Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(lecture rooms H18, H19, H20, and H21; poster A and D1)

Symposia co-organized by TT:

SYEL Energy Landscapes: Statistical Physics of (Spin-)Glasses, Biomolecules, Clusters and Optimization Problems

Organisation: Michael Kastner (Stellenbosch), Andreas Heuer(Universität Münster), Martin Weigel (Universität Mainz), Alexander Hartmann (Universität Oldenburg).
Joint symposium of the divisions DY, CPP, DF, TT — see SYEL for the full program of the Symposium

SYEL 1.1	Mon	10:00–10:30	H1	**Energy Landscapes of clusters, glasses, and biomolecules** — •David Wales
SYEL 1.2	Mon	10:30–11:00	H1	**Order parameters and energy landscapes for protein folding and misfolding** — •Steven Plotkin
SYEL 1.3	Mon	11:00–11:30	H1	**Nuclear Spins Reveal the Microscopic Nature of Tunneling Systems in Glasses** — •Christian Enss
SYEL 1.4	Mon	11:30–12:00	H1	**Energy landscapes and phase transitions** — •Lapo Casetti
SYEL 1.5	Mon	12:00–12:30	H1	**Phase transitions in spin glasses** — •Peter Young
SYEL 1.6	Mon	12:30–13:00	H1	**Statistical physics of inverse problems** — •Riccardo Zecchina

SYGN Spin-Orbit Coupling and Spin Relaxation in Graphene and Carbon Nanotubes

Organization: Milena Grifoni (Universität Regensburg), Markus Morgenstern (RWTH Aachen), Jürgen Smet (MPI-FKF, Stuttgart).
Joint symposium of the divisions TT, MA, HL, DS, MM — see SYNG for the full program of the Symposium

SYGN 1.1	Mon	14:00–14:35	H1	**Models for spin-orbit coupling in graphene** — •Francisco Guinea
SYGN 1.2	Mon	14:35–15:10	H1	**Spin-orbit coupling and spin relaxation in carbon nanotube quantum dots** — •Ferdinand Kuemmeth
SYGN 1.3	Mon	15:10–15:45	H1	**Spin-orbit interaction in carbon nanotubes probed in pulsed magnetic fields** — •Sungho Jhang
SYGN 1.4	Mon	16:00–16:35	H1	**Wigner molecules and spin-orbit coupling in carbon-nanotube quantum dots** — •Massimo Rontani
SYGN 1.5	Mon	16:35–17:10	H1	**Spin relaxation and decoherence in graphene quantum dots** — •Guido Burkard
SYGN 1.6	Mon	17:10–17:45	H1	**Spin transport in graphene field effect transistors** — •Bart van Wees

Focused Sessions:

TT 13 Topological Defects in Electronic Systems (Joint Session with MA)

Organisation: Roderich Moessner (MPI-PKS Dresden)

TT 13.1	Tue	9:30–10:00	H20	**Skyrmions in Chiral Magnets** — •Ulrich K. Rössler
TT 13.2	Tue	10:00–10:30	H20	**Dirac Strings and Magnetic Monopoles in the Spin Ice, $Dy_2Ti_2O_7$** — •David Jonathan Pryce Morris
TT 13.3	Tue	10:30–11:00	H20	**Manifestations of monopole physics in spin ice materials** — •Claudio Castelnovo
TT 13.4	Tue	11:00–11:30	H20	**Skyrmion Lattices in Pure Metals and Strongly Doped Semiconductors** — •Christian Pfleiderer
TT 13.5	Tue	11:45–12:15	H20	**Skyrmion lattice in MnSi** — •Achim Rosch
TT 13.6	Tue	12:15–12:45	H20	**Topological Insulators in Applied Fields: Magnetoelectric Effects and Exciton Condensation** — •Joel Moore
TT 13.7	Tue	12:45–13:15	H20	**Probing non-Abelian statistics with quasiparticle interferometry** — •Kirill Shtengel
TT 13.8	Tue	13:15–13:45	H20	**Spin Hall effects in HgTe Quantum Well Structures** — •Laurens W. Molenkamp

TT 21 Quantum Criticality in Strongly Correlated Metals

Organisation: Frank Steglich (MPI-CPfS, Dresden)

TT 21.1	Wed	9:30–10:10	H20	**Quantum Criticality, Kondo Breakdown, and Fermi Surfaces** — •Qimiao Si
TT 21.2	Wed	10:10–10:50	H20	**Tuning magnetic quantum phase transitions** — •Hilbert v. Löhneysen
TT 21.3	Wed	10:50–11:30	H20	**Orbital-selective Mott transitions: Heavy Fermions and beyond** — •Matthias Vojta
TT 21.4	Wed	11:40–12:20	H20	**Interaction of the magnetic instability and the Fermi surface reconstruction in $YbRh_2Si_2$** — •Sven Friedemann
TT 21.5	Wed	12:20–13:00	H20	**Novel electronic states near discontinous quantum phase transitions** — •Philipp Gegenwart

TT 25 Iron-Based Superconductors

Organisation: Rüdiger Klingeler (IFW Dresden), Carsten Honerkamp (Universität Würzburg)

TT 25.1	Wed	14:00–14:30	H20	**Fermiology of Fe-Pnictide Superconductors Revealed by Quantum Oscillations** — •James Analytis
TT 25.2	Wed	14:30–15:00	H20	**Magnetic degeneracy and hidden metallicity of the spin density wave state in Fe-based superconductors** — •Ilya Eremin
TT 25.3	Wed	15:00–15:30	H20	**Muon spin relaxation and Moessbauer studies of iron pnictide superconductors** — •Hans-Henning Klauss
TT 25.4	Wed	15:45–16:15	H20	**Interplay among lattice, orbital and spin degrees of freedom in iron pnictides** — •Roser Valenti
TT 25.5	Wed	16:15–16:45	H20	**Lattice dynamics and magnetism in layered iron based superconductors** — •Thomas Brückel
TT 25.6	Wed	17:00–17:15	H20	**ARPES studies on FeAs-based superconductors and their parent compounds** — •Jörg Fink
TT 25.7	Wed	17:15–17:30	H20	**Energy and temperature dependence of spin fluctuations in electron-doped iron arsenide superconductors** — •Dmytro Inosov
TT 25.8	Wed	17:30–17:45	H20	**Doping evolution of the electronic density of states and the gap symmetry in Co-doped 122 iron pnictides** — •Frédéric Hardy
TT 25.9	Wed	17:45–18:00	H20	**Mössbauer high pressure and magnetic field studies of the superconductor FeSe** — •Claudia Felser

TT 28 Time-Resolved Spectroscopy in Correlated Electron Systems: Experiment and Theory

Organisation: Marcus Kollar (Universität Augsburg), Dirk Manske (MPI-FKF, Stuttgart), Martin Wolf (FHI Berlin)

TT 28.1	Thu	9:30–10:00	H18	**Angle- and time-resolved photoelectron spectroscopy of charge density wave materials** — •Uwe Bovensiepen
TT 28.2	Thu	10:00–10:30	H18	**Many Body Theory for Time-Resolved Pump/Probe Photoemission and its Solution via Nonequilibrium Dynamical Mean-Field Theory** — •James Freericks
TT 28.3	Thu	10:30–10:45	H18	**Electron-phonon interaction in 122-iron pnictides investigated by femtosecond time-resolved ARPES.** — •Rocío Cortés
TT 28.4	Thu	10:45–11:15	H18	**Time resolved photoemission and THz spectroscopy of high temperature superconductors** — •Luca Perfetti
TT 28.5	Thu	11:30–12:00	H18	**Relaxation of strongly correlated electron systems: Insights from nonequilibrium dynamical mean-field theory** — •Martin Eckstein
TT 28.6	Thu	12:00–12:15	H18	**Quantum interference between photo-excited states in a solid-state Mott insulator** — •Simon Wall
TT 28.7	Thu	12:15–12:45	H18	**Two-Component Dynamics of the Order Parameter of High Temperature $Bi_2Sr_2CaCu_2O_{8+\delta}$ Superconductors Revealed by Time-Resolved Raman Scattering** — •Michael Alexander Rübhausen
TT 28.8	Thu	12:45–13:00	H18	**Ultrafast non-equilibrium dynamics in conventional and unconventional superconductors** — •Andreas Schnyder

Further Invited Talks:

TT 5.1	Mon	14:00–14:30	H18	**Field-Induced Berezinskii-Kosterlitz-Thouless Transition in a 2d Spin-Dimer System** — •Michael Lang
TT 7.8	Mon	16:00–16:30	H20	**Polar Kerr Effect of Unconventional Superconductors** — •Aharon Kapitulnik
TT 15.4	Tue	14:45–15:15	H18	**Superconductivity vs. Superinsulation in TiN Thin Films** — •Christoph Strunk
TT 17.6	Tue	15:30–16:00	H20	**Nature of Pairing in the FeAs Superconductors** — •Siegfried Graser
TT 19.8	Wed	11:15–11:45	H18	**Spectroscopy on Strongly Correlated Electron Materials** — •Liu Hao Tjeng
TT 23.4	Wed	14:45–15:15	H18	**Superconducting Flux Qubits in Circuit QED and Detection of Weak Microwave Signals** — •Achim Marx
TT 24.6	Wed	15:30–16:00	H19	**Fermi Surface Evolution in an Electron-Doped Cuprate Superconductor Revealed by High-Field Magnetotransport** — •Mark Kartsovnik
TT 32.4	Thu	14:45–15:15	H18	**Dispersion of the Excitations of Fractional Quantum Hall States** — •Jurgen Smet
TT 40.1	Fri	10:15–10:45	H20	**Heating, Heat Conduction and Cooling in Molecular Junctions** — •Abraham Nitzan
TT 38.4	Fri	11:00–11:30	H18	**Neutron Scattering Studies of Spin-Ladders** — •Bella Lake

Sessions:

CE: Correlated Electrons FS: Focused Session NE: Nanoelectronics
SC: Superconductivity TR: Transport MLT: Matter at Low Temperature

