydrostatic pressure on (BEDT-TTF)$_2$Cu$_2$Br$_3$ in a temperature range from 300 K to 4 K at various pressure values.

[1] Eur. J. Inorg. Chem. 2011, 1205-1211

TT 45.73 Thu 15:00 Poster B

Critical behavior at the antiferromagnetic phase transition of Azurite — •P. T. Cong, B. Wolf, R. S. Manna, A. Brühl, S. Köhler, and M. Lang — Physikalisches Institut, J.W. Goethe-Universität Frankfurt, SFB/TR49, 60438 Frankfurt(M)

The natural mineral azurite has been considered as a model substance for a 1D spin 1/2 Heisenberg diamond chain [1]. However, early studies of this material indicate the presence of 3D long-range antiferromagnetic (AF) order below $T_N \sim 1.88$ K [2]. Clear signatures of the transition into the ordered phase have been observed in ultrasound, thermal expansion and specific heat measurement at T_N. Here we present a detailed investigation of the critical behavior of the sound velocity and ultrasonic attenuation in the vicinity of T_N. While the critical velocity changes exhibit a uniform behavior for various magnetic fields, the critical attenuation shows a sudden change as the system moves from the ordered AF to the spin-flop state. We compare the critical behavior derived from the ultrasonic studies with that observed in the specific heat and thermal expansion.

[1] H. Kikuchi *et. al.*, Phys. Rev. Lett. **94**, 227201 (2005).
[2] H. Forstat *et. al.*, J. Chem. Phys. **31**, 929 (1959).

TT 45.74 Thu 15:00 Poster B

Surface Topology and Electronic Structure of Layered Strontium Ruthenates — •Robert Bienert[1], Melanie Klinke[1], Michael Waelsch[1], Sebastian Mietke[1], Jin Peng[2], Zhiqiang Mao[2], and René Matzdorf[1] — [1]Experimentalphysik II, Universität Kassel, Deutschland — [2]Department of Physics, Tulane University, New Orleans, USA

In complex materials the interplay of properties like crystal structure, electronic structure and magnetism results in very interesting physical phenomena. The Ruddlesden-Popper series of layered Strontium Ruthenates $Sr_{n+1}Ru_nO_{3n+1}$ describes one class of these materials.

The double and triple layer systems behave like a Fermi liquid up to the transition temperature of 15 K and 24 K, respectively. In both compounds the local density of states (LDOS) shows a peak within the dip-like feature around the Fermi energy E_F. Using low-temperature (LT) STM and STS we studied the temperature dependence of the LDOS in the range from 4.7 to 35 K. By increasing the temperature the peak within the dip in the LDOS at E_F is only affected by thermal broadening.

The surface unit cell of the Strontium Ruthenates exhibits a $c(2\times2)$ super structure, which is stable from 4.7 K up to room temperature as shown by our atomically resolved LT STM images and room temperature LEED experiments.

TT 45.75 Thu 15:00 Poster B

^{139}La-NMR in the T'-La_2CuO_4 antiferromagnetic phase — •Marco Günther[1], Katharina Weber[1], Hubertus Luetkens[2], Gwendolyne Pascua[2], Roland Hord[3], Barbara Albert[3], Lambert Alff[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon Spin Spectroscopy, PSI — [3]Eduard-Zintl-Institut, TU Darmstadt — [4]Institute of Materials Science, TU Darmstadt

We study the antiferromagnetic ordered phase of T'-La_2CuO_4, a recently synthesized parent compound of electron doped cuprate superconductors by means of I= $\frac{7}{2}$ ^{139}La-NMR spectroscopy and powder spectra simulation.

The observed field sweep spectra at temperatures range between 10-240 K are compared with simulations of the combined nuclear Zeeman- and quadrupole-hamiltonian. In this approach the experimentally found line broadening arises from a local hyperfine field parallel to the copper-oxygen planes and is interpreted as the order parameter showing magnetic order below 207 K. We construct the hyperfine fields in a local electronic antiferromagnetic dipole model. Our results are compared to other local probe experiments on parent compounds of cuprate superconductors.

TT 45.76 Thu 15:00 Poster B

Magnetic Impurity with Generalized Couplings to Antiferromagnetic Heisenberg Chains — •Björn Willenberg[1,3], Jan Grelik[2,3], Wolfram Brenig[1,3], and Holger Frahm[2,3] —

[1]Institute for Theoretical Physics, Technische Universität Braunschweig — [2]Institute for Theoretical Physics, Leibniz Universität Hannover — [3]Niedersächsische Technische Hochschule, NTH

We investigate magnetic spin-S impurities in contact to S=1/2 Heisenberg chains with open boundary conditions and an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo based on Stochastic Series Expansion. Results will be presented for thermodynamic properties as a function of temperature, exchange-coupling constants, anisotropy, magnetic fields, and system size. These include the energy, susceptibilities, magnetization and static correlation functions. For particular settings the models we investigate are integrable by Bethe Ansatz and we will compare findings from both methods in the limit of zero temperature.

TT 45.77 Thu 15:00 Poster B

Spin diffusion in the Heisenberg Chain: a quantum Monte-Carlo study — •Yousef Rahnavard[1,2], Björn Willenberg[1,2], and Wolfram Brenig[1,2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Niedersächsische Technische Hochschule, NTH

We study the long-wavelength, finite frequency spectrum of the spin density response of the antiferromagnetic Heisenberg chain. Current proposals for this, based on results from bosonization, transfer-matrix renormalization group, and quantum Monte-Carlo (QMC), suggest a diffusive spectrum in the isotropic case with a diffusion kernel independent of frequency and momentum which is diverging in the low temperature limit. Here we extend on the previous QMC work, which has been restricted to a single system size only. Results will be presented for the low frequency current relaxation rate versus momentum and temperature, for various system sizes from N=64 to 256. Moreover signatures of anomalous diffusion will be checked for by considering potential power-law frequency dependence of the diffusion kernel.

TT 45.78 Thu 15:00 Poster B

Helimagnets studied with neutron spin echo at RESEDA — •Jonas Kindervater[1,2], Wolfgang Häussler[1,2], Alexander Tischendorf[1,2], Andreas Bauer[1], Christian Pfleiderer[1], and Peter Böni[1] — [1]Technische Universität München, Physik Departement E21, 85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRMII), 85748 Garching, Germany

Using RESEDA (FRM II, Munich), several studies on magnetic fluctuations in ferro- and helimagnetic compounds have been performed. RESEDA uses the Neutron Resonance Spin Echo (NRSE) technique, being a variant of conventional Neutron Spin Echo (NSE). In NRSE as in NSE, the beam polarization is the measured quantity. It provides the intermediate scattering function yielding information on the slow dynamics of the sample. However, NRSE experiments on magnetic systems, which affect the beam polarization, are difficult or even not feasible at all. In this contribution, we present the results of elastic and quasi-elastic scattering experiments on manganese silicide. We summarize the data analysis, proofing the polarizing effect of the sample, and taking into account this feature in the normalization of the results from quasi-elastic measurements.

TT 45.79 Thu 15:00 Poster B

Orbitons and bi-orbitons in $GdVO_3$ and YVO_3 — •Luis Fels[1], Michael Voigt[1], Komalavalli Thirunavukkuarasu[1], Eva Benckiser[2,1], Giacomo Ghiringhelli[3], Marco Moretti Sala[3], Graeme R. Blake[4], Nandang Mufti[4], Agung A. Nugroho[4,5], Thomas T. M. Palstra[4], Pasquale Marra[6], Krzysztof Wohlfeld[6], Jeroen. van den Brink[6], Maurits Haverkort[2], Thorsten Schmitt[7], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung — [6]IFWDresden — [7]Paul Scherrer Institut, Villigen

Here we report on optical measurements and high-resolution RIXS on $GdVO_3$ and YVO_3 single crystals. The goal of the measurements is the observation of so called orbitons which are, in analogy to magnons, collective orbital excitations on top of an orbitally ordered state. In both investigated compounds a G-type orbital ordered (OO) phase occurs, but only in YVO_3 an additional low temperature phase with C-type OO exists.

In the optical conductivity $\sigma(w)$ of $GdVO_3$, a striking feature is seen at 0.4 eV in the OO phase which is interpreted as bi-orbiton in agreement with further investigations on YVO_3 and $HoVO_3$ [1]. With the RIXS measurements it was possible to observe a significant dispersion of the intra-t_{2g} excitations at roughly 0.2 eV. However, the origin of this dispersion, whether it is due to a collective character of the excitations or a local effect, is still unclear.

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TT 45.80 Thu 15:00 Poster B

Ground state properties of antiferromatgnetic anisotropic S=1 Heisenberg spin chains — •David Peters — Institut für Theoretische Physik, RWTH Aachen, 52064 Aachen

Using (infinite) density matrix renormalization group techniques, ground state properties of antiferromagnetic S=1 Heisenberg spin chains with exchange and single–site anisotropies in an external field are studied. The phase diagram is known to display a plenitude of interesting phases. We elucidate quantum phase transitions between the supersolid and spin–liquid as well as the spin–liquid and the ferromagnetic phases. Analyzing spin correlation functions in the spin–liquid phase, commensurate and (two distinct) incommensurate regions are identified.

TT 45.81 Thu 15:00 Poster B

Transport of an electron through a spin structure inside a quantum wire — •Christoph Hübner and Daniela Pfannkuche — I. Institut für Theoretische Physik, Hamburg, Germany

Transport properties of a quantum wire with embedded impurities is investigated in the framework of a numerically exact scattering formalism. The itinerant electrons are considered to interact with the impurities via a finite range exchange interaction. This leads to scattering of an initial wave package into different modes and spin states. We can map the integral Lippmann-Schwinger equation onto a system of linear equations. The solution of this equations is called the T-matrix. This matrix is directly related to the time dependent spacial and spin probability distribution of the itinerant electrons. The conductance of the quantum wire is associated with the transmission coefficients via the Landauer-Buettiker formula. It can be shown that the coefficients linearly depend on the elements of the T-matrix. Focus of our investigation lies on the cooperative dynamics of the impurities mediated by the conduction electrons. Screening effects of impurity momenta by localization of electrons are also of interest.

TT 45.82 Thu 15:00 Poster B

Thermal expansion investigation on EuB_6 — •Rudra Sekhar Manna[1], Frank Schnelle[1], Mariano de Souza[1], Michael Lang[1], Pintu Das[1], Adham Amyan[1], Jens Müller[1], Stephan von Molnár[2], Peng Xiong[2], and Zachary Fisk[3] — [1]Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Department of Physics, Florida State University, Tallahassee, Florida 32306, USA — [3]Dept. of Physics, University of California, Irvine, California 92697, USA

EuB_6 is a semimetallic correlated electron system, which exhibits a complex sequence of electronic and magnetic phase transitions at $\sim$ 15.5 K (T_1) and 12.5 K (T_2). The material also shows a colossal magnetoresistance effect which is largest at T_1. The paramagnetic to ferromagnetic transition in this system is suggested to take place via the formation of magnetic polarons. In this work, we investigate by means of thermal expansion and magnetostriction measurements to which extent lattice degrees of freedom are involved in these phase transitions. We find two corresponding anomalies in the thermal expansion, the one occurring at T_2 being much larger than that at T_1. The anomalies are very sensitive to magnetic fields. By applying a small magnetic field of less than 50 mT the anomaly at T_1 is fully suppressed, while the lower-temperature anomaly at T_2 shifts to higher temperature as the field is increased and finally fades out at a field $B > 5$ T. These measurements are complemented by measurements of the magnetostriction at various temperatures from below T_2 to above T_1 which highlight the extraordinarily large magnetoelastic effects in this material.

TT 45.83 Thu 15:00 Poster B

Realization of a Setup for Ultrasonic Experiments under He-Gas Pressure and Test Measurements on MnF_2 — •Sebastian Becker, Pham Thanh Cong, Bernd Wolf, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

Ultrasonic measurements are a powerful tool for investigating strongly correlated materials. The extension of these experiments to hydrostatic pressures, which opens up interesting possibilities for a detailed thermodynamic characterization, is challenging and has been rarely

documented in the literature. Here we discuss the realization of an experimental setup, where ultrasonic measurements can be performed in a temperature range 1.2 - 300 K, at hydrostatic (He-gas) pressure values up to 10 kbar, and magnetic fields up to 16 T. The setup has been tested by measuring the ultrasonic attenuation and sound velocity on single crystalline MnF_2 in the temperature range 50 K $\leq$ T $\leq$ 300 K at various pressures. From these measurements the pressure dependence of the Néel temperature was derived to (380 $\pm$ 165) mK/kbar which compares favourably with literature results.

TT 45.84 Thu 15:00 Poster B

ESR spectrum of the spin-1/2 Heisenberg-Ising chain — •Michael Brockmann[1], Frank Göhmann[1], Michael Karbach[1], Andreas Klümper[1], and Alexander Weisse[2] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Max-Planck-Institut für Mathematik, 53072 Bonn, Germany

We analyze the ESR absorption spectrum of the spin-1/2 Heisenberg-Ising chain, also known as XXZ chain. The moments of the absorbed intensity can be calculated exactly due to the integrability of this model. They can be used to define the shift of the resonance as well as the width of the spectral line, both induced by the anisotropy of the interactions. If the frequency of the incident microwave is varied for fixed Zeeman field, the first four moments are sufficient to explore the exact resonance shift and line width at arbitrary temperatures and Zeeman fields in the full range of anisotropy parameters. In current ESR experiments, however, the Zeeman field is varied for fixed frequency. For this case we can still present results for the shift at small anisotropies and a high-temperature expansion for the line width.

We performed numerical calculations which agree well with exact data. Additionally, we are able to extract an empirical parameter-free model for the line shape at high temperatures which is extremely accurate over a wide range of anisotropy parameters and is exact at the free-fermion point and at the isotropic point. The anisotropic model shows strong absorption even in the zero-field limit. We derive the exact two-spinon ground-state contribution to the spectral line which accounts for more than 96% of the spectral weight at moderate anisotropy.

TT 45.85 Thu 15:00 Poster B

Interplay of structural and electronic properties in itinerant $A\mathbf{Fe}_4X_2$ systems — •Til Goltz[1], Nandang Mufti[2], Christoph Geibel[2], Theo Woike[3], Hubertus Luetkens[4], Johannes Spehling[1], and Hans-Henning Klauss[1] — [1]Institute of Solid State Physics, TU Dresden, Germany — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Institute of Structural Physics, TU Dresden, Germany — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland

The $A\mathrm{Fe}_4X_2$ (A=Y, Lu, Zr; X=Ge, Si) family of transition metal tetrels has shown to be a promising candidate for studying the change of the electronic ground state under chemical substitution [1]. Within the $ZrFe_4Si_2$-type structure ($P4_2/mnm$), the iron atoms are arranged in chains of edge-linked tetrahedra [2]. Their structure is prone for reduced dimensionality or frustration and is thus expected to lead to emergent phenomena near a quantum critical point. Since neutron scattering data on YFe_4Ge_2 show a simultaneous structural and magnetic transition [3], electronic and structural properties seem intimately connected within the whole $A\mathrm{Fe}_4X_2$ family. On the poster, we discuss the electronic and structural properties, extracted from our μSR, Mössbauer, X-Ray and thermodynamic data in the context of a structural driven magnetic phase transition.

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TT 45.86 Thu 15:00 Poster B

Strong evidence against orbital fluctuations in $R\mathbf{VO}_3$ — •Julia Reul[1], Agung Nugroho[2], Thomas Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

Spin and orbital degrees of freedom play a decisive role for the low-energy physics of strongly correlated transition-metal oxides. Whereas the spin is a true low-energy degree of freedom with propagating low-energy excitations, it is still questionable if the same holds true for the orbital degree of freedom. In a typical situation the orbitals are strongly coupled to the lattice, which makes it sufficient to consider classical orbitals with rigid orbital order. However, different groups have pointed out that orbital fluctuations may be strong in the $3d^2$ Mott-Hubbard insulators $R\mathrm{VO}_3$ (R =rare earth ion or Y).