TT 1.1–1.10	Mon	10:15–13:00	H18	**TR: Graphene 1**
TT 2.1–2.8	Mon	10:15–12:30	H19	**SC: Applications and Measuring Devices**
TT 3.1–3.6	Mon	10:15–11:45	H20	**TR: Fluctuations and Noise**
TT 4.1–4.9	Mon	10:15–12:45	H21	**CE: Quantum Impurities, Kondo Physics**
TT 5.1–5.12	Mon	14:00–17:30	H18	**CE: Low-dimensional Systems - Materials 1**
TT 6.1–6.16	Mon	14:00–18:15	H19	**TR: Nanoelectronics II: Spintronics and Magnetotransport**
TT 7.1–7.14	Mon	14:00–18:00	H20	**SC: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence**
TT 8.1–8.14	Mon	14:00–17:45	H21	**CE: (General) Theory**
TT 9.1–9.60	Mon	14:00–18:00	Poster A	**SC: Poster Session**
TT 10.1–10.7	Mon	14:00–18:00	Poster A	**Measuring Devices, Cryotechnique: Poster Session**
TT 11.1–11.12	Tue	9:30–12:45	H18	**CE: Low-dimensional Systems - Materials 2**
TT 12.1–12.13	Tue	9:30–13:00	H19	**CE: Metal-Insulator Transition 1**
TT 13.1–13.8	Tue	9:30–13:45	H20	**FS: Topological Defects in Electronic Systems**
TT 14.1–14.12	Tue	9:30–12:45	H21	**TR: Graphene 2**
TT 15.1–15.8	Tue	14:00–16:15	H18	**MLT: Quantum Liquids, Bose-Einstein Condensates, Ultracold Atoms, ... 1**
TT 16.1–16.9	Tue	14:00–16:15	H19	**CE: Quantum-Critical Phenomena 1**
TT 17.1–17.7	Tue	14:00–16:15	H20	**SC: Iron-Based Superconductors - Theoretical Approaches**
TT 18.1–18.8	Tue	14:00–16:15	H21	**TR: Quantum Coherence and Quantum Information Systems 1**
TT 19.1–19.12	Wed	9:30–13:00	H18	**CE: Metal-Insulator Transition 2**
TT 20.1–20.13	Wed	9:30–13:00	H19	**SC: Fabrication and Characterization of Iron-Based and Other Superconductors**
TT 21.1–21.5	Wed	9:30–13:00	H20	**FS: Quantum Criticality in Strongly Correlated Metals**
TT 22.1–22.14	Wed	9:30–13:15	H21	**CE: Spin Systems and Itinerant Magnets**
TT 23.1–23.10	Wed	14:00–17:00	H18	**TR: Quantum Coherence and Quantum Information Systems 2**
TT 24.1–24.16	Wed	14:00–18:45	H19	**SC: Properties, Electronic Structure, Mechanisms**
TT 25.1–25.9	Wed	14:00–18:00	H20	**FS: Iron-Based Superconductors**
TT 26.1–26.17	Wed	14:00–18:45	H21	**CE: Heavy Fermions**
TT 27.1–27.84	Wed	14:00–18:00	Poster D1	**CE: Poster Session**
TT 28.1–28.8	Thu	9:30–13:00	H18	**FS: Time-Resolved Spectroscopy in Correlated Electron Systems: Experiment and Theory**
TT 29.1–29.13	Thu	9:30–13:00	H19	**TR: Nanoelectronics I: Quantum Dots, Wires, Point Contacts 1**
TT 30.1–30.13	Thu	9:30–13:00	H20	**CE: Low-dimensional Systems - Models 1**
TT 31.1–31.13	Thu	9:30–13:00	H21	**SC: Tunnelling, Josephson Junctions**
TT 32.1–32.14	Thu	14:00–18:00	H18	**MLT: Quantum Liquids, Bose-Einstein Condensates, Ultracold Atoms, ... 2**
TT 33.1–33.15	Thu	14:00–18:00	H19	**TR: Nanoelectronics I: Quantum Dots, Wires, Point Contacts 2**
TT 34.1–34.13	Thu	14:00–17:30	H20	**SC: Iron-Based Superconductors - 122**
TT 35.1–35.14	Thu	14:00–17:45	H21	**TR: Nanoelectronics III: Molecular Electronics 1**
TT 36.1–36.34	Thu	14:00–18:00	Poster A	**TR: Poster Session**
TT 37.1–37.31	Thu	14:00–18:00	Poster A	**MLT: Poster Session**
TT 38.1–38.8	Fri	10:15–12:45	H18	**CE: Quantum-Critical Phenomena 2**
TT 39.1–39.9	Fri	10:15–12:45	H19	**SC: Iron-Based Superconductors - 1111**
TT 40.1–40.9	Fri	10:15–13:45	H20	**TR: Nanoelectronics III: Molecular Electronics 2**
TT 41.1–41.8	Fri	10:15–12:30	H21	**CE: Low-dimensional Systems - Models 2**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:30-20:00 H19

TT 1: TR: Graphene 1

Time: Monday 10:15–13:00 Location: H18

TT 1.1 Mon 10:15 H18

Orbitally controlled Kondo effect of Co ad-atoms on graphene — •Tim Wehling[1], Alexander Balatsky[2], Mikhail Katsnelson[3], Alexander Lichtenstein[1], and Achim Rosch[4] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Institute for Molecules and Materials, Radboud University of Nijmegen, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [4]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Based on ab-initio calculations we identify possible scenarios for the Kondo effect due to Co ad-atoms on graphene. For a Co atom absorbed on top of a carbon atom, the Kondo effect is quenched by spin-orbit coupling below an energy scale of $\sim$15 K. For Co with spin $S = 1/2$ located in the center of a hexagon, an SU(4) Kondo model describes the entanglement of orbital moment and spin at higher energies, while below $\sim$ 60 meV spin-orbit coupling leads to a more conventional SU(2) Kondo effect. The interplay of the orbital Co physics and the peculiar band-structure of graphene is directly accessible in Fourier transform tunneling spectroscopy or in the gate-voltage dependence of the Kondo temperature displaying a very strong, characteristic particle-hole asymmetry.

TT 1.2 Mon 10:30 H18

Revivals of quantum wave packets in graphene — •Viktor Krückl[1] and Tobias Kramer[1,2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

We investigate the propagation of wave-packets on graphene in a perpendicular magnetic field. The wave-packet evolution in graphene differs drastically from the one in an electron gas and shows a rich revival structure similar to the dynamics of highly excited Rydberg states [1]. We present a detailed analysis of the occurring collapses, revivals and fractional revivals analytically as well as numerically. In order to study the impact of disorder on the effect we apply our novel numerical scheme to solve the wave-packet propagation on the effective single-particle Dirac-Hamiltonian of graphene in the presence of random impurity potentials.

[1] Viktor Krueckl and Tobias Kramer, New J. Phys. **11** 093010 (2009)

TT 1.3 Mon 10:45 H18

Externally induced spin relaxation in graphene — •Jan Bundesmann[1], Michael Wimmer[1,2], and Klaus Richter[1] — [1]Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, 2300 RA Leiden, The Netherlands

In the fast growing research field of spintronics graphene seems to be a promising candidate. From theory weak spin-orbit interaction is expected in pure carbon-based materials. However, experimental results and theoretical predictions differ by several orders of magnitude: spin lifetimes in the experiment are much smaller than, e. g., the ones obtained from recent DFT calculations [1].

In our calculations we will include also externally induced spin-orbit interactions. Sources for this might be impurities in the substrate or adsorbed atoms. For this investigation we set up a tight-binding model for graphene including intrinsic and Rashba-type spin-orbit interactions. By local variation of the Rashba parameter we model systems with the above introduced sources of spin-orbit interaction and study spin-orbit effects on quantum transport.

[1] M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl and J. Fabian; arxiv:0904.3315

TT 1.4 Mon 11:00 H18

Coulomb interaction in graphene: Relaxation rates and transport — •Michael Schütt[1], Pavel Ostrovsky[2], Igor Gornyi[2], and Alexander Mirlin[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

We study electron transport in graphene with Coulomb interaction at finite temperatures by using Keldysh diagrammatics. In the case of clean graphene we obtain the total scattering rate, the transport scattering rate, and the energy relaxation rate at the Dirac point. Since the total scattering rate diverges graphene exhibits a non-Fermi-liquid behavior similar to disordered metals. Unlike metals clean graphene has a finite conductivity due to the Coulomb interaction. For conductivity we obtain the same analytic behavior as was found using the Boltzmann approach [1,2]. We analyze the plasmon spectrum of graphene and formulate quantum kinetic equations to describe transport in the crossover between the Coulomb interaction dominated regime and the disorder dominated regime.

[1] L. Fritz et al., Phys. Rev. B 78:085416 (2008).
[2] A. Kashuba, Phys. Rev. B 78:085415 (2008).

TT 1.5 Mon 11:15 H18

Is it possible to detect edge states in graphene quantum dots? — •Michael Wimmer[1], Anton R. Akhmerov[1], and Francisco Guinea[2] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Instituto de Ciencia de Materiales de Madrid, Spain

We analyze the single particle states at the edges of graphene quantum dots of arbitrary shapes. By combining analytical and numerical arguments, we show that localized edge states, distinct from extended ones, exist in dots of all dimensions. The number of these states is proportional to the circumference of the dot measured in lattice constants. Perturbations breaking electron-hole symmetry shift the edge states away from zero energy but do not change their total amount.

15 min. break

TT 1.6 Mon 11:45 H18

Graphene: Relativistic transport in a nearly perfect quantum liquid — •Lars Fritz[1], Markus Mueller[2], Joerg Schmalian[3], and Subir Sachdev[4] — [1]Universitaet zu Koeln, Institut fuer theoretische Physik, Zuelpicher Strasse 77, 50937 Koeln — [2]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy — [3]Department of Physics and Astronomy Iowa State University Ames, Iowa 50011, USA — [4]Harvard University, 17 Oxford Street, Cambridge, MA 02138, USA

Electrons and holes in clean, charge-neutral graphene behave like a strongly coupled relativistic liquid. The thermo-electric transport properties of the interacting Dirac quasiparticles are rather special, being constrained by an emergent Lorentz covariance at hydrodynamic frequency scales. At small carrier density and high temperatures, graphene exhibits signatures of a quantum critical system with an inelastic scattering rate set only by temperature, a conductivity with a nearly universal value, solely due to electron-hole friction, and a very low viscosity. In this regime one finds pronounced deviations from standard Fermi liquid behavior. These results, obtained by Boltzmann transport theory at weak electron-electron coupling, are fully consistent with the predictions of relativistic hydrodynamics.

TT 1.7 Mon 12:00 H18

Hyperfine interaction and electron-spin decoherence in graphene and carbon nanotube quantum dots — •Jan Fischer[1], Bjoern Trauzettel[2], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We analytically calculate the nuclear-spin interactions of a single electron confined to a carbon nanotube or graphene quantum dot [1]. While the conduction-band states in graphene are p-type, the accordant states in a carbon nanotube are sp-hybridized due to curvature. This leads to an interesting interplay between isotropic and anisotropic hyperfine interactions. By using only analytical methods, we are able to show how the interaction strength depends on important physical parameters, such as curvature and isotope abundances. We show that for the investigated carbon structures, the ^{13}C hyperfine coupling strength is less than 1 μeV, and that the associated electron-spin decoherence time can be expected to be several tens of microseconds or longer, depending on the abundance of spin-carrying ^{13}C nuclei. Furthermore, we find that the hyperfine-induced Knight shift is highly anisotropic, both in graphene and in nanotubes of arbitrary chirality.

[1] J. Fischer, B. Trauzettel, D. Loss, Phys. Rev. B 80, 155401

(2009)

TT 1.8 Mon 12:15 H18

Spin transport in graphene with inhomogeneous spin-orbit coupling — •Dario Bercioux[1] and Alessandro De Martino[2] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

Recent theoretical [1] and experimental [2] works have shown that spin-orbit couplings in graphene can play a relevant role. Motivated by these results, we address the problem of spin transport in graphene through spin-orbit nanostructures, *i.e.* regions of inhomogeneous spin-orbit coupling on the nanometer scale. In analogy with the case of usual two-dimensional electron gases, we discuss the phenomenon of spin-double refraction [3,4] and its consequences on the spin polarization. In particular we study the transmission properties of a single- and a double-interface between a normal region and a region with finite spin-orbit coupling, and analyze the polarization properties of these systems. In addition, for the case of the single interface, we consider the formation of bound states localized at the interface, analogous to the states occuring at the edges of graphene in the weak topological insulator regime discussed by Kane and Mele [5].