Optical spectroscopy offers an efficient method to study the nature of the orbital degree of freedom, because the spectral weight of excitations across the Mott-Hubbard gap depends sensitively on nearest-neighbor spin-spin and orbital-orbital correlations. We study the temperature dependence of the optical spectral weight by means of ellipsometry in the frequency range 0.75 - 5.5 eV. A comparison of our experimental results for R = Y, Gd and Ce with a theory based on a low-energy spin orbital superexchange Hamiltonian [1,2] leads us as to the conclusion of rigid orbital order in $R\mathrm{VO}_3$.

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TT 45.87 Thu 15:00 Poster B

Skyrmions in two and three dimensional Dzyaloshinskii-Moriya magnets — •Stefan Buhrandt and Lars Fritz — Universität zu Köln, Institut für theoretische Physik, Zülpicher Strasse 77, 50937 Köln

Using classical Monte Carlo we study the phase diagram of ferromagnetic O(3) spin models with Dzyaloshinskii-Moriya interaction and spin anisotropies in applied magnetic fields. We determine the phase diagram for the two dimensional problem by simulated annealing upon investigation of the spin structure factor. We also study the evolution of the phase diagram upon becoming increasingly three dimensional. We especially focus on the evolution of the skyrmion crystal phase upon increasing the dimensionality.

TT 45.88 Thu 15:00 Poster B

Magnetic structures and magnon dispersion of $\mathbf{LaSrFeO}_4$ — •N. Qureshi[1], H. Ulbrich[1], Y. Sidis[2], A. Cousson[2], and M. Braden[1] — [1]University of Cologne — [2]LLB, Saclay (France)

We have conducted an extensive study on the single-layered perovskite $LaSrFeO_4$, a transition metal oxide of the Ruddelsden-Poppers series. This system orders antiferromagnetically at T_N=380 K and undergoes two further magnetic phase transitions at 90 K and 30 K [1,2] whose nature is still unclear. Our neutron diffraction experiments shed some light on this open issue: We have observed that there is no significant difference between the three magnetic structures. Although, the presence of four magnetic domains renders it impossible to determine the Fe moment direction within the basal plane using unpolarized neutrons. Hence, we conclude that the transitions must be connected to a spin reorientation within the basal plane. Additionally, we have investigated the magnon dispersion along two main symmetry directions. We find that the dispersions are well described by a Heisenberg antiferromagnet Hamiltonian including isotropic nearest and next-nearest neighbour interaction as well as an effective magnetic anisotropy field. The resulting values fit well into the series of the isostructural homologues. In $LaSrFeO_4$ the Fe ions nominally present a three-valent $3d^5$ state yielding S=2.5 and L=0. However, the results of our neutron study give rise to the assumption of a non-quenched orbital moment.

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TT 45.89 Thu 15:00 Poster B

Mott-Hubbard excitations in hole doped $R\mathbf{TiO}_3$ (R = rare earth ion or Y) studied via spectroscopic ellipsometry — •Ignacio Vergara, Julia Reul, Alexander Gössling, Alexander Komarek, and Markus Grüninger — Universität zu Köln

Hole doping of the $3d^1$ Mott-Hubbard insulators $R\mathrm{TiO}_3$ (R = rare earth ion or Y) leads to an interesting phase diagram including spin, charge and orbital order. Temperature dependent (20 K<T<500 K) spectroscopic ellipsometry (0.75 - 5.5 eV) offers a very sensitive method to study these phenomena as the Mott-Hubbard excitations from the lower to the upper Hubbard-Band $|d^n\rangle|d^n\rangle \rightarrow |d^{n+1}\rangle|d^{n-1}\rangle$ are sensitively dependent on nearest-neighbor spin-spin and orbital-orbital correlations.

The optical spectra of the undoped $3d^1$ compounds $R\mathrm{TiO}_3$ show a complex multipeak structure which has been attributed to the Mott-Hubbard excitations into the different $3d^2$ multiplets, while the temperature dependence has been analyzed on the basis of nearest-neighbor spin-spin correlations [1]. We now study the impact of hole doping on the optical spectra. In a perfect charge ordered scenario of a half doped compound, the hopping of an electron to the neighboring lattice site should not result in a double occupancy. Thus, instead

of the Hubbard energy U the excitation should only cost the nearest-neighbor repulsion V.
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TT 45.90 Thu 15:00 Poster B

High-precision magnetisation measurements in pulsed fields — •Lars Postulka, Lukas Hinz, Bernd Wolf, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

To determine the magnetic behaviour of materials at magnetic fields as high as 50 T, pulsed fields are required. This implies the handling of huge changes of magnetic flux during the magnetic field pulse. For ac-susceptibility measurements, the typical realisation of the experimental setup is done with a pair of compensated coils. In one of these coils a sample is positioned which leads to a change of the inductance and therefore to an induced voltage. However, the large changes of magnetic flux produce a non-negligible background signal if these coils are not identical. Therefore, a modification of the typical sample holder has been constructed which enables reference measurement without a sample to be performed in a convenient way. In addition, we have added an electronic circuit to the experimental setup with which we can adjust the signal of the empty sample holder to zero voltage. The calibration and testing has been done at different temperatures by using a well-characterized material, the paramagnet $CuSO_4 \cdot 5H_2O$.

TT 45.91 Thu 15:00 Poster B

Ground-state energy and beyond: High-accuracy results for the Hubbard model on the Bethe lattice in the strong-coupling limit — •Martin Paech[1,2], Eva Kalinowski[2], Walter Apel[3,1], Gunther Gruber[4], Rita Loogen[4], and Eric Jeckelmann[1] — [1]Leibniz Universität, Hannover, Germany — [2]Academy of Computer Science and Management, Bielsko-Biała, Poland — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Philipps-Universität, Marburg, Germany

We present critical parameters for the Mott-Hubbard transition on the half-filled Bethe lattice with infinite coordination number with unprecedented accuracy of order 15 in $1/U$. This became possible by an essentially improved C implementation of our parallelized diagrammatic-combinatorial computer algorithm for the strong-coupling expansion [1].

Furthermore, we give insight into an on-going graph-theoretical analysis, which is related to an implementation of the algorithm kernel in the functional programming language Haskell [2]. This analysis is a technical prerequisite e. g. for the calculation of the band gap, for precise information about the density of states, or for investigations in finite dimensions and of systems away from half filling.
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TT 45.92 Thu 15:00 Poster B

Strong dynamic correlations and Korringa Ratio of Na_xCoO_2 — •Lewin Boehnke and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The Korringa Ratio forms a valuable link between experimental and theoretical investigations of strongly correlated materials systems as it links the Knight shift and nuclear relaxiation time to dynamical spin properties of the conduction electrons of an itinerant magnet system.

While it has been studied phenomenologically [1] or for weakly interacting systems [2], rigorous calculations for strongly correlated systems are hindered by the need for accurate dynamical lattice susceptibilities which used to be numerically prohibitive in memory usage and runtime.

We employ the recently introduced Orthogonal Polynomial basis for one- and two-Particle Green's functions [3] to obtain reliable dynamic lattice correlation functions within the Dynamical Mean Field Theory [4] for the layered triangular system Na_xCoO_2. This system exhibits a vast variety of charge- and spin-instability tendencies, which is very well confirmed by our calculations. Most of these can not be reproduced without explicitly including vertex contributions.
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TT 45.93 Thu 15:00 Poster B

Perspectives of LDA+Slave-boson mean-field theory for realistic low-energy physics — •Christoph Piefke, Malte Behrmann, Sergej Schuwalow, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) is used to investigate large parameter spaces of arbitrary strongly interacting systems [1,2,3] based on realistic LDA calculations [4,5]. The multiorbital Hubbard-Hamiltonian is mapped onto an itinerant quasiparticle part and localized bosonic degrees of freedom. This decouples complex interactions, quartic in the original electron-operators, at the cost of a set of constraints. At saddle-point, a self-consistent mean-field solution is obtained. Practical computations using RISB are limited by the fact that the degrees of freedom of the modelation grow exponentially with the number of correlated orbitals. To circumvent this limitation, one reduces the number of variational parameters using symmetries. We demonstrate some of the recently implemented techniques and improvements in the context of itinerant systems with magnetic degrees of freedom and/or geometric frustration.
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TT 45.94 Thu 15:00 Poster B

Bosonization approach to singular low-energy contributions in the thermodynamics of Fermi liquids — •Hendrik Meier[1], Catherine Pépin[2,3], and Konstantin Efetov[1,3] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Institut de Physique Théorique, CEA-Saclay, France — [3]International Institute of Physics, Universidade Federal do Rio Grande do Norte, Brazil

Applying a recently suggested method of bosonization in an arbitrary dimension [2] to the two-dimensional Fermi liquid, we derive an effective supersymmetric field theory for the low-energy spin and charge excitations emerging in the vicinity of the non-flat Fermi surface. Using this field theory to study the anomalous contribution δc to the specific heat in the limit $T \to 0$, we find the leading logarithmic corrections to $\delta c/T^2$ by means of a one-loop renormalization group analysis. The final result is represented as the sum of two separate terms that can be interpreted as coming from singlet and triplet superconducting excitations.

Last, it is discussed how the bosonization method may become a useful analytical tool to study different problems in the field of strongly correlated systems.
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TT 45.95 Thu 15:00 Poster B

Two-stage thermalization of weakly interacting quantum systems — •Michael Stark and Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

An isolated quantum many-body system, which is suddenly forced out of equilibrium, is said to thermalize if it relaxes to a new equilibrium state and if this is the thermal state predicted by statistical mechanics. Weakly interacting systems are usually first trapped in a prethermalized state and can thermalize only at a later stage [1]. The prethermalization stage can be described by a generalized Gibbs ensemble built from approximate constants of motion in the vicinity of the non-interacting point [2]. In a subsequent stage the crossover from the prethermalized to the thermal state occurs. This two-stage scenario provides an understanding of thermalization from a pure initial state to a final thermal ensemble state for not too large interaction.
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TT 45.96 Thu 15:00 Poster B

Merging *GW* and dyanmical mean-field theory — •Ciro Taranto[1], Alessandro Toschi[1], Merzuk Kaltak[2], Martijn Marsman[2], Georg Kresse[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Computational Materials Physics, University of Vienna, Sensengasse 8/12 A-1090 Vienna, Austria

The combined approach of local density approximation (LDA) and dynamical mean-field theory (DMFT) is the tool of choice for the study of strongly correlated materials. Nevertheless the predictive power of this approach is hampered by two principal difficulties: the extimate of the screened Coulomb interaction and the so called double-counting correction. Both of these problems are rooted in the conceptual difficulty of formulating the DMFT and the LDA in a common (diagrammatic) context. For this reasons we believe that the *GW*+DMFT [1] approach, which can be formulated also diagramatically [2], can represent a major improvement to the LDA+DMFT one. Specifically we show how one can interface the *GW* approach with the DMFT in a possibly self-consistent cycle. We also present our preliminary *GW*+DMFT results on the test-material $SrVO_3$.

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TT 45.97 Thu 15:00 Poster B

Symmetry properties of the U-matrix — •Hermann Ulm and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich

We present a simple method of calculating Gaunt coefficients in the basis of spherical harmonics. Considering these coefficients as a 3-dimensional tensor gives us flexibility in choosing basis. We tabulate the Gaunt coefficients in spherical, semi cubic, cubic bases for *d*- and *f*-electrons. Moreover, it allows us to study the symmetry properties of the full $\hat{U}$-matrix easily. We finally present an elegant way of calculating relations between U and J parameters and Slater integrals and give a proof of their invariance.

TT 45.98 Thu 15:00 Poster B

Response functions of correlated materials — •Amin Kiani Sheikhabadi[1] and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation (IAS), Forschungszentrum Jülich, Jülich, Germany — [2]Peter Grünberg Institut (PGI), Forschungszentrum Jülich, Jülich, Germany

Two-particle correlation functions provide a bridge between experimentals and theory. For strongly correlated systems, response functions can be determined with the LDA+DMFT method. In this approach the response functions are extracted from the local two-particle vertex and the local Green's functions. Here we use such method and a Hirsch-Fye QMC impurity solver to calculate the response functions of correlated transition-metal oxides. As representative case, we present results for $KCuF_3$.

TT 45.99 Thu 15:00 Poster B

Reduced Density Matrix Functional Theory- A suitable vehicle to import explicit correlations — •Ebad Kamil — Institute for Theoretical Physics, University of Goettingen, Goettingen, germany

A variational formulation for the calculation of interacting fermions system based on density matrix functional theory is presented. This formulation allows importing explicit many particle effects into standard density functional theory based calculations and also avoids ambiguities of double counting terms inherent to other approaches.

Local approximation for explicit correlations is introduced and the resulting impurity problem is solved using techniques of open quantum system.

TT 45.100 Thu 15:00 Poster B

Vortex arrays in two-species Bose–Einstein condensates with interspecies attraction — •Pekko Kuopanportti[1], Jukka A. M. Huhtamäki[1], and Mikko Möttönen[1,2] — [1]Department of Applied Physics/COMP, Aalto University, P.O. Box 14100, FI-00076 AALTO, Finland — [2]Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 AALTO, Finland

One of the defining properties of superfluids is that they respond to rotation by forming quantized vortices. A convenient environment to controllably study vortices is dilute Bose–Einstein condensates (BECs) of alkali-metal atoms. To date, numerous experiments have shown that when a BEC is set into quick rotation, a triangular vortex lattice is typically formed. The density of vortices in the lattice, n_v, is governed by the Feynman relation $n_\mathrm{v} = m\Omega/(\pi\hbar)$, where m is the mass of the constituent boson and Ω is the rotation frequency.

In this theoretical work, we investigate vortex lattices in a rotating two-component BEC where the components have unequal atomic masses and interact attractively with each other. Because the atomic masses are unequal, the Feynman relation implies that the vortex densities in the two components should also differ from one another. On the other hand, the intercomponent attraction results in an effective attraction between vortices in different components. We show that together these two effects lead to exotic ground-state vortex structures such as square vortex lattices and arrays of two-quantum vortices. The obtained states invariably obey the Feynman relation, and they should be experimentally realizable with the current state of the art.

TT 45.101 Thu 15:00 Poster B

Quantum dynamics of few ultra-cold atoms in a periodically shaken double-well superlattice — •Martin Esmann[1,4], Niklas Teichmann[1], Jon Pritchard[3], and Christoph Weiss[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — [2]Department of Physics, Durham University, Durham, DH1 3LE, UK — [3]Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK — [4]Physics Department, Harvard University, Cambridge, MA 02138, USA

An analog of fractional photon-assisted tunneling (PAT) is investigated both numerically and analytically. The system under consideration is a periodically shaken optical superlattice of effectively decoupled double wells with few interacting ultra-cold Bosons per well. While previous results based on a perturbative approach suggest that the coherent transfer between the individual wells induced by PAT is a small effect [1], we introduced a resonance approximation [2] to show that for the right choice of parameters fractional PAT resonances yield major contributions to the transfer of particles. Our technique is particularly useful to investigate conditions for perfect transfer employing PAT resonances and first experimental results were recently obtained [3] in good agreement with our predictions [2,4].

[1] N. Teichmann et. al., Phys. Rev. A, 79:063620, 2009.
[2] M. Esmann et al., Phys. Rev. A, 83:063634, 2011.
[3] Y.-O. Chen et al., Phys. Rev. Lett., 107:210405, 2011.
[4] M. Esmann et al., Laser Phys. Lett., doi: 10.1002/lapl.201110109.

TT 45.102 Thu 15:00 Poster B

Viscosity of a two dimensional Fermi gas at strong coupling — •Carolin Küppersbusch[1], Lars Fritz[1], and Tilman Enss[2] — [1]Universität zu Köln, Institut für theoretische Physik, Zülpicher Strasse 77, 50937 Köln — [2]Physik Department, Technische Universität München, 85747 Garching, Germany

We consider a two dimensional Fermi gas which is experimentally realized in balanced and imbalanced fermionic ultra cold atom systems. An experimentally accessible quantity that has received a lot of interest recently as a measure of the interaction strength is the shear viscosity. This quantity describes the resistance of the system towards establishing a flow gradient. Using a Boltzmann equation we calculate the viscosity in all temperature and interaction ranges from a full numerical solution. In the high temperature limit we compare our results with the analytic solution of the non-degenerate Fermi gas.

TT 45.103 Thu 15:00 Poster B

Search for Floquet states in many-body quantum systems — •Armin Seibert, Sergey Denisov, and Peter Hänggi — Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg

Even under equilibrium conditions, a typical many-body system is hard to handle due to the exponential growth of the number of system states with the number of particles – spins, cold atoms, qubits, etc –it contains. Recent advances on the front of computational many-body quantum physics, marked by the development of the density matrix renormalization group (DMRG) methods, allowed to get insight into the Hilbert space of 'big' time-independent systems. In order to study the same, but now driven, systems, one must use more sophisticated methods, which should combine existing know-how with specific algorithms developed for periodically driven quantum systems. We present a brief overview of our recent attempts to advance in the corresponding direction, which attempts have involved the combination of the DMRG algorithms, the Floquet theory and a newest computational facility such as a graphic-processing unit (GPU) supercomputer.

TT 45.104 Thu 15:00 Poster B

Collective Excitations of Quantum Solid Phases — •Guenther Meissner and Uwe Schmitt — Department of Physics, Saarland

University, P.O.B. 151150, D-66041 Saarbruecken, Germany

For collective excitations of quantum solid phases at low temperatures as, e.g., sound propagation in solid helium or in magnetic field-induced 2D Wigner solids, Born's classical theory of lattice dynamics breaks down. This happens due to large zero-point motions of the helium atoms with low mass and the cyclotron motions of the electrons with electrical charge. These deficiencies have been removed in our general quantum many-body approach, where the collective excitations are obtained quite generally from correlation functions allowing, e.g., also to include the balance between single-particle and collective excitations [1]. In the presence of random disorder the dispersion of the modes of these collective excitations is no longer gapless in zero wave vector limit. The gap has been considered in recent microwave resonance experiments being a confirmation of a disorder-pinned 2D Wigner quantum solid phase [2]. It will be shown, that from a theoretical point of view this interpretation in terms of quasi-particles of magnetic flux quanta and fractional charge is feasible, particularly, since the resonances observed near the fractional filling factor one third are very similar to those, found near the integer filling factor one.

[1] G. Meissner, Phys. Rev. Lett. 21, 435 (1968); Physica B 184, 66 (1993).
[2] Hahn Zhu, Yong P. Chen, P. Jiang, L.W. Engel, D.C. Tsui, L.N. Pfeiffer and K.W. West, Phys. Rev. Lett. 105, 126803 (2010) and references therein.

TT 45.105 Thu 15:00 Poster B

Statistical properties of interacting Rydberg gases — •David Breyel and Andreas Komnik — Institut für theoretische Physik, Universität Heidelberg

The main goal of our work is answering the question whether it is possible to detect the formation of a crystal in a gas of interacting Rydberg atoms by purely statistical means. We model the cycles of cloud formation and subsequent Rydberg atom number measurement using exact diagonalisation technique and plot the probability to produce N Rydberg atoms in a histogram. The resulting distribution is sub-Poissonian with distinct features due to interaction effects. We extract the density correlation function, which unambiguously points towards a condensed phase formation in the Rydberg cloud.

TT 45.106 Thu 15:00 Poster B

Embedded cluster approach for strongly correlated systems out of equilibrium — Michael Knap, Anna Fulterer, Martin Nuss, Wolfgang von der Linden, and •Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We present a numerical approach to compute nonequilibrium properties of strongly-correlated quantum many-body systems. The method is based on the nonequilibrium Green's function formalism combined with a treatment of strong correlations via cluster perturbation theory and its variational extensions. Upon including appropriate virtual bath parameters the method bridges to nonequilibrium dynamical mean-field theory.

We present results for steady-state transport across different spatially extended strongly-correlated regions, such as (i) a quantum wire, and (ii) a Hubbard layer displaying d-wave superconductivity. In the latter case, we discuss the effect of the bias voltage on superconducting properties. Time transient behavior is also discussed.

TT 45.107 Thu 15:00 Poster B

Variational cluster approach for strongly correlated bosonic systems in and out of equilibrium — •Enrico Arrigoni, Benjamin Kollmitzer, Michael Knap, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We present a variational cluster approach to treat strongly-correlated lattice bosons in the superfluid phase. To this end, we reformulate the method within a pseudoparticle formalism, whereby cluster excited states are described in terms of particle-like excitations. The approximation amounts to solving a multi-component noninteracting bosonic system by means of a multi-mode Bogoliubov transformation. A criterion for the stability of the solution is discussed.

For the two-dimensional Bose-Hubbard model the method provides excellent agreement with Quantum Monte Carlo results even in the vicinity of the tip of the Mott lobe, both on the insulating as well as in the superfluid phase.

We illustrate the application of the method to strongly-correlated bosonic systems out of equilibrium within a Keldysh Green's function formulation.

TT 45.108 Thu 15:00 Poster B

Characterization of Mott-insulating and superfluid phases in the one-dimensional Bose-Hubbard model — •S. Ejima[1], H. Fehske[1], F. Gebhard[2], K. zu Münster[2], M. Knap[3], E. Arrigoni[3], and W. von den Linden[3] — [1]University Greifswald, Germany — [2]University Marburg, Germany — [3]TU Graz, Austria

We study the one-dimensional Bose-Hubbard model, the generic model for ultracold Bose gases, by means of various analytical and numerical techniques. Firstly, we determine the Kosterlitz-Thouless transition between the Mott insulator and the superfluid phase for the lowest two Mott lobes by analyzing the von Neumann entanglement entropy within a density matrix renormalization group (DMRG) approach. The phase boundaries are found to be in excellent agreement with those extracted from the scaling of the Luttinger liquid parameter. Secondly, we investigate the dynamical properties of the Bose-Hubberd model in both phases using analytical (strong-coupling expansion) and numerical (variational cluster approximation (VCA) and dynamical DMRG) methods. The results obtained for the single-particle photoemission spectra and the density of states agree very well in the strong-coupling regime. But even for intermediate couplings and within the superfluid phase, VCA reproduces the unbiased dynamical DMRG data surprisingly well, albeit the former one is based on a dynamical mean-field approach. Thirdly, including higher-order corrections in the strong coupling approach for the dynamical density-density correlation function, we discuss how the properties of the Mott insulator change in passing from the strong to the intermediate coupling regime.

TT 45.109 Thu 15:00 Poster B

Instability of a repulsive Bose gas near the BEC transition — •Michael Maennel[1], Klaus Morawetz[1,2], and Pavel Lipavsky[3,4] — [1]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany — [2]International Institute of Physics, Universidade Federal do Rio grande do Norte, 59.072-970 Natal-RN, Brazil — [3]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

We investigate a Bose gas with finite-range interaction using a scheme to eliminate self-interaction in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature, without the use of anomalous functions. In the vicinity of the onset of Bose-Einstein condensation (BEC) chemical potential and pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore for sufficiently strong interaction the equation of state becomes multivalued near the BEC transition. For a Hatree-Fock or Hartree-Fock-Bogoliubov approximation such a multivalued region can be avoided by a Maxwell construction. However, for the T-matrix approximation there remains a multivalued region even after a Maxwell construction.

TT 45.110 Thu 15:00 Poster B

One-dimensional many-body quantum transport of Bose-Einstein condensates — •Julien Dujardin, Arturo Argüelles, and Peter Schlagheck — Département de Physique, Université de Liège, 4000 Liège, Belgium

We calculate the transport properties of an ultracold gas of Bose-Einstein condensed atoms that is coupled from a magnetic trap into a one-dimensional waveguide [1,2]. A central aim of such guided atom lasers [1] is to study the role of atom-atom interaction in many-body transport processes across finite scattering regions within the waveguide resembling tunnel junctions or quantum dots. Our theoretical approach to solve this problem is based on a scattering formalism for which we consider the system to consist of two semi-infinite noninteracting leads and a finite interacting scattering region. We calulate the atom density, the current, and the transmission in the steady-state regime and compare these observables to the mean-field regime where the dynamics of the Bose gas is described by a Gross-Pitaevskii equation [2].

[1] W. Guerin et al., PRL 97, 200402 (2006).
[2] T. Ernst et al., PRA 81, 013631 (2010).

TT 45.111 Thu 15:00 Poster B

Crystal Structure and Magnetic Properties of

NaCu[$(Cu_3O)(PO_4)_2Cl$] — Teng-Teng Jin[1], Wei Liu[2], Shuang Chen[3], Yurii Prots[3], Walter Schnelle[3], Jing-Tai Zhao[1], Rüdiger Kniep[3], and •Stefan Hoffmann[3] — [1]Shanghai Institute of Ceramics, Shanghai, P. R. China — [2]Ocean University of China, Qingdao, P. R. China — [3]MPI CPfS, Dresden, Germany

A new copper(II) phosphate chloride, NaCu[$(Cu_3O)(PO_4)_2Cl$], has been synthesized and structurally characterized. Complex chains of copper-centered polyhedra give rise to a low-dimensional magnetic behavior similar to $Cu_3O(MoO_4)_2$ [1,2]. Field and temperature dependent measurements of the specific heat and the magnetic susceptibility revealed two transitions T_{N1} = 11.3(3) K and T_{N2} = 6.5(2) K. T_{N1} signals the long-range ordering of the Cu spins in the chains. The phase transition at T_{N2} is accompanied by the formation of a weak ferromagnetic moment typical for basically anti-ferromagnetic structures with spin canting.

[1] T. Hamasaki et al. Phys. Rev. B 2008, 77, 134419-1-134419-7.
[2] S. Vilminot; G. Andre; M. Kurmoo Inorg. Chem. 2009, 48, 2687-2692.

TT 46: Superconductivity: Tunnelling, Josephson Junctions, SQUIDs 2

Time: Thursday 17:45–20:00 Location: H 2053

TT 46.1 Thu 17:45 H 2053

Josephson junction with magnetic-field tunable current-phase relation — •Edward Goldobin[1], Hanna Sickinger[1], Markus Turad[1], Roman Mints[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalische Institut and Center for Collective Quantum Phenomena in LISA$^+$, University of Tübingen, 72076 Tübingen, Germany — [2]Tel Aviv University, Tel Aviv 69978, Israel

We consider an asymmetric 0-π Josephson junction consisting of 0 and π regions of different lengths L_0 and L_π in an applied magnetic field H. This system can be described by an effective sine-Gordon equation for the spatially averaged phase ψ. We demonstrate that the effective current-phase relation contains a negative term $\propto \sin(2\psi)$ as well as an additional term $\propto H\cos\psi$ [1]. Thus, the current phase relation and the ground state(s) are *tunable* by magnetic field. The first experimental evidences will be presented.

[1] E. Goldobin, et al., Phys. Rev. Lett. **107**, 227001 (2011).

TT 46.2 Thu 18:00 H 2053

Quantum phase slip interference device based on a shaped superconducting nanowire — •Alexander Zorin and Terhi Hongisto — Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

As was predicted by Mooij and Nazarov, the superconducting nanowires may exhibit, depending on the impedance of external electromagnetic environment, not only quantum slips of phase, but also the quantum-mechanically dual effect of coherent transfer of single Cooper pairs. We propose and realize a transistor-like superconducting circuit including two serially connected segments of a narrow (10nm by 18nm) nanowire joint by a wider segment with a capacitively coupled gate in between. This circuit is made of amorphous NbSi film and embedded in a network of on-chip Cr microresistors ensuring a high external impedance ($\gg h/e^2 \approx 25.8$ kΩ) and, eventually, a charge bias regime. Virtual quantum phase slips in two narrow segments of the wire lead in this case to quantum interference of voltages on these segments making this circuit dual to the dc SQUID. Our samples demonstrated appreciable Coulomb blockade voltage (analog of critical current of the SQUID) and remarkable periodic modulation of this blockade by an electrostatic gate (analog of flux modulation in the SQUID). The obtained experimental results and the model of this QPS transistor will be presented.

TT 46.3 Thu 18:15 H 2053

Influence of heating in on-chip resistors on frequency-to-current conversion in short arrays of small Josephson junctions — •Felix Maibaum, Sergey V. Lotkhov, and Alexander B. Zorin — Physikalisch-Technische Bundesanstalt Braunschweig

Small Josephson junctions can exhibit charge quantization effects and Bloch oscillations which are very much the electromagnetic dual to the behaviour of larger junctions. As such they can exhibit constant-current steps at I=2ef when an external drive of frequency f is applied, dual to the well known constant-voltage Shapiro steps exhibited by larger junctions. This is of interest for a possible current standard. Observation of these steps demonstrating phase lock of the Bloch oscillations with the external drive requires a high-impedance environment for the junctions, which is provided by on-chip resistors close to the junctions. Those resistors will inevitably be heated by the produced current. We experimentally determine the temperature dependance of miniature on-chip resistors on heating current and present circuit simulations incorporating this data as well as realistic values for stray capacitances and junction parameters. These simulations show that with harmonic drive there is practically no parameter window where observation of a flat current plateau is possible. However, a pulsed drive analogous to what is employed for AC voltage standards could enable direct frequency-to-current conversion with current technology. We also discuss potential problems not addressed in the simulations, in particular non-equilibrium quasiparticles in the superconductor.

TT 46.4 Thu 18:30 H 2053

Single crystal gold nanowire Josephson junctions and superconducting quantum interference devices — •Yusuf H. Günel[1,2], Nick Borgwardt[1,2], Huijun Yao[3], Gregor Panaitov[4], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2,5] — [1]Peter Grünberg Institute -9, Forschungszentrum Jülich, 52425 Jülich, Germany, — [2]JARA-Fundamentals of Future Information Technology — [3]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, People's Republic of China — [4]Peter Grünberg Institute -8, Forschungszentrum Jülich, 52425 Jülich, Germany, — [5]II. Physikalisches Institut, RWTH Aachen University, Aachen, Germany

We have used single crystal Au nanowires, grown by electrochemical deposition method, contacted by two Niobium (Nb) superconducting material to form a Josephson junction. The fabricated devices have been characterized in a filtered ^{3}He cryostat in a temperature range from 0.3 K up to 6 K as well as a magnetic field up to 7 T. The critical current of the Josephson devices has been investigated as a function of temperature and magnetic field. Furthermore, we have observed clear sub-harmonic gap structures in the differential resistance measurements, indicating multiple Andreev reflection.

As an important application of Josephson junctions, we have also fabricated and characterized the properties of superconducting quantum interference devices (SQUIDs) formed by two individual Nb/Au-nanowire/Nb Josephson junctions.

15 min. break.

TT 46.5 Thu 19:00 H 2053

Measurements of single fluxon radiation spectra in annular Josephson junctions — •Kirill G. Fedorov and Alexey V. Ustinov — Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We report measurements of single fluxon radiation from annular Josephson junctions using a low noise cryogenic microwave amplifier. Measurements in the frequency domain show very rich fine structure of the fluxon current-voltage characteristic. Distinct resonances that are found in the fine structure are explained by fluxon interaction with small-amplitude plasma waves. The linewidth of fluxon radiation is investigated for different bias points and temperatures down to mK range. We present a comparison of the existing theories for fluxon radiation linewidth with our data.