[1] D. Huertas-Hernando, *et al.*, Phys. Rev. Lett. **103**, 146801 (2009).
[2] A. Varykhalov, *et al.*, Phys. Rev. Lett. **101**, 157601 (2008).
[3] V. M. Ramaglia, *et al.*, Eur. Phys. J. B **36**, 365 (2003).
[4] V. M. Ramaglia, *et al.*, J. Phys.: Condens. Matter **16**, 9143 (2004).
[5] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).

TT 1.9 Mon 12:30 H18

Edge effects in quantum transport and quasiparticle spectra of graphene nanostructures — •Jürgen Wurm[1,2], Klaus Richter[1], and Inanç Adagideli[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

In this work, we focus on the spectral and transport properties of graphene nanostructures. In recent work, we studied the effects of edges on the transport and spectral properties of graphene quantum dots, as well as on the conductance of graphene nanoribbons numerically [1,2]. Some edges can lead to effective time reversal symmetry breaking, others are effective intervalley scatterers. In this work, we develop a theory that is capable of handling such effects in graphene nanostructures. We do this in two steps. First, we derive an exact expression for the Green function of a graphene flake, where each term in this expansion corresponds to the specific number of times the quasiparticle hits the edge. Second, we use the Green function to calculate: (i) the spectra for closed systems and (ii) the conductance of open systems. In particular, we focus on phase coherent effects, such as the weak localization correction to the average conductance, and the universal conductance fluctuations. Moreover, we show how the size of these effects depends on the edges.

[1] J. Wurm et al., Phys. Rev. Lett. **102**, 056806 (2009)
[2] J. Wurm et al., New J. Phys. **11**, 095022 (2009)

TT 1.10 Mon 12:45 H18

Charge transport in disordered superconductor-graphene junctions — •Georgo Metalidis[1], Dmitry Golubev[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany

We consider the charge transport through superconductor-graphene tunnel junctions, including the effect of disorder. Coherent scattering on elastic impurities in the graphene layer can give rise to multiple reflections at the graphene-superconductor interface, and can thereby increase the probability of Andreev reflection, leading to an enhancement of the subgap conductance above its classical value. Although the phenomenon is known already from heterostructures involving normal metals, we have studied how graphenes peculiar dispersion relation influences the effect.

TT 2: SC: Applications and Measuring Devices

Time: Monday 10:15–12:30 Location: H19

TT 2.1 Mon 10:15 H19

Josephson-Cantilever with integrated THz antenna — •Christian Brendel, Heiko Neeland, Tobias Vosskoetter, Jan M. Scholtyssek, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany

We imaged the three dimensional microwave power distributions at the open end of multimode circular waveguides and in the free space in the THz range. The measurement setup consists of a grating-tuned CO_2 laser (emission 9 - 11 μm) to pump a FIR laser with an output frequency range from 584 GHz up to 4.2 THz. As scanning sensor we employ a Josephson junction from the high-temperature superconductor $YBa_2Cu_3O_7$ on a vibrating cantilever prepared from a $LaAlO_3$-bicrystal. The setup is mounted inside a vacuum chamber on x-, y- and z-tables with submicrometer resolution and is cooled to a temperature of about 50 K by a cryocooler. We realized a quasi-optic THz-lens system and determined the beam parameters at the Josephson-cantilever position. The small change of the differential resistance in the Shapiro step is proportional to the microwave power. To improve the signal to noise ratio in the measured curent voltage curve we developed new Josephson cantilever designs with different THz antenna strutures.

We wish to acknowledge the financial support of C. Brendel by the Braunschweig International Graduate School of Metrology.

TT 2.2 Mon 10:30 H19

Metallic magnetic calorimeters for high-resolution x-ray spectroscopy — •Jan-Patrick Porst, Sebastian Kempf, Andrea Kirsch, Andreas Pabinger, Christian Pies, Philipp Ranitzsch, Sönke Schäfer, Falk von Seggern, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, 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 change of magnetic flux in a dc-SQUID. During the last years we have started to develop MMCs for a wide variety of applications, ranging from beta- and gamma-spectrometry over the spatially resolved detection of accelerated molecule fragments to arrays of high resolution x-ray detectors. For x-ray energies up to 6 keV an energy resolution of 2.7 eV (FWHM) has been demonstrated and we expect that this can be pushed below 1 eV with the next generation of devices. We summarize the physics of MMCs and the presently used readout schemes as well as the typically observed noise contributions and their impact on the energy resolution. We discuss general design considerations, the micro-fabrication and the performance of micro-fabricated devices. In this field large progress has been achieved in the last years and the thermodynamic properties of most materials approach bulk values allowing for optimal and predictable performance.

TT 2.3 Mon 10:45 H19

Moving a vortex by the tip of a magnetic force microscope — •Ernst Helmut Brandt — Max-Planck-Instiut für Metallforschung

In a recent paper [1] a magnetic force microscope (MFM) was employed to image and manipulate individual vortices in a thick single crystal of $YBa_2Cu_3O_7$. When the magnetic tip performed a zig-zag motion, wiggling fast along x and moving slowly along y, a large enhancement of the excursion of the vortex end at the upper surface (in the crystalline a-b plane) was observed along y, the vortex path covered an elliptical area with axes ratio $\max(y)/\max(x) \gg 1$. As a first step towards a more detailed theory, we consider the vortex as an elastic string which is uniformly pinned by point defects and is driven by the magnetic force exerted on the vortex near the surface by the tip of the MFM. The tip is approximated by a magnetic monopole and the anisotropy of $YBa_2Cu_3O_7$ in the a-b plane is accounted for. When the tip moves with wiggles, the vortex is curved and twisted, its motion penetrating to a maximum depth z_0 below which the vortex remains rigidly pinned in its straight initial position. Our theory [2] reproduces

the path of the vortex end observed in the experiments [1].

[1] O. M. Auslaender et al., Nature Physics **5**, 35 (2009).

[2] E. H. Brandt, G. P. Mikitik and E. Zeldov, Phys. Rev. B **80**, 054513, 1-10 (2009).

TT 2.4 Mon 11:00 H19

Barriers for vortex avalanche propagation in MgB_2 thin films — •Sebastian Treiber[1] and Joachim Albrecht[2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Hochschule Aalen, German

At temperatures below 10K the critical state in MgB_2 thin films gets unstable. This leads to chaotic motion of magnetic vortices and dendritic flux density patterns. Since the critical current is zero inside the dendrites this effect leads to a strong suppression of possible transport currents.

We prepared MgB_2 films containing areas of different current densities and thermal conductivities, respectively. Magneto-optical investigations revealed that the propagation of vortex avalanches can be manipulated by this local variations. It is found that boundaries to areas of higher current density or enhanced thermal conductivity can act like a barrier for the dendrites. The investigations also show that the critical current density around the dendrites is not constant which can not be described by classical critical state models.

TT 2.5 Mon 11:15 H19

Energy relaxation processes in YBCO thin films studied by frequency and time-domain techniques — •Petra Probst[1], Dagmar Rall[1,2], Matthias Hofherr[1], Stefan Wünsch[1], Konstantin Ilin[1], and Michael Siegel[1] — [1]Institut für Mikro- and Nanoelektronische Systeme, Karlsruher Institute of Technology, Hertzstrasse 16, 76187 Karlsruhe, Germany — [2]Lichttechnisches Institut, Karlsruher Institute of Technology, Engesserstrasse 13, 76131 Karlsruhe, Germany

The development of ultra-fast detectors with time resolutions in the picosecond range requires the analysis and understanding of the dynamics in the energy relaxation processes in thin films. A systematic study of the energy relaxation processes in YBCO thin films on sapphire substrate has been performed. Pulsed-laser deposited YBCO samples between 20 and 60 nm film thickness were fabricated and characterized by means of frequency and time domain techniques by excitation of the samples with optical radiation. The characteristic energy relaxation time was extracted from the thin film sample response according to the two-temperature model. The extracted time constants of the two techniques showed good agreement. We have observed an increase of the energy relaxation time from 500 ps to 4 ns with increase of the film thickness from 20 to 60 nm, respectively. The obtained dependence of the characteristic time on film thickness we attribute to the escape of non-equilibrium phonons from the YBCO films into substrate. Details of the experimental methods and results on the energy relaxation in thin YBCO films and the applied theoretical model will be discussed.

15 min. break

TT 2.6 Mon 11:45 H19

AC loss data for YBCO double-pancake coils — Christian Stiehler[1], •Vadim Grinenko[1], Konstantin Nenkov[1], Michal Vojenciak[2], Günter Fuchs[1], Bernhard Holzapfel[1], and Ludwig Schultz[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01067 Dresden, Germany — [2]Institute of Electrical Engineering, Slovak Academy of Sciences, Dubravsk'a cesta 9, 841 04 Bratislava, Slovak Republic

Since the second generation of superconducting tapes, YBCO coated conductors, are commercially available, large scale AC applications seem to be very promising provided that AC loss of the 2G tapes can be reduced. In this work, critical current measurements as well as AC loss experiments of YBCO double-pancake coils and 2G tapes were performed. An analysis of the magnetic field distribution at the coil's exterior, especially in critical points, shows no self-field limitation of the critical current density. Magnetisation loss data were obtained for YBCO double-pancake coils by applying magnetic AC fields at 77 K. It is demonstrated that the AC loss can be reduced by means of magnetic shielding. Furthermore, AC transport losses have been measured at temperatures between 65 and 77 K for frequencies between 36 and 288 Hz. The AC loss data were found to be dominated by hysteresis losses. The obtained results are compared with AC loss data reported for YBCO pancake coils.

TT 2.7 Mon 12:00 H19

Development of a micro-Hall magnetometer for the study of light-induced effects in magnetic molecules — •Robert Lusche, Jan Dreiser, and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany

Controlling magnetic properties in magnetic molecules with light is an intriguing effect and has recently attracted renewed interest [1]. In order to measure the magnetization in the presence of light we rely on micro-Hall-senors in our setup. Micro-Hall probes have been proven to be a simple and robust tool for magnetic measurements over a large range of experimental conditions. Here we present the design of our home-built micro-Hall magnetometer including an irradiation unit. It can be operated at temperatures down to 1.4 K and with magnetic fields of up to 5.5 T, and provides a resolution better than 10^{-7} emu. We demonstrate and characterize the performance by measurements on known spin-crossover complexes, and present first measurements on novel photomagnetic complexes.

[1] A. Bleuzen *et al.*, Inorg. Chem. **48**, 3453 (2009).