TT 46.6 Thu 19:15 H 2053

Strain tuning atomic tunneling systems in a Josephson junction — •Grigorij J. Grabovskij, Torben Peichl, Jürgen Lisenfeld, Georg Weiss, and Alexey V. Ustinov — Karlsruhe Institute of Technology, Physikalisches Institut, 76131 Karlsruhe

The so-called tunneling model assumes transitions of atoms between different localized configurations of the disordered structure of the solid. A transition like that is attributed to the two-level system (TLS) formed by the two lowest energy states of atoms tunneling in a double-well potential. The development of superconducting circuits based on

Josephson junctions as active elements grants access to single microscopic defect states located inside the disordered tunneling barrier. The spectra of Josephson phase qubits show avoided level crossings corresponding to individual coherent TLSs. We performed an experiment in which a chip with a phase qubit was bent using a piezo actuator. The tiny displacement of atoms on the chip surface, which is estimated to be of the order of the nuclei size, changes the potential of TLSs. We observed a change of the TLS resonance frequency as a function of the strain field that confirms the tunneling model assumptions for TLSs and yields unique data for the TLS potential.

TT 46.7 Thu 19:30 H 2053

Experiments with SQUID-based Metamaterials — •Susanne Butz[1], Philipp Jung[1], Sergey V. Shitov[2,3], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institute of Radio Engenieering and Electronics (IREE RAS), Moscow 125009, Russia — [3]National University of Science and Technology MISIS, Moscow 119049, Russia

Metamaterials consist of elements that are artifically created to obtain a specific, predetermined interaction with an electromagnetic wave. The size of individual elements is much smaller than the wavelength of the incoming radiation. Conventionally, split ring resonators are used to interact with the magnetic field component of the wave. The interaction with the electric component is realized by thin metallic wires. We designed a Josephson junction based metamaterial where the split ring resonators are replaced by rf-SQUIDs. The benefits compared to conventional metamaterials are that the losses are reduced and that the inductance of the Josephson junction can be tuned by an external magnetic field. This, in turn, changes the resonance frequency of the metamaterial, making the magnetic permeability, μ_r, tunable in situ. We will report on first experiments investigating such a SQUID metamaterial composed of a coplanar waveguide coupled to a one-dimensional array of rf-SQUIDs. The experimental results will be compared with numerical simulations.

TT 46.8 Thu 19:45 H 2053

Versatile Multi-Layer Josephson Junction Process for Vortex Molecules — •Johannes Maximilian Meckbach[1], Simon Bühler[1], Michael Merker[1], Konstantin Il'in[1], Michael Siegel[1], Kai Buckenmaier[2], Tobias Gaber[2], Uta Kienzle[2], Benjamin Neumaier[2], Edward Goldobin[2], Reinhold Kleiner[2], and Dieter Koelle[2] — [1]Institut für Mikro- und Nanoelektronische Systeme, KIT, Germany — [2]Physikalisches Institut - Experimentalphysik II, Universität Tübingen, Germany

In long Josephson junctions magnetic flux may penetrate the barrier resulting in a so-called Josephson-Vortex carrying one flux quantum Φ_0. In recent years a new type of Josephson-Vortex became available, which carries any arbitrary fraction $\Phi = -\Phi_0\kappa/2\pi$ of magnetic flux. These fractional vortices ($\wp$-vortices) spontaneously appear at discontinuities of the Josephson phase along the junction, which in turn are created using a pair of current injectors.

We present a new Nb/Al-AlO_x/Nb process for the fabrication of Josephson junctions of very high quality. Placing two injector pairs along the strongly underdamped long junctions allows the investigation of fractional vortex molecules. The topological charge of each vortex and their interaction can be altered even during experiment by changing the individual injector currents. Vortex molecule states have been measured using asymmetric DC-SQUIDs coupled to the vortices by overlying pick-up loops. To uphold the $\wp$-vortices we use persistent currents, which can be altered using heat switches. Fractional vortex molecules are promising candidates for a new type of qubits.

TT 47: Correlated Electrons: Spin Systems and Itinerant Magnets 2

Time: Friday 9:30–12:45 Location: H 0104

TT 47.1 Fri 9:30 H 0104

Single-Crystal Growth and Low Temperature Properties of the Itinerant Antiferromagnet $Cr^{11}B_2$ — Andreas Bauer[1], •Alexander Regnat[1], Saskia Gottlieb-Schönmeyer[1], Michael Wagner[1], Christian Bluhm[2], Sabine Wurmehl[2], Bernd Büchner[2], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, James-Franck-Straße, D-85748 Garching, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany

We report the preparation and low temperature properties of the itinerant antiferromagnet $Cr^{11}B_2$. Large single crystals were grown by means of optical float-zoning, where the feed rods were prepared in a solid state reaction using high purity Cr and B powder in a bespoke tungsten crucible. ^{10}B depleted boron was used to permit detailed neutron scattering studies. The crystal grown has the highest residual resisitvity ratio reported to date in the literature of 31 and 11 for current along the crystallographic c- and a-directions, respectively [1]. Measurements of the low temperature specific heat, magnetization and electrical resistivity are consistent with SDW type antiferromagnetic order below T_N=88 K [2], which is remarkably insensitive to large applied magnetic fields.

[1] Tanaka et al., J Less-Comm Met, **50**, 15 (1967)
[2] Funhashi et al., Solid State Commun, **23**, 859 (1977)

TT 47.2 Fri 9:45 H 0104

The strength of frustration and quantum fluctuations in $LiVCuO_4$ — •Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Johannes Richter[3], Jiři Málek[1,4], Miriam Schmitt[5], Jeroen van den Brink[1], and Helge Rosner[5] — [1]IFW Dresden — [2]Institute for Problems of Materials Science, Kiev, Ukraine — [3]Universität Magdeburg — [4]Institute of Physics, ASCR, Prague, Czech Republic — [5]MPI für Chemische Physik fester Stoffe

We present an empirical and microscopical analysis of the in-chain exchange constants of the edge-shared frustrated chain cuprate $LiVCuO_4$. We argue that the ferromagnetic nearest neighbour coupling J_1 clearly exceeds the antiferromagnetic (AFM) next-nearest neighbour coupling J_2. The measured saturation field is significantly affected by a weak 3D AFM interchain coupling leaving room for a possible Bose-Einstein condensation for several T below. The obtained exchange parameters are in agreement with the results for a realistic five-band extended HUBBARD Cu 3*d* O 2*p* model, LSDA+U predictions as well as with inelastic neutron scattering and magnetization data. The single chain frustration rate $\alpha = J_2/|J_1| \approx 0.75$, including all error bars, is definitely smaller than 1. This corresponds to strongly coupled interpenetrating AFM Heisenberg chains in contrast with opposite statements in the literature. A proper account of strong quantum fluctuations and frustration is necessary for a correct assignment of the exchange integrals, which cannot be achieved by a simple renormalization of J_2 from the spin-wave theory.

TT 47.3 Fri 10:00 H 0104

The Physics of Charge Ice in Relation to the Spin Ices — Aroon O'Brien[1,2], •Paul McClarty[1], Frank Pollmann[1], and Roderich Moessner[1] — [1]Max Planck Institute PKS, Dresden, Germany — [2]School of Physics, The University of Sydney, Sydney, Australia

We consider a classical system of charges on the sites of a pyrochlore lattice in the presence of long-range Coulomb interactions. This model, which we call the charge ice model, appeared in the early literature exploring the Verwey transition in magnetite. We revisit this model in the context of recent work on Coulomb phases in condensed matter. In particular, we find many parallels and some subtle differences between the properties of charge ice and those of another model with long-range interactions - the dipolar spin ice model - which has been studied extensively and accounts very well for much of the phenomenology of the spin ice magnets. The Coulomb phase of both models is inherited from their short-range interacting counterparts. We study in detail the degeneracy breaking brought about by the long-range interactions as well as its effects on the thermal properties of the Coulomb phase. Finally, we comment on possible experimental signatures of the Coulomb physics in mixed valence materials.

TT 47.4 Fri 10:15 H 0104

Search for quantum spin ice in $Tb_2Ti_2O_7$ at milli-Kelvin temperatures — S. Legl[1], •C. Krey[1], S.R. Dunsiger[1], C. Pfleiderer[1], H.A. Dabkowska[2], J. Rodriguez[2], and G.M. Luke[2] — [1]Physik Department E21, Technische Universität München, Ger-

many — [2]Department of Physics and Astronomy, McMaster University, Hamilton, Canada

Spin ice attracts great interest as a state in which emergent fractionalized excitations and magnetic-field induced topological forms of order may occur. However, little is known about the importance of quantum fluctuations for the spin ice state. We report a search for so-called quantum spin ice, i.e., a spin ice state driven by quantum fluctuations [1]. Using a vibrating coil magnetometer as combined with a dilution refrigerator [2], we performed comprehensive magnetization measurements in high-quality single crystals of $Tb_2Ti_2O_7$. As an isostructural sibling of the conventional spin ice systems $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$ strong quantum fluctuations are believed to suppress long-range magnetic order in $Tb_2Ti_2O_7$ despite strong antiferromagnetic interactions. We find that $Tb_2Ti_2O_7$ clearly remains paramagnetic down to the lowest temperatures studied without the magnetic field dependence predicted theoretically for quantum spin ice.

[1] Molavian et al., Journal of Physics: Condensed Matter, 21(17):172201 (2009).
[2] Legl et al., Rev. Sci. Instrum. 81, 043911 (2010).

TT 47.5 Fri 10:30 H 0104

Quantum Ice : a Quantum Monte Carlo study — •Olga Sikora[1,2], Owen Benton[1], Nic Shannon[1,2,3], Karlo Penc[4], Frank Pollmann[5], and Peter Fulde[5,6] — [1]H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK — [2]Okinawa Institute of Science and Technology, Okinawa, Japan 904-0495 — [3]Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, UK — [4]Research Institute for Solid State Physics and Optics, H-1525 Budapest, Hungary — [5]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [6]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Spin ice systems with fascinating "magnetic monopole" excitations are characterized by macroscopic degeneracy previously discovered in water ice. At very low temperatures we might expect this degeneracy to be lifted by quantum tunneling between different ice configurations.

Here we present the results of large-scale Green's function Monte Carlo simulation of ice-type models which include quantum tunneling. We find compelling evidence of an extended quantum U(1)-liquid ground state with deconfined monopole excitations in both the quantum dimer model [1,2] and the quantum ice model on the diamond lattice [3]. We discuss the fate of "pinch point" singularities seen in neutron scattering experiments on spin ice materials, showing how these are "hollowed out" in the quantum ice model [3,4].

[1] O. Sikora et al., Phys. Rev. Lett. 103, 247001 (2009)
[2] O. Sikora et al., Phys. Rev. B 84, 115129 (2011)
[3] N. Shannon et al., arXiv:1105.4196
[4] O. Benton et al., in preparation.

TT 47.6 Fri 10:45 H 0104

Thermal Transport in the Spin-Ice compound $Dy_2Ti_2O_7$ — •Gerhard Kolland, Oliver Breunig, Simon Scharffe, Johanna Frielingsdorf, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

The magnetic Dy sites in $Dy_2Ti_2O_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. A strong crystal field results in an Ising anisotropy of the magnetic moments of the Dy sites, which align along their local easy axis in the [111]-direction, pointing into or out of the tetrahedra. As a consequence, the spin system is geometrically frustrated. Possible ground-states at temperatures below 1 K are given by the "ice-rule": two spins point into and two out of a tetrahedron. This behaviour is analogous to the hydrogen displacement in water ice, revealing a residual entropy for $T \to 0$. Excited states can be created by flipping one spin – leading to the configurations of "1-in/3-out" and "3-in/1-out". In zero magnetic field, these excitations can easily propagate and are discussed as magnetic monopoles [1]. We measured the thermal conductivity down to 300 mK for external magnetic fields up to 8 T. The thermal conductivity is strongly field dependent and anisotropic with respect to the field direction. To investigate the influence of the magnetic excitations on the heat transport we compare our data to the thermal conductivity of $Dy_{2-x}Y_xTi_2O_7$ with $x = 1, 2$.

Work supported by the DFG through SFB 608.

[1] Castelnovo et. al. (2008). Nature, **451**(7174), 42-5

TT 47.7 Fri 11:00 H 0104

Spin transport in the XXZ chain at finite temperature and momentum — •Robin Steinigeweg[1] and Wolfram Brenig[2] — [1]J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia — [2]Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, D-38106 Braunschweig, Germany

We investigate the role of momentum for the transport of magnetization in the spin-1/2 Heisenberg chain above the isotropic point at finite temperature and momentum. Using numerical and analytical approaches, we analyze the autocorrelations of density and current and observe a finite region of the Brillouin zone with diffusive dynamics below a cut-off momentum, and a diffusion constant independent of momentum and time, which scales inversely with anisotropy. Lowering the temperature over a wide range, starting from infinity, the diffusion constant is found to increase strongly while the cut-off momentum for diffusion decreases. Above the cut-off momentum diffusion breaks down completely.

15 min. break.

TT 47.8 Fri 11:30 H 0104

Emergent critical phase in 2D frustrated Heisenberg model — •Peter Philipp Orth[1], Premala Chandra[2], Piers Coleman[2], and Jörg Schmalian[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

It is well-known that a discrete Ising ($\mathbb{Z}_2$) order parameter emerges in the frustrated square lattice J_1-J_2-Heisenberg model, which may be broken at finite temperature. We ask whether a different discrete symmetry $\mathbb{Z}_q$ with $q > 2$ may be found in other frustrated Heisenberg models, giving rise to a different finite temperature phase transition. Indeed, we identify an emergent $\mathbb{Z}_6$ symmetry at low temperatures in a frustrated Heisenberg model on a 2D lattice that contains both the sites of the triangular and its dual honeycomb lattice. Our analysis combines a spin-wave expansion, susceptible to short-distance physics, with renormalization group arguments of the corresponding long-wavelength non-linear sigma model. Our results are even more appealing since the $\mathbb{Z}_6$ clock model has a rich finite temperature phase diagram with two distinct Berezinskii-Kosterlitz-Thouless (BKT) phase transitions separated by a massless critical phase. We also discuss possible realizations of this system using cold-atoms in optical lattices.

TT 47.9 Fri 11:45 H 0104

Unconventional phase transition in the classical triangular-lattice Heisenberg antiferromagnet in applied magnetic field — •Luis Seabra[1], Tsutomu Momoi[2], Philippe Sindzingre[3], and Nic Shannon[4] — [1]Max-Planck-Institut für Physik komplexer System, Dresden, Germany — [2]Condensed Matter Theory Laboratory, RIKEN, Wako, Japan — [3]LPTMC, Université P. et M. Curie, Paris, France — [4]H. H. Wills Physics Laboratory, University of Bristol, U. K.

The classical Heisenberg antiferromagnet on a two-dimensional triangular lattice is a paradigmatic problem in frustrated magnetism. Its "120 degree" classical ground state gives rise to three distinct low-temperature phases under the combined effect of magnetic field and thermal fluctuations. However, many of the details of the magnetic phase diagram remain surprisingly obscure. We address this problem using modern Monte Carlo simulation techniques. At low to intermediate values of magnetic field, we find evidence for a continuous three-state Potts phase transition from the paramagnet into the one-third magnetisation plateau. We also find evidence for conventional Kosterlitz-Thouless transitions from the magnetisation plateau into the canted "Y-state", and into the 2:1 canted phase. However, at higher fields, the phase transition from the paramagnet into the 2:1 canted phase, while continuous, does not appear to fall into any conventional universality class, being instead described by continuously varying exponents. We argue that this deserves further study as an interesting example of a finite-temperature phase transition with compound order-parameter symmetry.