TT 2.8 Mon 12:15 H19

Coherent broadband continuous-wave THz spectrometry: A powerful tool for low-energy solid-state spectroscopy at low temperature and high magnetic field — •Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Axel Roggenbuck[2], Andreas Janssen[1], Anselm Deninger[2], Iván Cámara Mayorga[3], Joachim Hemberger[1], Rolf Güsten[3], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln, Germany — [2]TOPTICA Photonics AG, Lochhamer Schlag 19, D-82166 Gräfelfing, Germany — [3]Max-Planck Institute for Radio Astronomy, Auf dem Hügel 69, D-53121 Bonn, Germany

We present the development of a continuous-wave THz spectrometer and its application at low temperatures and high magnetic fields. The spectrometer employs photomixing of two NIR-DFB diode lasers for generation and phase sensitive detection of THz radiation of frequency from 60 GHz to 1.8 THz. A phase modulation technique and photocurrent correction are used to accurately determine amplitude and phase at a given frequency, and to correct for instabilities, respectively. The complex optical functions can be evaluated from the full THz phase information, and a very high spectral resolution in the MHz range can be achieved. Furthermore, this compact spectrometer can be integrated within a magnetic cryostat eliminating the need for optical windows. In this way, the investigations at high magnetic fields up to 16 T and low temperatures up to 2 K can be achieved without loss of intensity. Thus, a new door is opened for exploring low-energy electronic excitations of novel materials, lying in the sub-phonon energy regime.

TT 3: TR: Fluctuations and Noise

Time: Monday 10:15–11:45 Location: H20

TT 3.1 Mon 10:15 H20

Interactions, Coherence, and Multistability in Transport Statistics of coupled Quantum Dots — Gernot Schaller, •Gerold Kiesslich, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

We present a novel generalized coarse-graining n-resolved master equation technique [1]. By introducing a virtual detector counting the number of transferred electrons in single-electron transport the coherences and the Lamb shift can be conveniently included. For illustration, we consider transport through interacting levels that are either serially or parallely coupled to two leads. We show for the parallel setup that the coherences can lead to strong current suppression, giant Fano factors and bistable transport statistics. In the serial case a finite coarse graining time can resolve the shortcomings of the Born-Markov-secular

approximation such as unphysical currents.

[1] G. Schaller, G. Kießlich, and T. Brandes, in press, Phys. Rev. B, arXiv:0908.3620

TT 3.2 Mon 10:30 H20

Spin-induced charge correlations in transport through interacting quantum dots with ferromagnetic leads — •Stephan Lindebaum, Daniel Urban und Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

We study the full counting statistics of electronic transport through a single-level quantum dot weakly coupled to two leads, with either one or both of them being ferromagnetic[1]. Starting from a generalized master equation we use a diagrammatic real-time theory to calculate the cumulant generating function to first order in the tunnel-coupling strength. In both considered systems, we find that the interplay of Coulomb interaction and finite spin polarization implies spin-correlation induced charge correlations that give rise to super-Poissonian transport behavior. In the case of two ferromagnetic leads, we analyze the non-trivial dependence of the cumulants on the angle between the non-collinear polarization directions of the leads. We find even diverging second and higher cumulants for spin polarizations approaching unity. But already the system with one ferromagnetic and one normal lead displays super-Poissonian behavior and, in addition, positive cross correlations between the current fluctuations of the two spin species, if the electrons are injected from the normal electrode.

[1] S. Lindebaum, D. Urban, and J. König, Phys. Rev. B **79**, 245303 (2009).

TT 3.3 Mon 10:45 H20

Calculating Shot Noise based on Numerical Time Evolution of Transport States — •Alexander Branschädel[1] and Peter Schmitteckert[2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

A method to calculate shot noise in one-dimensional systems based on the time evolution of transport states using numerical simulation techniques is presented. We consider the single resonant level model, consisting of a single impurity attached to non-interacting leads, with spinless fermions, where we include nearest neighbour interaction between the impurity site and the leads. The time evolution is obtained either using exact diagonalisation for the non-interacting case or by means of time-dependent Density Matrix Renormalisation Group (td-DMRG) algorithms. We present results for the shot noise for finite bias voltage in the low frequency limit as well as the full frequency dependency and compare with analytical calculations.

TT 3.4 Mon 11:00 H20

Quasiprobability and weak measurement of current noise in a quantum point contact — •Adam Bednorz[1,2] and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Deutschland — [2]Institute of Theoretical Physics, University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

The charge flow (counting statistics) through mesoscopic junctions is well described by Bernoulli statistics in the long time (low frequency) limit [1] which follows from a projective detection model. The problem becomes more complicated and interesting, when considering the measurement of noncommuting observables, e.g. current and phase or time-resolved current [2]. The latter case can be resolved in terms of the weak measurement [3]. The idea is similar to the concept of weak values [4]. We show that the outcome of the weak measurement can be interpreted in terms of a quasiprobability. Namely, the total probability distribution of the measured values of observables is a convolution of a large, white, Gaussian detection noise and a quasiprobability (independent of the detector). We show that the quasiprobability can take negative values. The negative quasiprobability can be measured, if the Gaussian noise is subtracted, by a measurement of the fourth cumulant at high frequencies.

[1] G.B. Lesovik and L.S. Levitov, Phys. Rev. Lett. 72, 538 (1994).
[2] W. Belzig and Y.V. Nazarov, Phys. Rev. Lett. 87, 197006 (2001).
[3] A. Bednorz and W. Belzig, Phys. Rev. Lett. 101, 206803 (2008).
[4] Y. Aharonov, D.Z. Albert and L. Vaidman, Phys. Rev. Lett. 60, 1351 (1988).

TT 3.5 Mon 11:15 H20

Noise conductance of carbon nanotube transistors — Julien Chaste[1], Emiliano Pallecchi[1], Pascal Morfin[1], Gwendal Fève[1], Takis Kontos[1], Jean-Marc Berroir[1], Pertti Hakonen[2], and •Bernard Plaçais[1] — [1]Ecole Normale Superieure, Laboratoire Pierre Aigrain, 24 rue Lhomond 75005 Paris, France — [2]Helsinki University of Technology, Low Temperature laboratory, Espoo, Finland

The presentation deals with radio-frequency noise and transmission measurements of high-gain single wall carbon nanotube transistors at cryogenic temperatures [1]. The gate capacitance, drain conductance, transconductance and current-noise are analyzed by relying on a ballistic 1-dimensional scattering model whose parameter is the channel quantum capacitance that controls gate coupling. At 4 Kelvin, current and noise are thermally activated. The bias-dependent electronic temperature can be measured from the gate voltage dependence of transconductance. A "noise conductance" can be then deduced which is found to obey a simple law as function of drain conductance and transconductance as predicted by the 1D model. Finally we estimate the charge resolution of nanotube devices for applications as fast single-shot electron detectors.

[1] J. Chaste, E. Pallecchi, P. Morfin, G. Fève, T. Kontos, J.-M. Berroir, P. Hakonen, B. Plaçais, submitted (2009).

TT 3.6 Mon 11:30 H20

Inelastic noise spectroscopy in molecular junctions with multiple electronic states — •Federica Haupt[1], Tomas Novotny[2], and Wolfgang Belzig[1] — [1]Department of Physics, Konstanz University, Konstanz, Germany — [2]Department of Condensed Matter Physics, Charles University, Prague, Czech Republic

Inelastic transport spectroscopy and shot noise measurements are essential investigation tools in the field of molecular electronics. In fact, while the first allows to extract information on the presence and the orientation of a molecule in a junction, the latter can be used to analyze its individual conductance channels. So far noise measurements have been limited to the elastic transport regime, but more information is expected to be provided by inelastic noise spectroscopy.

In this work we investigate the effects due to inelastic phonon scattering on the current noise in molecular junctions with multiple electronic states. This case is particularly interesting because electron-phonon interaction may results in an effective coupling of different electronic states. Using the extended Keldysh-Green's function formalism we derive a general expression for the zero frequency noise in the case of weak electron-phonon coupling. We compare this result to the case in which transport is dominated by a single electronic state. Finally, we apply our theory to an experimentally relevant set-up.

TT 4: CE: Quantum Impurities, Kondo Physics

Time: Monday 10:15–12:45 Location: H21

TT 4.1 Mon 10:15 H21

Kondo physics in chaotic and regular mesoscopic systems — •Rainer Bedrich[1], Sebastien Burdin[2], and Martina Hentschel[1] — [1]Max Planck Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Condensed Matter Theory Group, CPMOH, UMR 5798, Université de Bordeaux I, 33405 Talence, France

We study the mesoscopic Kondo box, consisting of a quantum spin 1/2 interacting with an electronic bath as can be realized by a magnetic impurity coupled to electrons on a quantum dot using a mean-field approach for the Kondo interaction. Its numerical efficiency allows us to analyze the Kondo temperature, the local magnetic susceptibility, and the conductance statistics for a large number of samples as a function of the temperature, the Kondo coupling, and the number of electrons on the dot. Here, in contrast to the Kondo effect occurring in a bulk material, the metallic host is characterized by a finite mean level spacing, generating deviations from the universal behavior. We contrast the behavior of chaotic systems, described within the random matrix theory, to that of regular systems, e.g. rectangular quantum

dots. Besides the system geometry we find that the boundary of the dot affects the physical properties in a significant way.

TT 4.2 Mon 10:30 H21

Lattice density-functional theory of the single-impurity Anderson model — •Waldemar Töws and Gustavo Pastor — Institut für Theoretische Physik, Universität Kassel, Germany

A lattice density-functional theory of the single-impurity Anderson model is presented. In this approach the basic variable is the single-particle density matrix $\gamma_{ij\sigma}$ with respect to the lattice sites. The central interaction-energy functional $W[\gamma]$ is shown to be invariant under unitary transformations of orbitals in the conduction band. This property is exploited to find a unitary transformation such that the localized impurity orbital experiences charge fluctuations only to a particular single-particle state of the conduction band. A simple analytical approximation to $W[\gamma]$ is then derived from the solution of the resulting two-level problem. This so-called two-level approximation can be shown to be exact in the limit of a totally degenerated conduction band as well as in the limit of widely separated discrete conduction-band levels. The minimization of the total energy functional $E[\gamma]$ with respect to $\gamma_{ij\sigma}$ yields the ground-state properties such as the kinetic, interaction and total energy, as well as the occupation and spin polarization of the impurity orbital. The results obtained with the two-level-approximation for finite rings having $N \leq 12$ sites are in agreement with exact Lanczos diagonalizations in all interaction regimes, from weak to strong correlations. In particular the singlet-triplet gap, which determines the Kondo temperature, is correctly described. This constitutes a remarkable qualitative improvement over mean-field approximations. Advantages and limitations of this approach are discussed.

TT 4.3 Mon 10:45 H21

A weak coupling CTQMC study of the single impurity and periodic Anderson models with s-wave superconducting baths — •David J. Luitz and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

We apply the unbiased weak-coupling continuous time quantum Monte Carlo (CTQMC) method to review the physics of a single magnetic impurity coupled to s-wave superconducting leads described by the BCS reduced Hamiltonian. As a function of the superconducting gap Δ, we study the first order transition between the singlet and doublet (local moment) states by examining the crossing of the Andreev bound states in the single particle spectral function. Within DMFT, this impurity problem provides a link to the periodic Anderson model with superconducting conduction electrons (BCS-PAM). The first order transition observed in the impurity model is reproduced in the BCS-PAM and is signalized by the crossing of the low energy excitations in the local density of states. The momentum resolved single particle spectral function in the singlet state reveals the coherent, Bloch-like, superposition of Andreev bound states. In the doublet or local moment phase the single particle spectral function is characterized by incoherent quasiparticle excitations.

TT 4.4 Mon 11:00 H21

Spectral function of the Anderson impurity model at finite temperatures — •Aldo Isidori[1], Hermann Freire[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany — [2]Instituto de Física, Universidade Federal de Goiás, 74.001-970, Goiânia-GO, Brasil

Using the functional renormalization group (FRG) and the numerical renormalization group (NRG), we calculate the spectral function of the Anderson impurity model at zero and finite temperatures. In our FRG scheme spin fluctuations are treated non-perturbatively via a suitable Hubbard-Stratonovich field, but vertex corrections are neglected. Although at zero temperature this FRG scheme does not quantitatively reproduce the known exponential narrowing of the Kondo resonance for large values of the interaction, a comparison with the numerically exact NRG results shows that the FRG gives a reasonable description of the spectral line-shape both at high energies and for temperatures larger than the Kondo scale.

15 min. break

TT 4.5 Mon 11:30 H21

The Kondo exciton: a quantum quench towards strong spin-reservoir correlations — Hakan E. Türeci[1], •Markus Hanl[2], Martin Claassen[1], Andreas Weichselbaum[2], Theresa Hecht[2], Bernd Braunecker[3], Alexander Govorov[4], Leonid Glazman[5], Jan von Delft[2], and Atac Imamoglu[1] — [1]ETH-Zürich — [2]Ludwig-Maximilians-Universität München — [3]University of Basel — [4]Ohio University — [5]Yale University

We consider a semiconductor quantum dot coupled to a Fermionic reservoir, and study the dynamics after a quantum quench induced by the sudden creation of an exciton via optical absorption of an incident photon of definite frequency [1]. The subsequent emergence of correlations between the spin degrees of freedom of the dot and reservoir, ultimately leading to the Kondo effect, can be probed via a simple optical absorption experiment. The resulting lineshape is found to unveil three very different dynamical regimes, corresponding to short, intermediate and long times after the initial excitation, which are in turn described by the three fixed points of the single-impurity Anderson Hamiltonian. At low temperatures and just beyond the absorption threshold, the lineshape is dominated by a power-law singularity, with an exponent that is a universal function of magnetic field and gate voltage. Analytical results obtained by fixed-point perturbation theory are in excellent agreement with numerical renormalization group results.

[1] arXiv:0907.3854v1 [cond-mat.str-el]

TT 4.6 Mon 11:45 H21

Non-equilibrium Scaling Properties of a Double Quantum Dot System: Comparison between Perturbative Renormalization Group and Flow Equation Approach — •Verena Koerting[1], Peter Fritsch[2], and Stefan Kehrein[2] — [1]Niels Bohr Institute, Universitetsparken 5, DK-2100 København Ø, Denmark — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

Since the discovery of Kondo physics in quantum dots, its far-from-equilibrium properties have generated considerable theoretical interest. By now several new theoretical methods have analyzed the interesting interplay of non-equilibrium physics and correlation effects in this model.

In this talk the differences and commons between the flow equation method out of equilibrium [1] and the frequency-dependent poor man's scaling approach [2] will be presented. We will focus on the non-equilibrium properties of a double quantum dot system, which will turn out to be a particularly suitable testing ground while being experimentally interesting in its own right.

[1] S. Kehrein, PRL 95, 056602 (2007).

[2] A. Rosch, J. Paaske, J. Kroha, and P. Wölfle, PRL 90, 076804 (2003).

TT 4.7 Mon 12:00 H21

Relaxation vs decoherence: Spin and current dynamics in the anisotropic Kondo model at finite bias and magnetic field — •Mikhail Pletyukhov, Dirk Schuricht, and Herbert Schoeller — Institut für theoretische Physik A, RWTH Aachen, Germany

Using a nonequilibrium renormalization group method we study the real-time evolution of spin and current in the anisotropic Kondo model (both antiferromagnetic and ferromagnetic) at finite magnetic field h_0 and bias voltage V. We derive analytic expressions for all times in the weak-coupling regime $\max\{V, h_0, 1/t\} \gg T_c$ (T_c = strong coupling scale). We find that all observables decay both with the spin relaxation and decoherence rates $\Gamma_{1/2}$. Various V-dependent logarithmic, oscillatory, and power-law contributions are predicted. The low-energy cutoff of logarithmic terms is generically identified by the difference of transport decay rates. For small times $t \ll \max\{V, h_0\}^{-1}$, we obtain universal dynamics for spin and current.

TT 4.8 Mon 12:15 H21

Discretization artifacts in the TD-NRG — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

One approach to study the nonequilibrium dynamics of quantum impurity systems is the time-dependent numerical renormalization-group (TD-NRG). Like the conventional NRG the TD-NRG relies on a logarithmic discretization of the bath continuum by mapping the bath onto a Wilson chain. We demonstrate in the real-time dynamics of a toy model, the resonant level model, that the group velocity of the wave propagation along the Wilson Chain is strongly position depen-

dent. The induced reflection of waves corrupt the calculation of the time-dependent impurity occupation. The time period for which the occupation number is calculated reliably can be extended by using a hybrid approach combining different discretizations of the bath continuum.

TT 4.9 Mon 12:30 H21

Nonequilibrium functional RG with frequency dependent vertex function – a study of the single impurity Anderson model — •Severin Jakobs[1,2], Mikhail Pletyukhov[1,2], and Herbert Schoeller[1,2] — [1]Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA – Fundamentals of Future Information Technologies, Germany

We investigate nonequilibrium properties of the single impurity Anderson model by means of the functional renormalization group (fRG) within Keldysh formalism. We present how the level broadening $\Gamma/2$ can be used as flow parameter for the fRG. This choice preserves important aspects of the Fermi liquid behaviour that the model exhibits in case of particle-hole symmetry. An approximation scheme for the Keldysh fRG is developed which accounts for the frequency dependence of the two-particle vertex in a way similar but not equivalent to a recently published approximation to the equilibrium Matsubara fRG. Our method turns out to be a rather flexible tool for the study of weak to intermediate on-site interactions $U \lesssim 3\Gamma$. In equilibrium we find excellent agreement with NRG results for the linear conductance at finite gate voltage, magnetic field, and temperature. In nonequilibrium, our results for the current agree well with TD-DMRG. For the nonlinear conductance as function of the bias voltage, we propose reliable results at finite magnetic field and finite temperature. Furthermore, we demonstrate the exponentially small scale of the Kondo temperature to appear in the second order derivative of the self-energy.

TT 5: CE: Low-dimensional Systems - Materials 1

Time: Monday 14:00–17:30 Location: H18

Invited Talk TT 5.1 Mon 14:00 H18

Field-Induced Berezinskii-Kosterlitz-Thouless Transition in a 2d Spin-Dimer System — •Michael Lang[1], Ulrich Tutsch[1], Bernd Wolf[1], Tonia Kretz[2], Hans-Wolfram Lerner[2], Matthias Wagner[2], Stefan Wessel[3], Tanusri Saha-Dasgupta[4], Harald Jeschke[5], and Roser Valenti[5] — [1]Phys. Institut, Univ. Frankfurt, SFB/TR49, D-60438 Frankfurt (M) — [2]Inst. f. Anorg. Chemie, Univ. Frankfurt SFB/TR 49, D-60438 Frankfurt(M) — [3]Inst. f. Theor. Phys. III, Univ. Stuttgart, D-70550 Stuttgart — [4]S.N. Bose National Centre f. Basic Science, 700098 Kolkata, India — [5]Inst. f. Theor. Phys., Univ. Frankfurt, SFB/TR49, D-60438 Frankfurt(M)

Weakly-coupled spin-1/2 dimer systems exposed to a sufficiently strong magnetic field offer exciting possibilities for studying critical phenomena under well-controlled conditions [1]. A prominent example is the Bose-Einstein condensation of magnetic triplet excitations in three dimensionally (3D)-coupled systems. Here we report on a chemically-constructed multilayer bulk magnet composed of molecule-based pairs of spin S = 1/2 dimers, where, by the application of a magnetic field, a gas of magnetic excitations is formed. Based on magnetic susceptibility measurements combined with Density Functional Theory and Quantum Monte Carlo calculations, we conclude that these excitations have a distinct 2D character and that the field-induced state, revealed at low temperatures of 39 mK, is a manifestation of the Berezinskii-Kosterlitz-Thouless topological order.

[1] T. Giamarchi et al., Nature Physics 4, 198 (2008).

TT 5.2 Mon 14:30 H18

Exploring the doping dependence of the Mott transition on X-ray irradiated crystals of κ-$(ET)_2Cu[N(CN)]_2]Cl$ — •Ulrich Tutsch[1], Ammar Naji[1], Takahiko Sasaki[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TRR49, D-60438 Frankfurt (M) — [2]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi 980-8577, Japan

The quasi two-dimensional organic charge-transfer salt κ-$(ET)_2Cu[N(CN)_2]Cl$ has a Mott-insulating ground state at ambient pressure, which can be transformed into a superconducting ground state ($T_c \approx 13\,K$) by applying moderate pressures of $\sim 30\,MPa$ (300 bar). Our objective is to study how the first-order Mott-transition line and its second-order critical end point change on doping the material away from half filling. We use X-ray irradiation in order to introduce charge carriers in this material [1] and take the shifts in the room-temperature resistivity as a measure of the amount of doping. We will present resistivity data for the temperature range $5\,K \leq T \leq 60\,K$ and for pressures up to 50 MPa for a κ-$(ET)_2Cu[N(CN)]_2]Cl$ crystal at various doping levels and discuss the accompanied changes in the p-T-phase diagram.

[1] T. Sasaki *et al.*, J. Phys. Soc. Jpn. 76, 123701 (2007)

TT 5.3 Mon 14:45 H18

Finite size effects and magnetic order in the spin-1/2 honeycomb lattice compound $InCu_{2/3}V_{1/3}O_3$ — •M. Yehia[1], E. Vavilova[1,2], U. Löw[3], A. Möller[4,5], T. Taetz[5], R. Klingeler[1], V. Kataev[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [3]Technische Universität Dortmund, Theoretische Physik I, 44221 Dortmund, Germany — [4]University of Houston, Department of Chemistry and Texas Centre for Superconductivity Houston, TX 77204, USA — [5]Institut für Anorganische Chemie, Universität zu Köln, 50939 Köln, Germany

A two dimensional spin honeycomb lattice on the basis of $InCu_{2/3}V_{1/3}O_3$ was studied by means of high field electron spin resonance, nuclear magnetic resonance and magnetic susceptibility. Previous structural studies suggest the occurrence of uncorrelated finite size in-plane domains, which is expected to inhibit long range magnetic order. Surprisingly, ESR data reveal the development of two collinear AFM sublattices below $\sim$ 20 K whereas NMR results show the presence of the staggered internal field. This is consistent with the magnetization data which implies a reorientation of the spin sublattices at $\sim$ 5.7 T. Quantum Monte-Carlo calculations of spin clusters of the coupled honeycomb spin planes indicate the development of the staggered magnetization at a finite temperature. This may explain the occurrence of the AFM state in $InCu_{2/3}V_{1/3}O_3$ despite unfavorable for magnetic order structural effects.