TT 47.10 Fri 12:00 H 0104

Magnetic properties of the Kitaev-Heisenberg model and effects of spin vacancies — Fabien Trousselet, Giniyat Khaliullin, and •Peter Horsch — Max-Planck-Institut f. Festkörperforschung, Heisenbergstr.1, D-70619 Stuttgart

We study the ground state properties of the Kitaev-Heisenberg model in a magnetic field and explore the evolution of spin correlations in the presence of non-magnetic vacancies [1]. This model may be relevant for layered iridates A2IrO3 (A=Na or Li) [2]. By means of

exact diagonalizations, the phase diagram without vacancies is determined as a function of the magnetic field and the ratio between Kitaev and Heisenberg interactions. We show that in the (antiferromagnetic) stripe ordered phase the static susceptibility and its anisotropy can be described by a spin canting mechanism, accounting as well for the transition to the polarized phase when including quantum fluctuations perturbatively.

Effects of spin vacancies depend sensitively on the type of the ground state. In the liquid phase, the magnetization pattern and its spatial anisotropy around a single vacancy in a small field is determined. In the stripe phase, the combination of a vacancy and a small field breaks the six-fold symmetry of the model and stabilizes a particular stripe pattern. Similar symmetry-breaking effects occur even at zero field due to interaction effects between vacancies. This selection mechanism and intrinsic randomness of vacancy positions may lead to spin-glass behavior.

[1] F. Trousselet, G. Khaliullin and P. Horsch, PRB 84, 054409 (2011).
[2] Y. Singh and P. Gegenwart, PRB 82, 064412 (2010);

TT 47.11 Fri 12:15 H 0104

Critical scales in anisotropic spin systems from the functional renormalization group — •Stefan Göttel[1,2], Sabine Andergassen[1,2], Dirk Schuricht[1,2], Carsten Honerkamp[2,3], and Stefan Wessel[3,4] — [1]Institute for Theory of Statistical Physics, RWTH Aachen — [2]JARA-Fundamentals of Future Information Technology — [3]Institute for Theoretical Solid State Physics, RWTH Aachen — [4]JARA-High-Performance Computing

We apply a recently developed functional renormalization group scheme [Reuther *et. al*, Phys. Rev. B **81**, 144410 (2010)] for quantum spin systems to the spin-1/2 antiferromagnetic XXZ model on a two-dimensional square lattice. Based on an auxiliary fermion representation we derive flow equations which allow a resummation of the perturbation series in the spin-spin interactions. This way, the spin susceptibilities are calculated for different values of the anisotropy parameter, confirming the phase transition between planar and axial ordering at the isotropic point. As recently proposed in [Reuther *et. al*, Phys. Rev. B **84**, 100406(R) (2011)], we extract critical temperatures from the flow. In the Ising limit these results coincide with the Onsager solution, but violate the Mermin-Wagner theorem at the isotropic point and a satisfactory description of the behavior in the vicinity of the phase transition is not possible. A quantitative comparison with quantum Monte-Carlo shows major differences. We trace this problem back to an incorrectly generated selfenergy and discuss potential improvements.

TT 47.12 Fri 12:30 H 0104

Vacancies in non-collinear antiferromagnets — •Alexander Wollny[1], Lars Fritz[2], and Matthias Vojta[1] — [1]Institut für theoretische Physik, Technische Universität Dresden, 01062 Dresden — [2]Institut für theoretische Physik, Universität zu Köln, 50937 Köln

We study dilute magnetic impurities and vacancies in two-dimensional frustrated magnets with non-collinear order. Taking the triangular-lattice Heisenberg model as an example, we use quasiclassical methods to determine the impurity contributions to the magnetization and susceptibility. Most importantly, each impurity moment is *not* quantized, but receives non-universal screening corrections due to local relief of frustration. At finite temperatures, where bulk long-range order is absent, this implies an impurity-induced magnetic response of Curie form, with a prefactor corresponding to a *fractional* moment per impurity. We also discuss the behavior in an applied magnetic field, where we find a singular linear-response limit for overcompensated impurities.

TT 48: Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Vortices

Time: Friday 9:30–13:00 Location: H 2053

TT 48.1 Fri 9:30 H 2053

Epitaxial Fe/$BaFe_{2-x}Co_xAs_2$ multilayers — •Jan Engelmann[1,2], Silvia Haindl[1], Kazumasa Iida[1], Fritz Kurth[1], Christian Behler[1], Ruben Huehne[1], Bernhard Holzapfel[1], and Ludwig Schultz[1,2] — [1]IFW Dresden, P. O. Box 27 01 16, 01171 Dresden, Germany — [2]TU Dresden, Institut für Festkörperphysik, D-01069 Dresden, Germany

Heterostructures of superconducting/ferromagnetic layers have attracted attention in controlling superconductivity by changing the magnetic state. In this work we present multilayers consisting of iron and Co-doped $BaFe_2As_2$ (Ba-122) fabricated by UHV pulsed laser deposition. We have employed the advantage of a coherent interfacial bonding between the FeAs tetrahedron of the iron pnictides and bcc Fe which enables the growth of epitaxial bi- and multilayers of Fe and the new Fe-based superconductors of high crystalline quality [1, 2] The epitaxial growth of the heterostructures was controlled in-situ by reflection high-energy electron diffraction (RHEED) and ex-situ by X-ray analysis. We discuss selected results of transport measurements with respect to the influence of additional Fe layers.

[1] T. Thersleff et al., APL 97 (2010) 022506
[2] K. Iida et al., APL 97 (2010) 172507

TT 48.2 Fri 9:45 H 2053

Transport, magnetic and structural properties of $YBa_2Cu_3O_7/La_{0.7}Ca_{0.3}MnO_3$ heterostructures grown on SrTiO3 (110) substrates — •Luqman Mustafa[1], Soltan Soltan[1,2], Gennady Logvenov[1], Hanns-Ulrich Habermeier[1], and Bernhard Keimer[1] — [1]Max Planck Institute or Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Physics Department, Faculty of science, Helwan University, 11792-Helwan, Cairo, Egypt

YBCO/LCMO bi- and multi-layers were grown on STO (110) substrates by Pulsed Laser Deposition (PLD) technique with the goal to study the interface of an oxide ferromagnet and a cuprate superconductor where the CuO_2 planes are perpendicular to the film plane. The structure was investigated by X-ray diffractometry, transport and magnetic properties were studied by conventional four-point-probe and SQUID techniques respectively.

Depending on the preparation conditions the single layer YBCO as well as bilayers can be grown in the (110), (103)/(10-3), as well as mixed orientations. Large anisotropy of electrical conductivity in these films was observed in case of (110)-oriented YBCO layer and less pronounced anisotropy in case of (103)-oriented one. We present a detailed analysis of the anisotropy of the magnetization of such bi- and multi-layers emphasizing its relation to the orientation of the YBCO film.

TT 48.3 Fri 10:00 H 2053

Transport measurements in superconductor/Heusler bilayers — •Inga-Mareen Imort, Savio Fabretti, Patrick Thomas, Günter Reiss, and Andy Thomas — Fakultät für Physik, Universität Bielefeld, Bielefeld, Germany

Superconductivity and ferromagnetism are two contrary phenomena due to their electronic properties. The investigation of superconductor (S)/ferromagnet (F) heterostructures has attracted a lot of scientific interest since they allow studying the interplay between superconductivity and ferromagnetism. Additionally, applications seem possible such as F/S/F spin valves and S/F/S π-junctions. Using transport- and magnetotransport-measurements, we investigate the behavior of the superconducting transition temperature T_c in NbTi/Co_2FeSi bilayers as a function of different layer thicknesses and for varying magnetic moments of the Co_2FeSi layers. Using rf - magnetron sputtering, NbTi/Co_2FeSi bilayers were grown on single-crystalline MgO(001) substrates and in-situ annealed at different temperatures. The layered character of our samples has been tested by X-ray diffraction (XRD) scans. The electronic and magnetic transport measurements have been performed between 3 and 300 K with the magnetic field up to 4 T oriented in the film plane. The dependence of T_c on the NbTi- and Co_2FeSi-layer thickness enables an estimation of the interface transparency of the NbTi/Co_2FeSi barrier in the framework of recent theoretical models. This work has been supported by the NRW MIFW.

TT 48.4 Fri 10:15 H 2053

Superconductivity and Magnetism in the presence of interface-induced Rashba spin-orbit coupling — •Florian Loder, Arno P. Kampf, and Thilo Kopp — Zentrum für Elektron-

ische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, Deutschland

Two dimensional electron systems at oxide interfaces are often influenced by a Rashba type spin-orbit coupling (SOC), which is tunable by a transverse electric field. Ferromagnetism at the interface can simultaneously induce strong local magnetic fields. This combination of SOC and magnetism leads to anisotropic two-sheeted Fermi surfaces, on which superconductivity with finite-momentum pairing is favored. The superconducting order parameter is derived within a generalized pairing model realizing both, the FFLO superconductor in the limit of vanishing SOC and a mixed-parity pairing state with zero pair momentum if the magnetism vanishes. The nature of the pairing state is discussed in the context of interface superconductivity and ferromagnetism at LAO-STO interfaces [1,2].
[1] Lu Li, C. Richter, J. Mannhart, and R. C. Ashoori, Nature Physics 7, 762 (2011).
[2] J. A. Bert, B. Kallisky, C. Bell, M. Kim, Y. Hikita, H. Y. Hwang, and K. A. Moler, Nature Physics 7, 767 (2011).

TT 48.5 Fri 10:30 H 2053

Proximity effect in semiconductor films with spin-splitting and spin-orbit interaction — •Jens Michelsen and Roland Grein — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Superconducting heterostructures with spin-active materials have emerged as promising platforms for engineering topological superconductors featuring Majorana bound states at surfaces, edges and vortices. Here we present a method for evaluating, from a microscopic model, the band structure of a semiconductor film of finite thickness deposited on top of a conventional superconductor. Analytical expressions for the proximity induced gap openings are presented in terms of microscopic parameters and the proximity effect in presence of spin-orbit and exchange splitting is visualized in terms of Andreev reflection processes. An expression for the topological invariant, associated with the existence of Majorana bound states, is shown to depend only on parameters of the semiconductor film. The finite thickness of the film leads to resonant states in the film giving rise to a complex band structure with the topological phase alternating between trivial and non-trivial as the parameters are tuned of the film are tuned.

TT 48.6 Fri 10:45 H 2053

Proximity effect in noncentrosymmetric superconductors hybrid structures — •Gaetano Annunziata[1], Jacob Linder[2], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway

We analyze proximity effect in junctions of noncentrosymmetric superconductors (NCSs) and diffusive metals/ferromagnets within the quasiclassical theory of superconductivity. We show how by standard STM/STS measurements for LDOS in the proximate region [1] exploiting the directional dependence of pair-breaking effect of the exchange field on the triplet Cooper pairs [2,3], several superconducting scenarios for NCSs characterized by different kinds of edge states [4] can be discriminated, and that within a single scenario information on the relative magnitude of triplet and singlet gaps in NCSs can be obtained [5].
[1] T. Kontos, M. Aprili, J. Lesueur, F. Genêt, B. Stephanidis, and R. Boursier, Phys. Rev. Lett. **89**, 137007 (2002).
[2] P. M. R. Brydon and D. Manske, Phys. Rev. Lett. **103**, 147001 (2009).
[3] G. Annunziata, M. Cuoco, C. Noce, A. Sudbø, and J. Linder, Phys. Rev. B **83**, 060508(R) (2011).
[4] Y. Tanaka, Y. Mizuno, T. Yokoyama, K. Yada, and M. Sato, Phys. Rev. Lett. **105**, 097002 (2010).
[5] G. Annunziata, J. Linder and D. Manske, to be published.

TT 48.7 Fri 11:00 H 2053

Transport properties of a Josephson junction coupled to the dynamics of a nanomagnet — •Cecilia Holmqvist[1], Wolfgang Belzig[1], and Mikael Fogelström[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

The interplay between superconductivity and ferromagnetism in nanoscale junctions may lead to interesting effects that could be utilized in spintronics devices. Here, we present a theoretical study of a superconducting point contact coupled to a nanomagnet. The magnetization of the nanomagnet is brought into precession by an external magnetic field. The coupling between the Josephson effect and the magnetization precession modifies the current-phase relation [1]. Additionally, the critical current is enhanced at finite temperatures due to coupling between the continuum of states and the Andreev levels. The spin-dependent Andreev scattering also generates an ac spin current, that decays on the length scale of the superconducting coherence length. For a voltage-biased Josephson junction coupled to a precessing spin, the interplay between spin-scattering processes and multiple Andreev reflection, characterized by the Larmor and Josephson frequencies, respectively, leads to a modification of the current-voltage characteristics as well as the spin transport properties.
[1] C. Holmqvist, S. Teber, and M. Fogelström, Phys. Rev. B 83, 104521 (2011)

15 min. break.

TT 48.8 Fri 11:30 H 2053

Characterization and electronic transport properties of nanostructured Pb/Fe point contacts — •Jörg Gramich[1], Gernot Goll[1], Christoph Sürgers[2], and Hilbert v. Löhneysen[1,2] — [1]DFG-Centrum für Funktionelle Nanostrukturen, KIT Karlsruhe — [2]Physikalisches Institut, KIT Karlsruhe

We experimentally investigate the spin-polarized transport through nanostructured Pb/Fe point contacts at low temperatures. All samples are produced by *in-situ* evaporation of the metals on either side of a Si_3N_4 membrane with a nanostructured hole, resulting in clean metal interfaces. A direct measurement of the nanocontact size allows for the first time a comparison with theoretical models for contact-size estimates of heterocontacts. The ballistic transport regime for contacts with high Knudsen ratio is demonstrated by features in the spectra such as phonon peaks and the critical pair-breaking current of Pb. The spin polarization P of the current through the superconductor-ferromagnet contact is determined by means of Andreev reflection at the S/F interface. The observed systematic dependence on the contact radius a and superconducting transition temperature T_c is compared to previous measurements on Al/Fe nanocontacts.

TT 48.9 Fri 11:45 H 2053

A Numerical Study of the Superconducting Proximity Effect in Topological Surface States — •Roland Grein[1,2], Jens Michelsen[1], and Matthias Eschrig[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]SEPnet and Hubbard Theory Consortium, Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, United Kingdom

We study a microcopic model to investigate the superconducting proximity effect in the topological surface states of Bi_2Se_3 by means of the recursive Green's function technique. We find that the phenomenological Fu-Kane model, usually used to describe the proximity effect in these states, breaks down at energies close to the superconducting bulk-gap and in the case of strong coupling between the topological insulator and the superconductor[1].
[1] R. Grein, J. Michelsen, M. Eschrig, arXiv:1111.0445 (2011)

TT 48.10 Fri 12:00 H 2053

Nonlocal thermoelectric symmetry relations in ferromagnet-superconductor proximity structures — •Peter Machon[1], Matthias Eschrig[1,2], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Royal Holloway, University of London, Egham Hill, EGHAM, TW20 0EX, UK

The symmetries of thermal and electric transport coefficients in quantum coherent structures are related to fundamental thermodynamic principles by the Onsager reciprocity. We generalize Onsager's symmetry relation to nonlocal thermoelectric currents in a three terminal ferromagnet-superconductor heterostructur including spin-dependent crossed Andreev reflection and direct electron transfer processes. We proof this general symmetry by applying spin-dependent boundary conditions for quasiclassical Green's functions in both the clean and the dirty limit. We predict an anomalously large local thermopower and a nonlocal Seebeck effect, which can be explained by the spin-dependent spectral properties.