TT 5.4 Mon 15:00 H18

Low temperature magnetic response of CePt surface alloy — •Annemarie Köhl, Christian Praetorius, Sebastian Brück, and Kai Fauth — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We have used X-ray magnetic circular dichroism (XMCD) at Cerium edges to determine the low temperature paramagnetic local moment response of a CePt intermetallic surface alloy. The ultrathin alloy film is prepared in situ by evaporation of few atomic layers of Ce onto Pt(111) and subsequent annealing. LEED patterns of the resulting alloy hint at a (1.85×1.85) superstructure. The temperature dependent susceptibility is partially compatible with the response of the crystal field split Ce $4f^1$ state with a crystal field splitting of $\approx$ 60 K. Below 20 K our data are indicative of a magnetic phase transition at a critical temperature of $\approx$ 9 K. We discuss our results in view of the recent findings of Kondo lattice physics in the related $CePt_5$ surface alloy.

TT 5.5 Mon 15:15 H18

Magnetism in Azurite Studied by Muon Spin Rotation — Mathias Kraken[1], Josefin Engelke[1], Stefan Süllow[1], •Jochen Litterst[1], Anja Wolter[2], Bernd Wolf[3], Michael Lang[3], Chris Baines[4], and Hubertus Luetkens[4] — [1]IPKM, Technische Universität Braunschweig, Braunschweig, Germany — [2]IFW , Dresden, Germany — [3]Physikalisches Institut, Universität Frankfurt, Frankfurt am Main, Germany — [4]LEM, PSI, Villigen, Switzerland

The natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ represents a new type of low-dimensional frustrated quantum spin system with a diamond spin chain as basis. From specific heat [1] there is evidence for a phase transition at ca. 1.8 K which however is magnetically still ill-defined. Earlier muon spin rotation experiments [2] have indicated a magnetic transition yet no systematic study has been reported. We have per-

formed zero field and transverse field muon spin rotation experiments at Paul Scherrer Institut Villigen (Switzerland) in the temperature range from 0.02 K to 6 K on polycrystalline powder and a single crystal. We could corroborate the appearance of magnetic order below 1.9 K from spontaneous muon spin rotation with a frequency following a magnetization curve. The rotation profile is indicative of a modulated spin structure. In addition we find a pre-cursor phase between 1.9 K and about 3 K which we relate to the onset of magnetic correlations between Cu monomers via dimers.

[1] H. Kikuchi, et al., Phys. Rev. Lett. 94 (2005) 227201.

[2] H. Kikuchi, et al., Progress of Theoretical Physics Supplement. 159 (2005)1 2005

TT 5.6 Mon 15:30 H18

Neutron scattering investigations of the magnetic properties of azurite $Cu_3(CO_3)_2(OH)_2$ — •Kirrily Rule[1], Clare Gibson[1,2], Manfred Reehuis[1], Bachir Ouladiaff[3], Matthias Gutmann[4], Jens-Uwe Hoffmann[1], Sebastian Gerischer[1], Alan Tennant[1,2], Stefan Süllow[5], and Michael Lang[6] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]ISIS Facility, Rutherford Appleton Laboratory, Didcot UK — [5]Institut für Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [6]Physikalisches Institut, J.W. Goethe-Universität Frankfurt, Germany

Azurite, $Cu_3(CO_3)_2(OH)_2$, has been considered an ideal example of a one-dimensional (1D) diamond chain antiferromagnet. Early studies of this material imply the presence of an ordered antiferromagnetic phase below TN 1.9 K while magnetization measurements have revealed a 1/3 magnetization plateau. Until now, no corroborating neutron scattering results have been published to confirm the ordered magnetic moment structure. In this talk, we will present neutron diffraction data which reveal the presence of a commensurate magnetic order in azurite. The results of magnetic structural refinement from single crystal diffraction will also be discussed. Finally we will show some recent inelastic neutron scattering results which reveal new information about the dynamics in this material.

15 min. break

TT 5.7 Mon 16:00 H18

Consequence of the intra-chain dimer-monomer spin frustration and the inter-chain dimer-monomer spin exchange in the diamond-chain compound Azurite $Cu_3(CO_3)_2(OH)_2$ — •R. K. Kremer[1], J. Kang[2], C. Lee[2], and M.-H. Whangbo[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204

The spin lattice appropriate for Azurite $Cu_3(CO_3)_2(OH)_2$ was determined by evaluating its spin exchange interactions on the basis of first principles density functional calculations. It is found that Azurite cannot be described by an isolated diamond chain with no spin frustration, but by a two-dimensional spin lattice in which diamond chains with spin frustration interact through the interchain spin exchange in the *ab*-plane.[1] Our analysis indicates that the magnetic properties of Azurite at low temperatures can be approximated by two independent contributions, i.e., an isolated dimer and an effective uniform chain contributions. This prediction was verified by analyzing the magnetic susceptibility and specific heat data of Azurite.

[1] J. Kang, *et al.* J. Phys. Cond. Matter **21** 392201 (2009).

TT 5.8 Mon 16:15 H18

Effective spin-chain model for azurite: derivation from ab-initio computations (exchanged with TT 5.9) — Ingo Opahle[1], Hem C. Kandpal[2], Niels Jackson[1], Hena Das[3], Tanusri Saha-Dasgupta[3], Andreas Honecker[4], •Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [2]IFW Dresden — [3]Bose Institute, Kolkata, India — [4]Institut für Theoretische Physik, Universität Göttingen

The observation of complex spin dynamics and a 1/3 magnetization plateau has revived the interest in the famous pigment azurite $Cu_3(CO_3)_2(OH)_2$. We revisit the question of the underlying microscopic Hamiltonian using a combination of first principles methods. As a guiding tool, we employ NMTO downfolding which yields the relative importance at low energies of the many possible hybridization paths between the copper centers. In order to obtain the corresponding exchange coupling strengths we perform total energy calculations for many spin configurations and several supercells. We employ FPLAPW and FPLO basis sets with LDA+U functionals, and we investigate the dependence of the exchange couplings on the correlation strength U. We find that the low-energy Hamiltonian of azurite is a diamond chain with a monomer-monomer coupling and some nonzero interchain couplings. We show that the neglect of interchain couplings effectively leads to a less symmetric diamond chain.

TT 5.9 Mon 16:30 H18

Effective spin-chain model for azurite: comparison with experimental results (exchanged with TT 5.8) — •Andreas Honecker[1], Robert Peters[1], Thomas Pruschke[1], Roser Valentí[2], Harald Jeschke[2], Ingo Opahle[2], Hem Kandpal[2], Tanusri Saha-Dasgupta[3], Hena Das[3], Johannes Richter[4], Helge Rosner[5], Oleg Janson[5], Shijie Hu[6], Xiaoqun Wang[6], Bernd Wolf[2], and Michael Lang[2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Johann Wolfgang Goethe-Universität Frankfurt am Main — [3]Bose National Centre for Basic Sciences, Kolkata — [4]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg — [5]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [6]Department of Physics, Renmin University of China, Beijing

We analyze a spin-1/2 Heisenberg model with a generalized diamond chain exchange geometry which has been derived from ab-initio computations for the mineral azurite $Cu_3(CO_3)_2(OH)_2$. Using numerical results, we demonstrate that a consistent description can be obtained for various physical properties of azurite: (i) the low-temperature magnetization curve, (ii) inelastic neutron scattering on the 1/3 magnetization plateau, (iii) nuclear magnetic resonance measurements on the 1/3 magnetization plateau, and (iv) the magnetic susceptibility as well as the specific heat. Our results resolve previous controversies on the modeling of azurite. Furthermore, we explain why a one-dimensional model can be used in many situations although interchain exchange in azurite is actually non-negligible at a microscopic level.

TT 5.10 Mon 16:45 H18

The low-temperature structure of azurite — •Clare Gibson[1,2], Kirrily Rule[1], Manfred Reehuis[1], Bachir Ouladdiaf[3], Alan Tennant[1,2], Stefan Suellow[4], and Michael Lang[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [5]Phys. Inst., J.W. Goethe-Universität Frankfurt, Germany

The low-dimensional quantum magnet and natural mineral azurite, $Cu_3(CO_3)_2(OH)_2$, is considered to be a model of the distorted diamond chain lattice. Recently, much study has been devoted to determining the magnetic exchange parameters in this frustrated magnetic material. However, results have been contradictory [1,2,3] and the validity of the one-dimensional model has been called into question [4]. An accurate structural determination of azurite below the Nèel temperature may prove useful for the purpose of exchange parameter calculation in terms of precise knowledge of the magnetic superexchange pathways. We report on single crystal and powder neutron diffraction data taken over the temperature range 200 mK - 5 K to determine the low temperature lattice parameters and space group. Analysis reveals strain in the material which coincides with the magnetic ordering transition at 1.86 K.

[1] H. Kikuchi et al., Phys. Rev. Lett. 94, 227201 (2005)

[2] K.C. Rule et al., Phys. Rev. Lett. 100, 117202 (2008)

[3] G. Bo and G. Su, Phys. Rev. Lett. 97, 089701 (2006)

[4] J. Kang et al., J. Phys.: Condens. Matter 21, 392201 (2009)

TT 5.11 Mon 17:00 H18

Analyzing the complex spin-coupling structure in the single-molecule magnet Mn_{12}wheel by inelastic neutron scattering — •Joscha Nehrkorn[1], Oliver Waldmann[1], Taketo Tagushi[2], George Christou[2], Thierry Strässle[3], Philip L. W. Tregenna-Pigott[3], and Hannu Mutka[4] — [1]Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany — [2]Department of Chemistry, University of Florida, Gainesville, Florida 32611-7200, USA — [3]LNS, ETH Zürich & Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]Institut Laue-Langevin, 38042 Grenoble, France

Recently the single-molecule magnet (SMM) $[Mn_{12}(O_2CMe)_{14}(R\text{-}mda)_8]$, or Mn_{12}wheel in short, has attracted interest because of its unusual quantum tunneling transitions in the magnetization, which

were explained by describing it as a dimer of two magnetically coupled SMM subunits [1,2]. In order to analyze the underlying complicated spin structure we performed inelastic neutron scattering experiments. They show that the model of two coupled SMMs has to be refused. A microscopic model was devised which reproduces the data and provides values for the exchange coupling and magnetic anisotropy parameters. By using basic principles for bipartite lattices the low-energy sector can be reduced again to that of two coupled subunits, which, however, are substantially different than the two subunits in the originally proposed dimer model. The new model resolves some controversies as regarding the magnetic tunneling transitions.

[1] C. Ramsey *et al.*, Nature Physics **4**, 277 (2008)
[2] W. Wernsdorfer *et al.*, Phys. Rev. Lett **101**, 237204 (2008)

TT 5.12 Mon 17:15 H18

Molecular Magnets Confined in the Nanocage of a Globular Protein — •Peter Lemmens[1,4], Dirk Wulferding[1,4], Dirk Menzel[1], Tamoghna Mitra[2], Achim Müller[2], Rajib Kumar Mitra[3], Pramod Kumar Verma[3], and Samir Kumar Pal[3] — [1]IPKM, TU-BS, Braunschweig — [2]FC, Univ. Bielefeld — [3]SNBC, Kolkata, India — [4]IGSM, TU-BS, Braunschweig

We investigate the effect of confinement and energy transfer on the dynamics of a molecular magnet known as a model system to study quantum coherence. The polyoxovanadate V_{15} is incorporated into a protein cavity and the energy transfer probed by time resolved experiments. Work supported by DFG and B-IGSM.