TT 48.11 Fri 12:15 H 2053

Driven superconducting proximity effect in interacting quantum dots — •Ali G. Moghaddam[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]School of Chemical and Physical Sciences, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

We show that strong superconducting correlations can be induced in an interacting quantum dot (QD) using fast oscillations in the effective coupling between the dot and superconducting leads which drive the dot out of equilibrium. This is in contrast with the well-known equilibrium state suppression of proximity effect in interacting QDs. In fact although interaction prohibits the superposition of empty (0) and doubly-occupied (d) states, fast coherent dynamics accompanied by the fast variations in the tunnel coupling can produce a nonequilibrium finite probability for such a superposition. Subsequently the superconducting correlations are established inside the QD when the energy difference between 0 and d states coincide with the frequency of driving oscillations. Simultaneously the nonequilibrium occupation probabilities of 0 and d states cause a pumping current flowing to the normal lead connected to the dot. Finally we demonstrate coherent oscillations in both dot charge and current by applying a pulsed oscillatory field to the coupling of dot and superconductor which show the possibility of coherent manipulation in the subspace of 0 and d states by changing the pulse duration.

TT 48.12 Fri 12:30 H 2053

The role of thermal conductivity on the nucleation and propagation of magnetic flux avalanches — •Claudia Stahl[1], Sebastian Treiber[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart — [2]Hochschule Aalen, Beethovenstraße 1, 73430 Aalen

Below a certain threshold temperature the critical state of superconducting thin films can get unstable, which results in large magnetic flux avalanches. In thin MgB_2 films with an inhomogeneous current density distribution both the nucleation and propagation of magnetic flux avalanches are highly favoured [1].

Magnetization measurements and magneto - optical imaging are used to characterize inhomogeneous MgB_2 thin films.

Avalanches occur when the thermal transport gets much slower than the transport by electric conductivity. Increasing the thermal conductivity by a gold cover layer leads to a suppression of the instabilities. It is investigated how the two steps of the avalanche process, nucleation and propagation, are influenced by the thermal conductivity in inhomogeneous MgB_2 thin films. We found that the gold layer in particular influences the initial phase of the avalanche formation.

[1] S. Treiber, C. Stahl, G. Schütz, and J. Albrecht, *Physical Review B* **84**, 094533 (2011).

TT 48.13 Fri 12:45 H 2053

Superconducting vortex dynamics in cylindrical Nb micro- and nanotubes — •Vladimir M. Fomin[1], Roman O. Rezaev[1,2], and Oliver G. Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]Laboratory of Mathematical Physics, Tomsk Polytechnic University, 634050 Tomsk, Russia — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Advancements in fabrication of rolled-up micro- and nanotubes including superconductor layers (e.g., InGaAs/GaAs/Nb) open new ways for investigation of the vortex matter in superconductors with curved geometries. Geometry determines the dynamics of vortices in the presence of transport currents in open superconductor micro- and nanotubes subject to a magnetic field orthogonal to the axis. Vortices nucleate periodically at one edge of the tube, subsequently move along the tube under the action of the Lorentz force and denucleate at the opposite edge of the tube. Characteristic times of nonequilibrium vortex dynamics in an open tube are efficiently controlled by the tube radius. The magnetic field, at which the vortices begin to nucleate at the edge of the structure, is increased several times by rolling up a planar film in a tube. This effect is caused not only by a spatial dependence of the magnetic field component normal to the cylindrical surface, but also by correlations between the states of the superconducting order parameter in the opposite areas of the cylindrical surface.

TT 49: Correlated Electrons: Low-dimensional Systems - Materials 4

Time: Friday 9:30–12:00 Location: H 3005

TT 49.1 Fri 9:30 H 3005

Crossover from 1D to 2D in the Infrared Absorption of Cuprate Ladder Systems — •Kris Cöster[1], Stefan Wessel[2], Eva Benckiser[3], Michael Voigt[4], Markus Grüninger[4], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I , TU Dortmund, 44221 Dortmund, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University, 52056 Aachen, Germany — [3]Max-Planck-Institut für Fest körperforschung, 70569 Stuttgart, Germany — [4]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We study the optical spectra of n-leg cuprate ladder systems using infrared absorption and different theoretical tools. The n-leg spin ladders interpolate between the 1D spin chain with fractional excitations and the two-dimensional Heisenberg model on the square lattice relevant for the undoped mother compounds of the high-temperature superconductors. Theoretically, we use perturbative continuous unitary transformations and quantum Monte Carlo simulations to investigate the infrared absorption of n-leg Heisenberg ladders. This joined approach of theory and experiment allows a convincing physical identification of a sharp spectral mode arising from a two-particle bound state dominating the infrared absorption at low energies. This low-energy behaviour of the infrared absorption is a generic feature being present for all studied n-leg ladder systems with $n > 1$.

TT 49.2 Fri 9:45 H 3005

Spin and lattice dynamics in the low-dimensional quantum magnet $(NO)Cu(NO_3)_3$ — Vladimir Gnezdilov[1], •Dirk Wulferding[2], Peter Lemmens[2], Yurii Pashkevich[3], Olga Volkova[4], Igor Morozov[4], and Alexander Vasiliev[4] — [1]ILTPE NAS, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]DonFTI, Donetsk, Ukraine — [4]MSU, Moscow, Russia

We present excitation spectra of $(NO)Cu(NO_3)_3$, a topological realization of the 2D Nersesyan-Tsvelik model with possible RVB or VBC ground states. The phonons display a temperature dependence and anomalies due to strong spin-lattice coupling which has not been considered in previous investigations. In addition, a broad magnetic continuum is observed and used to investigate the spin dynamics. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

TT 49.3 Fri 10:00 H 3005

The magnetic ground state of the frustrated spin chain linarite — •Britta Willenberg[1,2], Markus Schäpers[3], Kirrily Rule[1], Stefan Süllow[2], Manfred Reehuis[1], Bachir Ouladdiaf[4], Hanjo Ryll[1], Klaus Kiefer[1], and Anja Wolter[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [3]Leibniz Institute for Solid State and Materials Research IFW, Dresden, Germany — [4]Institute Laue-Langevin, Grenoble, France

The natural mineral linarite, $PbCuSO_4(OH)_2$, is found to be a frustrated one dimensional spin system. In the material CuO_4 units form chains along the b axis, in which the Cu^{2+} ions are coupled ferromagnetically to the nearest neighbor with a coupling constant $J_1 \approx 100\,\mathrm{K}$ and antiferromagnetically to the next nearest neighbor with $J_2 \approx -36\,\mathrm{K}$ leading to a ratio J_2/J_1 = -0.36. Due to a residual interchain couplings a magnetically ordered state is observed for temperatures below $T_N = 2.8\,\mathrm{K}$. We will present neutron diffraction results on the magnetically ordered ground state. The propagation vector indicates an incommensurate magnetic moment structure. The refinement of the neutron diffraction data shows that the structure is formed by an elliptical helical arrangement of moments. Furthermore, we will present magnetization measurements for temperatures down to 0.25 K in applied magnetic fields along the b axis indicating a very rich magnetic phase diagram, likely as a result of magnetic frustration.

TT 49.4 Fri 10:15 H 3005

Magnetic properties and revisited exchange integrals of the frustrated chain cuprate $PbCuSO_4(OH)_2$ - linarite — •M. Schäpers[1], A. U. B. Wolter[1], F. Lipps[1], V. Kataev[1], S.-L. Drechsler[1], S. Nishimoto[1], R. Beyer[2], M. Uhlarz[2], J. Wosnitza[2], B. Willenberg[3,4], K. C. Rule[3], S. Süllow[4], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]HZB für Materialien und Energie, Berlin, Germany — [4]IPKM, TU Braunschweig, Braunschweig, Germany

We present a detailed experimental and theoretical study of the frustrated s = $\frac{1}{2}$ spin-compound linarite, $PbCuSO_4(OH)_2$, with competing ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions. Our experimental data are described using various theoretical approaches to obtain the magnetic exchange interactions. These main intrachain interactions are significantly larger as those derived previously [1, 2], causing a shift of the frustration ratio $\alpha \approx 0.36$ closer to the 1D critical point. ESR and NMR at elevated temperatures indicate a highly frustrated system with the onset of magnetic correlations far above the magnetic ordering temperature $T_N = 2.8$ K into a spin spiral ground state. Linarite shows a complex magnetic phase diagram with small saturation field, which makes it a prototype for investigating the recently predicted spin multipolar order close to the saturation field for such spin-chain compounds.

[1] M. Baran et al., Phys. Stat. Sol. (c) **3**, 220 (2006).
[2] Y. Yasui et al., JPSJ **80**, 033707 (2011).

TT 49.5 Fri 10:30 H 3005

Field-induced staggered moment stabilization in frustrated quantum magnets — •Burkhard Schmidt, Mohammad Siahatgar, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

For low-dimensional frustrated quantum magnets, the dependence of the staggered moment on an applied magnetic field is nonmonotonic: For small and intermediate fields, quantum fluctuations are gradually suppressed, leading to an increase of the staggered moment as a function of the field strength. For large applied magnetic fields, the classically expected field dependence is recovered, namely a monotonous decrease with increasing field strength. The staggered moment is eventually suppressed when reaching the fully polarized state at the saturation field. The quantitative analysis of this behavior is an excellent tool to determine the frustration parameter of a given compound. We apply linear spin-wave theory, numerical exact diagonalization, and a self-consistent RPA theory. As an example, we discuss the recently measured field dependence of the magnetic neutron scattering intensity of $Cu(pz)_2(ClO_4)_2$ in the framework of the $S = 1/2$ two-dimensional (2D) J_1-J_2 Heisenberg model. Our results show that $Cu(pz)_2(ClO_4)_2$ is a quasi-2D antiferromagnet with intermediate frustration $J_2/J_1 = 0.2$. With this ratio, the observed reentrant behavior of the magnetic ordering temperature as a function of the applied magnetic field can be understood as a consequence of the reduced quantum fluctuations as well.

15 min. break.

TT 49.6 Fri 11:00 H 3005

Comparative study of spin orbit dominated iridates — •Mehmet Fatih Cetin[1], Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Tomohiro Takayama[3], Kei Ohashi[3], Hidenori Takagi[3,4], Kwang-Yong Choi[5], and Chengtian Lin[6] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]ILTPE NAS, Ukraine — [3]AM, Univ. Tokyo, Japan — [4]RIKEN, Japan — [5]Dept. Phys., CA Univ., Seoul, Korea — [6]MPI-FKF, Stuttgart, Germany

Raman spectroscopy is used to compare the effect of SOC on the excitation spectra in Sr_2IrO_4, $Sr_3Ir_2O_7$, and $Na_4Ir_3O_8$, which are reported to be spin liquids or anomalous Mott insulators. There is a decisive dynamics of the quasi particles and crossover phenomena related to an entanglement of electronic and lattice degrees of freedom. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

TT 49.7 Fri 11:15 H 3005

Unconventional magnetic ordering in Spin-orbit Mott insulator with Honeycomb lattice — •Soham Manni[1], Yogesh Singh[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Goettingen, Germany — [2]IISER Mohali, Mohali, India

Iridates have recently attracted much attention due to a novel $S_{\text{eff}} = 1/2$ Mott insulating state, driven by the interplay of moderate electronic correlations with strong spin-orbit coupling. We focus on A_2IrO_3 (A=Na,Li) which is a layered system with Ir moments sitting on a Honeycomb lattice and study their magnetic properties [1, 2]. The temperature dependence of the susceptibility indicates a dominating antiferromagnetic exchange interaction with $\Theta_W = -116$ K and -33 K for the Na- and Ir system, respectively, while $T_N = 15$ K for both materials. Resonant X-ray scattering for the former system indicates an unconventional most likely zig-zag magnetic structure [3]. We discuss the results with respect to recent theoretical predictions for the Heisenberg-Kitaev model, including magnetic exchange beyond next-neighbor couplings and also present first results on the related Li_2RhO_3 system.

Work supported by the AvH foundation and the Erasmus Mundus EURINDIA project.

[1] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010).
[2] Y. Singh, S. Manni, P. Gegenwart, arXiv:1106.0429.
[3] X. Liu et al., Phys. Rev. B 83, 220403(R) (2011).

TT 49.8 Fri 11:30 H 3005

THz and infrared excitation spectrum below the Jahn-Teller transition in $Sr_3Cr_2O_8$ — •Zhe Wang[1], Michael Schmidt[1], Axel Günther[1], Franz Mayr[1], Diana Quintero-Castro[2,3], A. T. M. Nazmul Islam[2], Bella Lake[2,3], Hans-Albrecht Krug von Nidda[1], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

We report on optical excitations observed recently in $Sr_3Cr_2O_8$ by THz and infrared spectroscopy. Low-energy excitations below 3 THz are detected by THz time domain spectroscopy. These excitations can be divided into two different classes according to the temperature-dependent properties. One is emergent right below the Jahn-Teller transition temperature, which is determined by specific heat measurement to occur at 285 K [1,2]. The other appears only below 100 K, where the fluctuations are sufficiently suppressed, consistent with the temperature dependence of low-energy Raman modes [3]. Infrared transmission measurements reveal a broad crystal-field excitation, which can be associated with an electronic transition from E to T_2 orbital states.

[1] Zhe Wang et al., Phys. Rev. B 83, 201102 (2011)
[2] D. L. Quintero-Castro et al., Phys. Rev. B 81, 014415 (2010)
[3] D. Wulferding et al., Phys. Rev. B 84, 064419 (2011)

TT 49.9 Fri 11:45 H 3005

Optical spectroscopy of the Triangular Lattice Antiferromagnets $CuCrO_2$ and α-$CaCr_2O_4$ — •Michael Schmidt[1], Zhe Wang[1], Franz Mayr[1], Sandor Toth[2,3], Bella Lake[2,3], Nazmul Islam[2], Vladimir Tsurkan[1], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz Zentrum Berlin, Berlin 14109, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

We will compare and discuss our results obtained by optical spectroscopy on $CuCrO_2$ and α-$CaCr_2O_4$. While $CuCrO_2$ is famous for its multiferroicity [1], in α-$CaCr_2O_4$ a polarization can only be observed under the application of electric or magnetic field, despite having a closely related structure [2]. At near infrared and visible light frequencies we observe Cr^{3+} crystal field absorptions and below T_N excitons and exciton-magnon-transitions appear. The width of these exciton-magnon transitions is analyzed with respect to the existence of Z_2 vortices as proposed by Kojima et al. [3].

[1] S. Seki et al., Phys. Rev. Lett. 101, 067240 (2008)
[2] K. Singh et al., Phys. Rev. B 84, 064129 (2011)
[3] N. Kojima et al., J. Phys. Soc. Jpn. 62, 4137 (1993)

TT 50: Superconductivity: (General) Theory

Time: Friday 9:30–12:15 Location: H 3010

TT 50.1 Fri 9:30 H 3010

State of the art and new developments in superconducting density functional theory — •Antonio Sanna and Eberhard K. U. Gross — Max Planck Institute Halle

We will present the theoretical framework of superconducting density functional theory (SCDFT), a fully parameter-free approach to superconductivity. The advantages and disadvantages of this method will be presented, as well as more recent extensions and perspectives. First I will present the connection of the theory to Eliashberg's method, and discuss some exact limits. Then I will report on how this connection is used to improve the existing phononic functionals. Applications to several materials will be shown. The purely electronic part of the coupling in SCDFT will also be analyzed properties and limits of the static random phase approximation will be discussed. Finally I will report on recent extensions which include dynamical effects in the screened interaction.