TT 6: TR: Nanoelectronics II: Spintronics and Magnetotransport

Time: Monday 14:00–18:15 Location: H19

TT 6.1 Mon 14:00 H19

Transport through an interacting quantum dot tunnel coupled to a ferromagnet with time-dependent magnetisation — •Nina Winkler[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik and CeNIDE · Universität Duisburg-Essen — [2]School of Chemical and Physical Sciences · Victoria University of Wellington · New Zealand

We study adiabatic charge and spin pumping in an interacting quantum dot connected to one normal and one ferromagnetic lead. In general, this setup can work as a quantum pump when only the direction of the lead magnetisation is varied in time [1]. We focus on the adiabatic-pumping regime. To account for a time-dependent lead magnetisation, we generalise a diagrammatic real-time approach for adiabatic pumping through quantum dots with ferromagnetic leads [2, 3]. We perform a systematic expansion in both frequency and tunnel-coupling strength, treating the on-site Coulomb interaction on the quantum dot exactly. We investigate the adiabatic charge and spin transport through the structure when pumping by periodically changing the direction of the lead magnetisation up to second order in the tunnel-coupling strength.

[1] M.V. Costache *et al.*, Phys. Rev. Lett. **97**, 216603 (2006).
[2] J. Splettstoesser *et al.*, Phys. Rev. B **74**, 085305 (2006).
[3] J. Splettstoesser *et al.*, Phys. Rev. B **77**, 195320 (2008).

TT 6.2 Mon 14:15 H19

Kondo Effect in single wall carbon nanotubes with ferromagnetic contacts — •Markus Gaass, Andreas Hüttel, Dominik Preusche, Lorenz Herrmann, and Christoph Strunk — Universität Regensburg, Institut für Experimentelle und Angewandte Physik

We investigate the interplay of the Kondo effect and magnetic contacts in quantum dots formed by single wall carbon nanotubes. The regular spin-1/2 Kondo effect appears when the coupling between the electrodes and the quantum dot is high enough. If the leads are magnetized the Kondo resonance is exchange split at zero magnetic field. We fabricated single wall carbon nanotube transport devices with electric contacts made of PdNi which show a sufficient interface transparency to observe the Kondo effect. Without any applied field the Kondo resonance is indeed split. In some Coulomb valleys the splitting can be compensated by an external magnetic field on the order of 1 Tesla, in others it remains finite. In addition a fine structure in the spectra is observed which indicates a more complex level structure than expected for armchair carbon nanotubes.

TT 6.3 Mon 14:30 H19

A singlet - triplet T_+ based qubit — •Hugo Ribeiro[1], Jason Petta[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457, Konstanz, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA

We theoretically model a nuclear-state preparation scheme that increases the coherence time of a two-spin qubit in a double quantum dot. The two-electron system is tuned repeatedly across a singlet-triplet level-anticrossing with alternating slow and rapid sweeps of an external bias voltage. Using a Landau-Zener-Stückelberg model, we find that in addition to a small nuclear polarization that weakly affects the electron spin coherence, the slow sweeps are only partially adiabatic and lead to a weak nuclear spin measurement and a nuclear-state narrowing which prolongs the electron spin coherence. This resolves some open problems brought up by a recent experiment [1]. We also show that the electronic two-spin states singlet and triplet T_+ are promising candidates for the implementation of a qubit in GaAs double quantum dots (DQD). A coherent superposition of the two-spin states is obtained by finite time Landau-Zener-Stückelberg interferometry and the single qubit rotations are performed by means of an external magnetic field with a typical amplitude of about 100 mT, while coherent manipulation can be done within ~ 1 ns. We also study the nuclear induced decoherence, mainly due to hyperfine contact coupling between the electronic and nuclear spins, and compute the decoherence time $T_2^* \sim 10$ ns.

[1] D. J. Reilly *et al.*, Science **321**, 817 (2008).

TT 6.4 Mon 14:45 H19

Charge ratchet from spin flip: Space-time symmetry paradox — •Sergey Smirnov[1], Dario Bercioux[2], Milena Grifoni[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Freiburg Institute for Advanced Studies (FRIAS) and Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany

Traditionally the charge ratchet effect is considered as a consequence of either the spatial symmetry breaking engineered by asymmetric periodic potentials, or time asymmetry of the driving fields. Here we demonstrate that electrically and magnetically driven quantum dissipative systems with spin-orbit interactions represent an exception from this standard idea. In contrast to the so far well established belief, a charge ratchet effect appears when both the periodic potential and driving are symmetric. We show that the source of this paradoxical charge ratchet mechanism is the coexistence of quantum dissipation with the spin flip processes induced by spin-orbit interactions [1]. The queerness of the charge ratchet current consists in the fact that this current, in contrast to early predictions for systems without spin-orbit interactions, appears even when only one energy band provides electrons for transport and no harmonic mixing is present in the driving fields. Such purely spin-orbit charge currents are controlled by the gate voltage tuning the strength of the spin-orbit coupling. This peculiarity of the effect is very attractive from the experimental point of view.

[1] S. Smirnov, D. Bercioux, M. Grifoni and K. Richter, Phys. Rev. B 80, 201310(R) (2009).

TT 6.5 Mon 15:00 H19

Orbitally phase coherent spintronics — Cheryl Feuillet-Palma[1,2], Thomas Delattre[1,2], Pascal Morfin[1,2], Jean-Marc Berroir[1,2], Gwendal Feve[1,2], Christian Glattli[1,2,3], Bernard Placais[1,2], Audrey Cottet[1,2], and •Takis Kontos[1,2] — [1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France — [2]CNRS UMR 8551, Laboratoire associé aux universités Pierre et Marie Curie et Denis Diderot, France — [3]Service de physique de l'état Condensé, CEA, 91192

The scattering imbalance between up and down spins at the interface between a non-magnetic metal and a ferromagnetic metal is at the heart of the principle of the magnetic tunnel junctions or multilayers celebrated in the field of spintronics. Although these devices use the quantum mechanical spin degree of freedom and electron tunneling, they do not exploit a crucial degree of freedom involved in quantum mechanics: the phase of the electronic wave function. In most of the

devices studied so far, this aspect has not been developed owing to the classical-like motion of charge carriers in the conductors used. In this work, we report on spin dependent transport measurements in carbon nanotubes based multi-terminal circuits. We observe a gate-controlled spin signal in non-local voltages and an anomalous conductance spin signal, which reveal that both the orbital phase and the spin can be conserved along carbon nanotubes with multiple ferromagnetic contacts. This paves the way for spintronics devices exploiting both these quantum mechanical degrees of freedom on the same footing.

TT 6.6 Mon 15:15 H19

Bulk transport properties of two-dimensional HgTe nanostructures — •Elena G. Novik[1], Patrik Recher[2], Ewelina M. Hankiewicz[2], and Björn Trauzettel[2] — [1]Physikalisches Institut (EP3), University of Würzburg, 97074 Würzburg — [2]Institut für Theoretische Physik und Astrophysik, University of Würzburg, 97074 Würzburg

The topologically non-trivial insulators realized in HgTe quantum wells (QWs) have recently attracted considerable attention because of their unique property: the existence of the gap in the bulk and the gapless edge states on the sample boundaries. Depending on the width of the HgTe QW the structure can be a trivial insulator with normal band structure when the QW width is smaller than 6.3 nm, or a topologically non-trivial insulator with inverted band structure for thicker QWs. Here we show that it is possible to distinguish the topologically trivial from non-trivial insulator states on the basis of bulk transport properties only. Using the effective four-band model [1], we have calculated the bulk conductance through the two-dimensional metal/HgTe insulator/metal structure. Whereas for the trivial insulator the conductance increases monotonically with decreasing distance between the electron reservoirs L, a non-monotonic behaviour of the bulk transport depending on L has been found for the insulator in the inverted regime. Interestingly, the bulk transport contribution can even exceed the quantized conductance caused by edge state transport and should be taken into account for the interpretation of future experiments.

[1] B. A. Bernevig et al., Science, 314, 1757 (2006).

TT 6.7 Mon 15:30 H19

Magneto-resistance of atomic-sized contacts of magnetic metals — •Stefan Egle[1], Hans-Fridtjof Pernau[1], Cécile Bacca[1], Magdalena Huefner[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Solid State Physics Laboratory, ETH Zurich, Switzerland

In this talk, a comprehensive study of the magneto resistance (MR) behavior of atomic-size contacts is given, where two macroscopic electrodes are connected to a central nanobridge. An atomic contact can be adjusted by means of mechanically controllable break junction (MCBJ) technique. In order to separate the influence of the electrodes from the effect of the nanobridge itself, we employ different material systems. Namely, ferromagnetic cobalt electrodes are connected to a non-magnetic gold bridge and vice versa. The shape of the electrodes can be chosen symmetric or asymmetric and the nanobridge region can be suspended or non-suspended. Furthermore, we investigate the MR for different orientations of the magnetic field. The curves show a very rich behavior with magneto resistance ratios (MRR) up to 100% and more in the atomic contact regime, reaching up to a few 1000% in the tunneling regime. For all geometries used, the MRR values are of comparable size. Moreover, we study the possible influence of the micromagnetic order of the domains in the vicinity of the contact region as well as ballistic MR, GMR, TMR, atomically enhanced anisotropic MR (AAMR) and magnetostriction. We conclude that the AAMR is the most important contribution of the MR at large magnetic fields, while magnetostriction, TMR and GMR govern the low-field regime.

TT 6.8 Mon 15:45 H19

Oscillatory crossover from two dimensional to three dimensional topological insulators — •Chao-Xing Liu[1], HaiJun Zhang[2], Binghai Yan[3], Xiao-Liang Qi[4], Thomas Frauenheim[3], Xi Dai[2], Zhong Fang[2], and Shou-Cheng Zhang[4] — [1]EP3 and Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]IOP, Chinese Academy of Sciences, Beijing 100190, China — [3]Bremen Center for Computational Materials Science, Universität Bremen, 28359 Bremen, Germany — [4]Department of Physics, Stanford University, Stanford, CA 94305-4045

Topological insulators (TIs) are new states of quantum matter with the surface states protected by time-reversal symmetry, which can exist both in two-dimensional (2D) system and three-dimensional (3D) system. In this work, we would like to investigate the crossover regime from 3D TIs to 2D TIs when the sample thickness is reduced. Based on the four band effective model, we find that the crossover occurs in an oscillatory fashion as a function of the film thickness, alternating between topologically trivial and non-trivial 2D behavior. A physical picture is provided to understand the origin of the oscillation. Furthermore *ab initio* calculation is performed to study the realistic Bi_2Se_3 and Bi_2Te_3 thin film and confirm the analytical results. These results not only establisch the relation between the TIs with the different dimensions, but also provide a new path to search for new TIs.