TT 50.2 Fri 9:45 H 3010

Reliability study of the Migdal-Eliashberg theory for strong coupling superconductors — Johannes Bauer[1], Jong E Han[1,2], and •Olle Gunnarsson[1] — [1]Max-Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart, Germany — [2]Department of Physics, SUNY at Buffalo, Buffalo, New York 14260, USA

The Migdal-Eliashberg (ME) theory for strong electron-phonon coupling and retardation effects of the Morel-Anderson type form the basis for the quantitative understanding of conventional superconductors. In recent years, the validity of the ME theory for values of the electron-phonon coupling strength $\lambda > 1$ has been questioned by model studies. By distinguishing bare and effective parameters, and by comparing the ME theory with the dynamical mean field theory (DMFT), we clarify the range of applicability of the ME theory. Specifically, we show that ME theory is very accurate as long as the product of effective parameters, $\lambda\omega_{\rm ph}/D$, where $\omega_{\rm ph}$ is an appropriate phonon scale and D an electronic scale, is small enough [1]. The effectiveness of retardation effects for the competing Coulomb interaction is usually considered based on the lowest order diagram in the perturbation theory. We analyze these effects to higher order and find modifications to the usual result for the Coulomb pseudo-potential μ^*. Retardation effects are weakened due to a reduced effective bandwidth appearing in the expressions. Comparsion with the non-perturbative DMFT corroborates our findings [2].

[1] J Bauer, J E Han, and O Gunnarsson, Phys. Rev. B. 84, 184531 (2011).
[2] J Bauer, J E Han, and O Gunnarsson, in preparation (2011).

TT 50.3 Fri 10:00 H 3010

A Green function approach to superconductivity in nanofilms — •Rolando Saniz, Bart Partoens, and François Peeters — Universiteit Antwerpen, Antwerpen, Belgium

We reformulate the BCS theory of superconductivity in the Green function framework in such a way that it is readily applied to inhomogeneous systems. We study here nanofilms and go beyond previous models in that we take into account the effects of confinement on electron-phonon coupling, as well as on the electron and phonon fields. We show that, contrary to what has been advanced in recent years, the increases of the density of states as the film thickness increases will tend to suppress the critical temperature, and not enhance it. Instead, it is the increase of the phonon modes with increasing film thickness that can lead to increases of the critical temperature above the bulk value. Further, we show that the multigap character of superconductivity in nanofilms will result in general in a condensate composed of subcondensates with different coherence lengths. This is in analogy with the very recent suggestion that different coherence lengths exist in two-gap superconductors such as MgB_2.

TT 50.4 Fri 10:15 H 3010

Phase Diagram of Electron Systems near the Superconductor-Insulator Transition — •Thomas Nattermann[1], Valery Pokrovsky[2,3], and Gianmaria Falco[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]Department of Physics, Texas A&M University, College Station, Texas 77843-424 — [3]Landau Institute for Theoretical Physics, Chernogolovka, Moscow District, 142432, Russia

The zero temperature phase diagram of Cooper pairs exposed to disorder and magnetic field is determined theoretically from a variational approach. Four distinct phases are found: a Bose and a Fermi insulating, a metallic and a superconducting phase, respectively. The results explain the giant negative magneto-resistance found experimentally in In-O, TiN, Bi and high-T_c materials.

TT 50.5 Fri 10:30 H 3010

Is the $t-J$ model sufficient to describe magnetic excitations in cuprates? — •Wei Chen[1] and Oleg Sushkov[2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of New South Wales, Sydney 2052, Australia

We adopt theself-consistent Born approximation to study the renormalization of magnetic excitations in a two-dimensional antiferromagnetic state due to finite hole doping. We found that the incoherent motion of holes strongly influences high energy magnons, which causes a significant reduction of magnon bandwidth at large doping. However, by comparing with recent resonant inelastic x-ray scattering data, we conclude that the strongly correlated holes, as described by the $t-J$ model, are not sufficient to determine the magnetic excitations in underdoped cuprates.

15 min. break.

TT 50.6 Fri 11:00 H 3010

Two-particle self-consistent approach to anisotropic superconductivity — •Junya Otsuki — Department of Physics, Tohoku University, Sendai, Japan — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

A non-perturbative approach to anisotropic superconductivity is developed based on the idea of the two-particle self-consistent (TPSC) theory by Vilk and Tremblay [1]. An exact sum-rule which the momentum-dependent pairing susceptibility satisfies is derived. Effective pairing interactions between quasiparticles are determined so that an approximate susceptibility should fulfill this sum-rule, in which fluctuations belonging to different symmetries mix at finite momentum. The mixing leads to a suppression of the $d_{x^2-y^2}$ pairing close to the half-filling, resulting in a maximum of T_c away from half-filling.

[1] Y. M. Vilk and A.-M. Tremblay, J. Phys. I (Paris) **7** (1997) 1309.

TT 50.7 Fri 11:15 H 3010

Fulde-Ferrel-Larkin-Ovchinnikov phase separation in a one-dimensional superconducting lattice of strongly coupled fermions — •Vivian França and Andreas Buchleitner — Physikalisches Institut, Albert-Ludwigs Universität, Freiburg, Germany

The exotic coexistence of superconductivity and magnetism, first investigated by Fulde-Ferrell and Larkin-Ovchinnikov (FFLO), is predicted to show a spontaneous breaking of spatial symmetry. In spin-imbalanced fermionic systems, such inhomogeneous superfluidity would take place via a microscale phase separation, with alternating finite-momentum pairs and normal regions, the latter being composed by the excess species. After almost fifty years since the FFLO-phase was predicted, the microscale phase separation has not been observed.

We deduce an expression for the critical polarization below which the FFLO-state emerges in a one-dimensional lattice with spin-imbalanced populations and show that its ground-state is indeed microscale phase separated. For strongly interacting systems, we find that the microscale structure can be observed directly in the density profiles. Our results suggest that clear signatures of exotic superfluidity are accessible for state-of-the-art experiments with single-site resolution, as already achieved for bosons.

TT 50.8 Fri 11:30 H 3010

Competing many-body instabilities and unconventional superconductivity in graphene — •Christian Platt[1], Maximilian Kiesel[1], Dmitry Abanin[2], Werner Hanke[1], and Ronny Thomale[3] — [1]Institute for Theoretical Physics, University of Wuerzburg — [2]Department of Physics, Harvard University — [3]Department of Physics, Stanford University

The band structure of graphene exhibits van Hove singularities (VHS) at doping x = *1/8 away from the Dirac point. Near the VHS, interactions effects, enhanced due to the large density of states, can give rise to various many-body phases at experimentally accessible temperatures. We study the competition between different many-body instabilities in graphene using functional renormalization group (FRG). We predict a rich phase diagram, which, depending on long range hopping as well as screening strength and absolute scale of the Coulomb interaction, contains a d + id-wave superconducting (SC) phase, or a spin density wave phase at the VHS. The d + id state is expected to exhibit quantized charge and spin Hall response, as well as Majorana modes bound to vortices. In the vicinity of the VHS, we find singlet d + id-wave as well as triplet f -wave SC phases. [1] arXiv:1109.2953v1

TT 50.9 Fri 11:45 H 3010

Resonant inelastic x-ray scattering (RIXS) in an unconventional superconductor — •Pasquale Marra, Steffen Sykora, and Jeroen van den Brink — IFW, Dresden, Germany

The investigation of the pairing mechanism in unconventional superconductors has generated enormous interest in spectroscopic techniques which are sensitive with respect to the phase of the superconducting order parameter. We show that resonant inelastic x-ray scattering (RIXS) in combination with an appropriate high energy resolution would be a very promising method in that aspect.

Using a BCS model for unconventional superconductors we calculate the lowest order excitations which are relevant for the RIXS scattering amplitude. We compare different scenarios of pairing and show that the momentum-dependent low energy RIXS spectra are strongly influenced by coherence factors which are known to be phase-sensitive.

TT 50.10 Fri 12:00 H 3010

Supercurrent through cuprate grain boundaries in the presence of strong correlations — •Fabian Alexander Wolf, Siegfried Graser, Florian Loder, and Thilo Kopp — Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Strong correlations are known to severely reduce the mobility of charge carriers near half-filling and thus have an important influence on the current carrying properties of grain boundaries in high-T_c cuprates. We apply a Gutzwiller method to investigate the critical current through microscopically reconstructed grain boundaries for a wide range of misalignment angles. In good agreement with experimental data, we find a reduction of the current by one order of magnitude as compared to an analogous weak coupling evaluation. This reduction emerges from the interplay of charge fluctuations and strong correlations. See Reference arXiv:1106.5759.

TT 51: Transport: Nanoelectronics II - Spintronics and Magnetotransport (jointly with HL and MA)

Time: Friday 9:30–12:00 Location: BH 243

TT 51.1 Fri 9:30 BH 243

Adiabaticity mediated mesoscopic spin transport — •Tobias Dollinger, Henri Saarikoski, and Klaus Richter — Universität Regensburg, Germany

We examine mesoscopic transport in ballistic and diffusive waveguide geometries with Zeeman coupling by means of a numerical recursive Green's function algorithm and interprete the results using a semiclassical transport formalism. Our discussion is focused on analyzing magnetoconductance traces of two-dimensional systems with spatially nonuniform magnetic moment. We illustrate how controlling magnetic field textures within a sample allows for an efficient manipulation of spin transmission properties, which are determined by nonadiabatic transition probabilities.

TT 51.2 Fri 9:45 BH 243

Electronic transport through EuO spin filter tunnel junctions — •Nuttachai Jutong[1], Ivan Rungger[2], Stefano Sanvito[2], Udo Schwingenschlögl[3], and Ulrich Eckern[1] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]School of Physics and CRANN, Trinity College Dublin, Dublin, Ireland — [3]KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

Spin filter tunnel junctions based on europium monoxide (EuO), a ferromagnetic semiconductor, are investigated by means of density functional theory. In particular, the spin transport of Cu/EuO/Cu junctions is investigated by using the self-consistent ab-initio electron transport code SMEAGOL. The dependence of the transmission coefficient on the interface spacing and on the EuO thickness is studied, and explained in terms of the density of states and the complex band structure of EuO. Our calculation indicates that EuO epitaxially grown on Cu can act as a perfect spin filter, with polarization close to 100%, which is related mainly to the Eu-4f states. The transmission coefficient is sensitive to the interface spacing, since this spacing determines the charge transfer between EuO and the Cu leads.

TT 51.3 Fri 10:00 BH 243

Spin transistor action from Onsager reciprocity and SU(2) gauge theory — Inanc Adagideli[1], •Vitalij Lutsker[2], Matthias Scheid[2], Philippe Jacquod[3], and Klaus Richter[2] — [1]Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [3]Physics Department, University of Arizona, Tucson, USA

We construct a local gauge transformation to show how, in confined systems, a generic, weak non-homogeneous $SU(2)$ spin-orbit Hamiltonian reduces to two $U(1)$ Hamiltonians for spinless fermions at opposite magnetic fields, to leading order in the spin-orbit strength. Using an Onsager relation, we further show how the resulting spin conductance vanishes in a two-terminal setup, and how it is turned on by either weakly breaking time-reversal symmetry or opening additional transport terminals. We numerically check our theory for mesoscopic cavities as well as Aharonov-Bohm rings.

TT 51.4 Fri 10:15 BH 243

Magnetic impurities on Bi thin films — •Daniel Lükermann[1], Sergii Sologub[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover — [2]Institute of Physics, National Ac. of Sc. Ukraine, Nauky Av. 46, 03028 Kyiv, Ukraine

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. Furthermore, the surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements.
In order to elucidate the effect of spin-related scattering at impurities, magnetic and non-magnetic metals were adsorbed on thin films of epitaxially grown Bi(111) and investigated by means of conductance and magneto-conductance measurements. We observe a very strong reduction of conductance by roughly 30 % for adsorbate concentrations of less than 2% of a monolayer both for Bi- and Co-atoms, whereas Fe-atoms only show an effect of 15 %, ruling out the simple assumption of enhanced spin-flip-scattering of the spin-polarized carriers at magnetic impurities. An evaluation of magneto-conductance and Hall-effect data reveals that the charge transfer from the impurity atoms into the surface states of bismuth plays an important role and can not be neglected in interpreting the data.

TT 51.5 Fri 10:30 BH 243

Adiabatic pumping through an interacting quantum dot with spin-orbit coupling — •Stephan Rojek[1], Jürgen König[1], and Alexander Shnirman[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]Institut für Theorie der Kondensierten Materie and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany

We study adiabatic pumping through a two-level quantum dot coupled to two normal metallic leads in the presence of spin-orbit coupling. The variation of the two energy levels of the dot periodically in time leads

to finite charge and spin currents.

We calculate the pumped charge and spin using a diagrammatic real-time approach [1]. Going beyond the limit of noninteracting electrons on the quantum dot [2], we study the situation of strong Coulomb interaction. In both limits of noninteracting and strongly interacting electrons, spin-orbit coupling provides the possibility for pure spin current. We introduce an isospin to describe the level degree of freedom. This isospin feels an exchange field similar to the exchange field in a quantum-dot spin valve. The exchange field originates form the Coulomb interaction and its strength is sensitive to the symmetry in the tunneling matrix elements. New features concerning the pure spin pumping as well as the absolute pumped charge of the two-level quantum dot with spin-orbit coupling arises from the Coulomb interaction.

[1] J. Splettstoesser *et al.*, Phys. Rev. B **74**, 085305 (2006).
[2] V. Brosco *et al.*, Phys. Rev. B **82**, 041309(R) (2010).

15 min. break.

TT 51.6 Fri 11:00 BH 243

Anomalous Hall conductivity in Ni and its alloys — •D. Ködderitzsch, K. Chadova, J. Minar, and H. Ebert — Universität München, Department Chemie, Butenandtstraße 5-13, D-81377 München, Germany

The anomalous Hall conductivity (AHC) in Ni as discussed on the basis of the intrinsic contribution shows a strong overestimation of the AHC [1]. Recent studies using the LSDA+U approximation seem to remedy this problem [2]. However, still missing is taking into account the temperature dependence of the AHC which has recently been reinvestigated [3] and changes the picture.

Using our recently implemented [4] first-principles approach to describe transverse transport based on the Kubo-formalism in the Kubo-Středa formulation we study the anomalous Hall conductivity (AHC) in Ni. To take into account the effect of correlations we extended our method to employ the LSDA+U, as well as the LSDA+DMFT to go beyond the LSDA approximation to DFT. Furthermore, we study the influence of finite temperatures on the AHC by using an alloy-analogy for a quasistatic representation of the thermal displacements of the atoms. In addition, we performed calculations for dilute impurities in the Ni host.

[1] Nagaosa *et al.* Rev. Mod. Phys. **82**, 1539 (2010) and references therein
[2] Weischenberg *et al.* PRL **107**, 106601 (2011); Fuh and Guo PRB **84**, 144427 (2011)
[3] Xiao, Jin
[4] Lowitzer, Gradhand, Fedorov, Mertig, Ködderitzsch, Ebert, PRL **105**, 266604 (2010) and PRL **106**, 056601 (2011)

TT 51.7 Fri 11:15 BH 243

Investigation of magnetic point contacts irradiated by microwave and THz radiation — •Stefan Egle, Torsten Pietsch, and Elke Scheer — Department of Physics, University of Konstanz

The growing field of spintronics became one of the most intensively studied topics in modern solid-state physics. The possibility not only exploiting the charge of an electron, but also its spin (or magnetic moment), offers the possibility to explore various interesting effects. In this talk, we investigate magnetic point contacts and heterostructures, where a ferromagnet (F) acts as a spin polarizer, injecting hot electrons into a non-magnetic metal (N) or a diluted ferromagnet (f). Thereby, an external magnetic field in case of N is used to generate a Zeeman-splitting between spin-up and spin-down electrons. In case of F/f-contacts, this energy splitting ΔE is given by the exchange energy of f. These energies correspond to electromagnetic frequencies in the GHz (N) and THz regime (f). The highly non-equilibrium spin-population of F is then used to create a spin inversion in N or f, leading to a spin-flip photon emission. By matching the resonant condition hν=ΔE and using an external source in the microwave and THz range, theory predicts an induced spin lasing effect in N/f. Presently, we investigate the influence of the external irradiation on the electronic resistance via transport spectroscopy. In particular, we will present our measurements on the magnetotransport properties, studying the complex interplay between the crucial parameters, namely magnetization, current density and geometry of the point contacts. The results illustrate that a successful spin-population inversion can be detected.

TT 51.8 Fri 11:30 BH 243

Gate dependent TMR-effect in a SWCNT-based spin valve device with exchange biased ferromagnetic contacts — Andreas Prüfling, •Daniel Steininger, Maurice Ziola, Matthias Sperl, Andreas K. Hüttel, and Christoph Strunk — Universität Regensburg, Germany

We report on magneto-transport measurements on a single wall carbon nanotube based spin valve device with Permalloy ($Ni_{81}Fe_{19}$) and $Ni_{81}Fe_{19}/Fe_{50}Mn_{50}$ bilayer contacts. Sputtered thin films and EBL-patterned strip-arrays of these materials were characterized by means of vibrating sample- and SQUID magnetometry and optimized by varying both layer thickness ratios, and material grain size via the sputtering power. Utilizing the magnetic exchange bias effect in these ferromagnet/anti-ferromagnet bilayer systems, the difference in cooercive fields of our contacts is sufficently large to achieve controllable independent switching of two contacts by an external magnetic field. Magneto-transport measurements performed in the Coulomb blockade- and Kondo regime of a SWCNT quantum dot device show systematic gate dependence of the tunneling magnetoresistance (TMR) when the gate voltage is scanned through several Coulomb diamonds.

TT 51.9 Fri 11:45 BH 243

Rotating skyrmion lattices by spin torques and field gradients — •Karin Everschor[1], Markus Garst[1], Benedikt Binz[1], Christian Pfleiderer[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Physics-Department E21, Technical University Munich, Germany

Chiral magnets like MnSi form lattices of skyrmions, i.e. magnetic whirls, which react sensitively to small electric currents. The interplay of these currents and thermal gradients can induce either a rotation of the magnetic pattern by a finite angle or – for higher current densities or larger gradients – a steady rotation defined by a constant angular velocity. We develop a theory of rotational forces induced by gradients in magnetic field or temperature. Reactive forces (Magnus and Lorentz forces) arise from Berry phases while several mechanisms affect the dynamics of magnets by damping. We use the Landau Lifshitz Gilbert equation extended by extra damping terms in combination with a phenomenological treatment of pinning forces to develop a theory of the relevant rotational torques.

TT 52: Transport: Graphene 2 (jointly with MA, HL, DY, DS, O)

Time: Friday 9:30–12:45 Location: BH 334

TT 52.1 Fri 9:30 BH 334

Transport study of graphene with artificially induced defects — •Verena Martin, Johannes Jobst, Michael Krieger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We report on transport properties of ion irradiated graphene which is grown epitaxially on 6H semi-insulating silicon carbide (SiC) substrate. We investigate both monolayer graphene [1] and quasi-free standing epitaxial graphene [2]. Subsequent irradiation steps of argon and carbon ions with different ion energies into the graphene/SiC stack are performed at low temperature (4K) and room temperature. The resistivity of the graphene layer is monitored in situ. After each irradiation step temperature dependent measurements and magnetoresistance measurements are performed to study the effect of the damage. An increase of resistivity with decreasing temperature as well as a broadening of the weak localization peak could be correlated to an increase of the defect amount.

[1] K. Emtsev et al., Nat. Mater. **8**, 203 (2009)
[2] C. Riedl et al., Phys. Rev. Lett. **103**, 246804 (2009)

TT 52.2 Fri 9:45 BH 334

Inelastic Raman scattering on electronic excitations in graphene and carbon nanotubes — •Oleksiy Kashuba[1] and Vladimir Fal'ko[2] — [1]Institut für Theorie der statistischen Physik, RWTH Aachen, 52056 Aachen, Deutschland — [2]Department of

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Raman measurements in carbon allotropes are generally associated with the exploration of the vibrational modes. We present a theory of the non-resonant inelastic light scattering accompanied by the excitations of electron-hole pairs and predict the selection rules and polarization properties of the dominant Raman active modes. The prediction of the Raman plot profile for graphene at high magnetic field with pronounced peaks corresponding to the inter-Landau-level transitions [1,2] was confirmed by subsequent experiment [3]. We also provide a theory of Raman scattering on intersubband electron-hole pairs in large diameter carbon nanotubes predicting dominant polarisations and Raman spectra featuring a pattern of van Hove singularities [4].

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[3] C. Faugeras et. al., Phys. Rev. Lett. 107, 036807 (2011).
[4] O. Kashuba and V. I. Fal'ko, submitted to PRL (2011), arXiv:1111.1413

TT 52.3 Fri 10:00 BH 334

Transport in clean side-gated graphene nanoribbons — •Bernat Terrés[1,2], Jan Dauber[1,2], Uwe Wichmann[1], Stefan Trellenkamp[2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene is a two dimensional form of crystalline carbon with unique electrical properties. However, due to its gap-less nature it is hardly possible to implement concepts of state-of-the-art electronic devices. Recently, it has been shown that by tailoring graphene into narrow ribbons an effective band gap can be induced. Extensive studies have been reported on the transport mechanism in graphene nanoribbons and although being successfully demonstrated as tunneling barriers in quantum dots, graphene nanoribbons show a Coulomb blockade dominated transport behavior. In this work we report on the effects of a symmetrically applied side gate voltage on clean (hydrofluoric acid treated) graphene nanoribbons. In particular we show low-temperature experiments where the overall conductance can be tuned up to a level of about $8e^2/h$. Measurements show evidence that the local resonances in the transport gap can be strongly suppressed by adjusting the side-gate voltages. In summary, the high conductance values together with the observation of onsets of quantized conductance plateaus at integer multiples of $2e^2/h$ indicates that the disorder potential can be dramatically reduced, even though the transport mechanism is still mainly dominated by substrate and rough-edge induced disorder.

TT 52.4 Fri 10:15 BH 334

Coulomb drag in graphene: perturbation theory — •Boris Narozhny[1], Michael Titov[2,3], Igor Gornyi[3,4], and Pavel Ostrovsky[3,5] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK — [3]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [4]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [5]L.D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia

We study the effect of Coulomb drag between two closely positioned graphene monolayers. In the limit of weak electron-electron interaction and small inter-layer spacing d ($\mu_{1(2)}, T \ll v/d$) the drag is described by a universal function of the chemical potentials of the layers $\mu_{1(2)}$ measured in the units of temperature T. When both layers are tuned close to the Dirac point, then the drag coefficient is proportional to the product of the chemical potentials $\rho_D \propto \mu_1\mu_2$ (when any of the layers is precisely at the Dirac point, then the drag vanishes due to electron-hole symmetry). In the opposite limit of low temperature the drag is inversely proportional to both chemical potentials $\rho_D \propto T^2/(\mu_1\mu_2)$. In the mixed case where the chemical potentials of the two layers belong to the opposite limits $\mu_1 \ll T \ll \mu_2$ we find $\rho_D \propto \mu_1/\mu_2$. In the case of strongly doped graphene $\mu_{1(2)} \gg v/d \gg T$ the drag coefficient acquires additional dependence on d and we recover the usual Fermi-liquid result if the screening length is smaller than d.

TT 52.5 Fri 10:30 BH 334

Dirac boundary condition at the reconstructed zigzag edge of graphene — Jan van Ostaa, Anton Akhmerov, Carlo Beenakker, and •Michael Wimmer — Instituut-Lorentz, Universiteit Leiden, The Netherlands

Edge reconstruction modifies the electronic properties of finite graphene samples. We formulate a low-energy theory of the reconstructed zigzag edge by deriving the modified boundary condition to the Dirac equation. If the unit cell size of the reconstructed edge is not a multiple of three with respect to the zigzag unit cell, valleys remain uncoupled and the edge reconstruction is accounted for by a single angular parameter ϑ. Dispersive edge states exist generically, unless $|\vartheta| = \pi/2$. We compute ϑ from a microscopic model for the "reczag" reconstruction (conversion of two hexagons into a pentagon-heptagon pair) and show that it can be measured via the local density of states. In a magnetic field there appear three distinct edge modes in the lowest Landau level, two of which are counterpropagating.

TT 52.6 Fri 10:45 BH 334

Dielectric properties of graphene in the presence of spin-orbit interactions — •Andreas Scholz[1], John Schliemann[1], and Tobias Stauber[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Departamento de Fisica de la Materia Condensada and Instituto Nicolas Cabrera, Universidad Autonoma de Madrid. E-28049 Madrid. Spain

We study the dielectric function of graphene in the presence of pseudo-Rashba and intrinsic spin-orbit interactions (SOI) for arbitrary frequency, wave vector, doping, and spin-orbit coupling (SOC) parameters. In the static limit, the asymptotic behavior of the screened potential due to charged and magnetic impurities is derived. Due to the existence of a sharp Fermi surface in doped graphene, the screened potential exhibits characteristic (Friedel) oscillations. These oscillations are absent in the undoped case. An analytical expression for the plasmon dispersion is derived from the long-wavelength limit of the dielectric function and afterwards compared to the numerical result. For finite SOC parameters we find the existence of several new plasmon modes. Several limiting cases, namely the case of pure Rashba or pure intrinsic SOC, the case of equally large Rasbha and intrinsic coupling and of zero SOC are opposed.

15 min. break.

TT 52.7 Fri 11:15 BH 334

Monolithic Epitaxial Graphene Electronics — •Stefan Hertel[1], Daniel Waldmann[1], Johannes Jobst[1], Sergey Reshanov[2], Adolf Schöner[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]Chair of Applied Physics, Erlangen, Germany — [2]ACREO AB, Kista, Sweden

We developed a scheme to fabricate transistors with high switching performance by employing the whole system epitaxial graphene consisting of the graphene itself, but also include the semiconducting silicon carbide substrate and their common interface.

We used n-type SiC as conducting channel and tailored two different interfaces to the graphene: (a) monolayer epitaxial graphene [1] to provide ohmic contacts and (b) quasi-freestanding bilayer graphene [2](as achieved by hydrogen intercalation of MLG) to get Schottky-like contacts. We developed a method to produce both species side-by-side on the same chip. The resulting transistor works similar to a MeSFET with graphene as source and drain material but also as gate metal. In principal one single lithography step is sufficient to fabricate a transistor.

We demonstrate an epitaxial graphene transistor with on/off ratios exceeding 4 orders of magnitude at room temperature which can operate in both normally-on and normally-off operation mode, adjustable using a parametric backgate voltage. No damping was observed up to MHz frequencies.

[1] Emtsev et al., Nature Material **8**, 203-207 (2009).
[2] Speck et al., Applied Physics Letters **99**, 122106 (2011).

TT 52.8 Fri 11:30 BH 334

Field Effect Superconductivity in Multigraphene — •Ana Ballestar[1], Srujana Dusari[1], Jose Barzola-Quiquia[1], Pablo Esquinazi[1], Robson da Silva[2], and Yakov Kopelevich[2] — [1]Division of Superconductivity and Magnetism, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany — [2]Instituto de Fisica, Unicamp, 13083-970 Campinas, Sao Paulo, Brasil

We have studied the temperature and magnetic field dependence of the electrical resistivity of mesoscopic tens of nanometers thick multigraphene samples as a function of bias voltage applied perpendicular

to the graphene planes. We found that the resistivity changes asymmetrically with the bias voltage. For large and negative bias voltages the resistivity shows non-percolative superconducting-like transitions at $T \sim 15 \ldots 20$ K . The transition can be suppressed at high enough magnetic fields applied normal or parallel to the main plain of the samples. We discuss the obtained results in terms of electric field induced superconductivity at localized near surface regions of the graphite sample.

TT 52.9 Fri 11:45 BH 334

Graph theory meets ab-initio molecular dynamics: atomic structures and transformations at the nanoscale — •Fabio Pietrucci[1] and Wanda Andreoni[1,2] — [1]CECAM - EPFL Lausanne, Switzerland — [2]Institute of Theoretical Physics - EPFL Lausanne, Switzerland

We introduce a set of Social PeRmutation INvarianT (SPRINT) coordinates which describe the topology of the network of bonds among atoms [1]. These coordinates are obtained from the contact matrix, they are invariant under permutation of identical atoms, and provide a clear signature of the transition between ordered and disordered structures. In combination with first-principles molecular dynamics and metadynamics, the topological coordinates are employed to explore low-energy structures of silicon clusters and organic molecules, demonstrating the possibility of automatically simulating isomerization, association, and decomposition reactions without prior knowledge of the products or mechanisms involved.

Finally we discuss the application of this new approach to the simulation of carbon nanostructures: we obtain transformation pathways for the reconstruction of zig-zag edges of graphene ribbons to 5-7 rings, as well as the folding of graphene into fullerene-like cages. Our results show that it is now feasible the blind exploration of complex structural rearrangements of nanostructures at finite temperature and at density-functional theory level of accuracy.

[1] F. Pietrucci and W. Andreoni, Phys. Rev. Lett. 107 (2011) 085504.

TT 52.10 Fri 12:00 BH 334

Localization behavior of Dirac particles in disordered graphene superlattices — Qifang Zhao[1], Jiangbin Gong[1], and •Cord Müller[2] — [1]Department of Physics and Centre for Computational Science and Engineering, National University of Singapore — [2]Centre for Quantum Technologies, National University of Singapore

Graphene superlattices (GSLs) can be used to engineer band structures and, from there, charge transport properties, but these are sensitive to the presence of disorder. We study the localization behavior of massless 2D Dirac particles induced by weak disorder for both scalar-potential and vector-potential GSLs. By an analytical weak-disorder expansion, we investigate how the localization length depends on the incidence angle to a 1D GSL. Delocalization resonances are found for both scalar and vector GSLs. The sharp angular dependence of the Lyapunov exponent may be exploited to realize disorder-induced filtering devices [1].

[1] Q. Zhao, J. Gong, and C. A. Müller, `arXiv:1111.3436`

TT 52.11 Fri 12:15 BH 334

Thermal Transport in Graphene: a Large-scale Molecular Dynamics Study — •Luiz Felipe C Pereira and Davide Donadio — Max Planck Insitute for Polymer Research, Mainz, Germany.

Carbon-based materials show exceptional thermal properties. The thermal conductivity of carbon allotropes can range five orders of magnitude. In the bulk, amorphous carbon is a very poor heat conductor, with $\kappa \approx 0.01$ W/m/K, whereas diamond has the highest thermal conductivity among elemental solids, $\kappa \approx 2000$ W/m/K at room temperature. Carbon nanostructures extend the range even further. Thermal conductivities as large as 5000 W/m/K have been measured for suspended graphene and carbon nanotubes. Nonetheless, there is still much controversy over the thermal transport properties of graphene, both experimentally and theoretically. We have performed extensive equilibrium and non-equilibrium molecular dynamics simulations aimed at understanding the mechanism of heat transport in graphene. In order to address the influence of system size on the simulation results, an aspect frequently overlooked in similar computational studies, we perform large scale molecular dynamics simulations of micrometer-size models containing more than 10^6 atoms. Furthermore, we investigate the influence of uniaxial strain on the thermal conductivity of graphene, and show that the resulting strain-induced anysotropy has a profound influence on its thermal conductivity.

TT 52.12 Fri 12:30 BH 334

Effect of short-range interactions on the phase diagram of graphene — •David Mesterhazy[1], Jürgen Berges[1], and Lorenz von Smekal[2] — [1]Institut für Theoretische Physik, Universität Heidelberg — [2]Institut für Kernphysik, Technische Universität Darmstadt

We study low-energy theories of suspended monolayer graphene at the charge neutral point by means of functional renormalization group methods. In particular, the role of residual short-range interactions for the expected chiral phase transition is investigated. The resulting effective low-energy description can provide a firm basis for a study of the universal properties of the quantum phase transition. Furthermore, first results for the phase diagram at finite temperature are presented.