15 min. break

TT 6.9 Mon 16:15 H19

Spin accumulation with spin-orbit interaction — •Henri Saarikoski[1,2,3] and Gerrit E. W. Bauer[1] — [1]Kavli Institute of Nanoscience, Delft University of Technology, 2628-CJ Delft, The Netherlands — [2]Mathematical Physics, Lund Institute of Technology, SE-22100 Lund, Sweden — [3]Present address: University of Regensburg, 93040 Regensburg

Spin accumulation is a crucial but imprecise concept in spintronics. In metal-based spintronics it is characterized in terms of semiclassical distribution functions. In semiconductors with a strong spin-orbit coupling the spin accumulation is interpreted as a superposition of coherent eigenstates. We show that both views can be reconciled by taking into account the electron-electron interaction: a sufficiently strong self-consistent exchange field reduces a spin accumulation to a chemical potential difference between the two spin bands even in the presence of spin-orbit coupling. We demonstrate the idea on a clean two-dimensional electron gas (2DEG) by showing how the exchange field protects a spin accumulation from dephasing and introduces an easy-plane anisotropy. Spin can be injected either adiabatically, e.g. by a ferromagnetic contact with small electric bias, or diabatically, e.g. by pulsed optically induced excitation. We discuss spin-accumulation eigenstates that are accessible by adiabatic excitation as well as spin accumulation dynamics of rapidly excited states. We illustrate the general ideas at the hand of a 2DEGs with Rashba SOI, in which the disorder-scattering lifetime broadening is much smaller than the spin-orbit splitting at the Fermi-level.

TT 6.10 Mon 16:30 H19

Suppression of the Spin-Hall Effect by Magnetic Fields in Nanostructures — •Dietrich Rothe and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astrophysik, Würzburg, Germany

The spin-Hall effect (SHE) is the generation of the transverse spin-imbalance in semiconductors with strong spin-orbit interactions in the conducting ("metallic") regime. Although the SHE is caused by spin-orbit interaction and the time symmetry breaking perturbation should destroy the phenomenon, the influence of magnetic field was not so far discussed in detail.

In this contribution, we will analyze the influence of magnetic field on the magnitude of spin signal in the H-shaped structures where the spin signal can be excited and detected electrically [1,2].

We will show, within the non-equilibrium Green function formalism, that the magnetic field destroys the spin signal effectively in perpendicular magnetic fields while the signal is much less affected in parallel fields where only the Zeeman part of the field is present. The connection with experimental results will be discussed [1].

[1] C. Bruene, A. Roth , E. G. Novik, M. Koenig, H. Buhmann, E. M. Hankiewicz, W. Hanke, J. Sinova and L. W. Molenkamp, arXiv:0812.3768 (2008).

[2] E. M. Hankiewicz, L. W. Molenkamp, T. Jungwirth, and Jairo Sinova, Phys. Rev. B 70, 241301(R) (2004).

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TT 6.11 Mon 16:45 H19

Interference spin-blockade in symmetric nanojunctions — •Andrea Donarini, Georg Begemann, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

Nanojunctions with a high degree of spatial symmtry, like molecular junctions, but also specially designed multiple quantum dot structures, have a degenerate many body spectrum. The degeneracy is in fact protected by symmetry. The interference between the degenerate states

causes a novel current blocking mechanism that allows, in presence of polarized leads, the all electric control of the spin and orbital degree of freedom on the junction. We present here a general formalism to give necessary and sufficient conditions for interference blockade. As an example we analyze a triple dot single electron transistor (SET) [1]. In particular, we show how to prepare the system in each of the three spin states of the excited 2-electrons triplet state without application of any external magnetic field.

[1] Nano Letters, **9**, 2897 (2009).

TT 6.12 Mon 17:00 H19

Influence of Different Spin-Orbit Terms on Spin Transport in HgTe Quantum Wells — •Rolf W. Reinthaler[1], Dietrich Rothe[1], Chao-xing Liu[2], Laurens W. Molenkamp[2], and Ewelina M. Hankiewicz[1] — [1]Institut für Theoretische Physik und Astrophysik, Würzburg, Germany — [2]Physikalisches Institut (EP3), Würzburg, Germany

We derive, within kp theory, an effective four band model (conduction/heavy hole bands) describing physics of HgTe quantum wells with the Dirac-like and Rashba types spin-orbit interactions.

The physics of both contributions is discussed using the Landauer-Büttiker approach and with the semiclassical equations of motions within the wave packet formalism. We find that the spin-Hall conductance originating from the Rashba spin-orbit interaction scales quadratically with spin-orbit coupling strength and shows a precession pattern. On the other hand, the term obtained from Dirac part scales linearly with the spin-orbit strength and conserves the z-component of the spin.

The competition between the Dirac-like and Rashba spin-orbit terms is of particular interest. We find that for realistic material parameters the Dirac-like terms can influence the action of Rashba spin-orbit interactions and lead to the enhancement of the spin-Hall conductance.

We acknowledge the financial support by German DFG grant HA 5893/1-1.

TT 6.13 Mon 17:15 H19

Hyperfine mediated triplet-singlet transition probability in a double-quantum-dot system: Analogy with the double-slit experiment — •Fernando Dominguez, Carlos López-Monís, and Gloria Platero — Instituto de ciencia de los materiales de Madrid (ICMM)

Recent experiments and theoretical works have been devoted to the analysis of transport through double quantum dots in the spin blockade regime. There, the current is blocked unless spin scattering induces electron spin-flip, giving rise to electronic triplet-singlet transition. Hyperfine interaction is the main mechanism responsible for spin-flip and it will be considered in the present work. We present an elementary measurement theory scheme in order to analyze the electronic triplet-singlet transition mediated by the hyperfine interaction in a double quantum dot. We show that the local character of the hyperfine interaction and the nuclear back-action process (flip-flop) are crucial for canceling destructive interferences of the triplet-singlet transition probability. It is precisely this cancellation which distinguishes the transition probability mediated by hyperfine interaction from the effect due to an anisotropic magnetic field.

[1] Phys. Rev. B 80, 201301 R (2009)

TT 6.14 Mon 17:30 H19

Ballistic transport in 1D magnetic systems based on the FLAPW Method and Wannier functions — •Björn Hardrat[1], Neng-Ping Wang[2], Yuriy Mokrousov[3], Frank Freimuth[3], and Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, D-24098 Kiel, Germany — [2]Physics Departement, Ningbo Univeristy, Fenghua Road 818, 315211 Ningbo, P.R. China — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52435 Jülich, Germany

We report the development of a ballistic transport code for one-dimensional magnetic systems based on Wannier functions (WF) constructed within the full-potential linearized augmented plane-wave (FLAPW) method. We describe the details of the construction of first-shot (fsWF) or maximally localized (MLWF) WFs from the FLAPW wavefunctions choosing a monoatomic Pt chain as a model system. For the calculation of ballistic transport, we apply the Landauer formalism using Green's functions, which allows us to obtain the conductance of the system. As first applications of the approach, we study the transition from the contact to the tunneling regime in monoatomic Pt wires, with and without spin-orbit coupling (SOC), as well as in ferromagnetic Co wires, for which we calculated the tunneling magneto resistance (TMR). Furthermore we investigate the effect of single defect Pt and Co scatterers on the transmission through such monowires.

TT 6.15 Mon 17:45 H19

Dynamic spin-Hall effect and driven spin helix for linear spin-orbit interactions — •Mathias Duckheim[1], Dmitrii L. Maslov[2], and Daniel Loss[1] — [1]Department of Physics, University of Basel, CH-4056 Basel, Switzerland — [2]Department of Physics, University of Florida, Gainesville, FL 32611 -8440, USA

We derive boundary conditions for the electrically induced spin accumulation in a finite, disordered 2D semiconductor channel. While for DC electric fields these boundary conditions select spatially constant spin profiles equivalent to a vanishing spin-Hall effect, we show that an in-plane ac electric field results in a non-zero ac spin-Hall effect, i.e., it generates a spatially non-uniform out-of-plane polarization even for linear intrinsic spin-orbit interactions. Analyzing different geometries in [001] and [110]-grown quantum wells, we find that although this out-of-plane polarization is typically confined to within a few spin-orbit lengths from the channel edges, it is also possible to generate spatially oscillating spin profiles which extend over the whole channel. The latter is due to the excitation of a driven spin-helix mode in the transverse direction of the channel. We show that while finite frequencies suppress this mode, it can be amplified by a magnetic field tuned to resonance with the frequency of the electric field. In this case, finite size effects at equal strengths of Rashba and Dresselhaus SOI lead to an enhancement of the magnitude of this helix mode. We comment on the relation between spin currents and boundary conditions.

TT 6.16 Mon 18:00 H19

Frequency-Dependent Spin Conductance and Spin Noise of Quantum Dots in the Kondo Regime — •Ireneusz Weymann[1,2], Catalin Pascu Moca[3], and Gergely Zarand[3] — [1]Physics Department, ASC, and CeNS, Ludwig-Maximilians-University, Theresienstrasse 37, 80333 Munich, Germany — [2]Physics Depertement, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, H-1521 Budapest, Hungary

We analyze the equilibrium and non-equilibrium frequency-dependent spin noise and spin conductance of a quantum dot in the Kondo regime. The equilibrium spin noise is characterized by two universal functions that we determine perturbatively for large frequencies, and compute numerically at zero temperature using numerical renormalization group.

The parallel and antiparallel noise components show markedly different frequency dependence. The antiparallel spin conductance develops a resonance for frequencies of the order of the Kondo temperature as a result of dynamical spin accumulation. For temperatures well above the Kondo scale, a low-frequency anomaly appears in the spin current correlations below the Korringa relaxation rate.

TT 7: SC: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

Time: Monday 14:00–18:00 Location: H20

TT 7.1 Mon 14:00 H20

Spin-dependent boundary conditions for isotropic superconducting Green's functions — •Wolfgang Belzig[1], Audrey Cottet[2], Daniel Huertas-Hernando[3], and Yuli Nazarov[4] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Ecole Normale Supérieure, Laboratoire Pierre Aigrain, Paris, France — [3]Department of Physics, Norwegian University of Science and Technology,Trondheim, Norway — [4]Kavli Institute of NanoScience, Delft University of Technology, Delft, The Netherlands

The quasiclassical theory of superconductivity provides the most suc-

cessful description of diffusive hetero- structures comprising superconducting elements, namely, the Usadel equations for isotropic Green's functions. Since the quasiclassical and isotropic approximations break down close to interfaces, the Usadel equations have to be supplemented with boundary conditions for isotropic Green's functions (BCIGF), which are not derivable within the quasiclassical description. For a long time, the BCIGF were available only for spin- degenerate tunnel contacts, which posed a serious limitation on the applicability of the Usadel description to modern structures containing ferromagnetic elements. We close this gap and derive spin- dependent BCIGF for a contact encompassing superconducting and ferromagnetic correlations [1]. This finally justifies several simplified versions of the spin-dependent BCIGF, which have been used in the literature so far [2].

[1] A. Cottet, D. Huertas-Hernando, W. Belzig and Yu. V. Nazarov, Phys. Rev. B **80**, 184511 (2009)

[2] D. Huertas-Hernando, Yu. V. Nazarov, W. Belzig, Phys. Rev. Lett. **88**, 047003 (2002)

TT 7.2 Mon 14:15 H20

Doppler shift in Andreev reflection from a moving superconducting condensate in Nb/InAs Josephson junctions — Rohlfing Franziska[1], •Tkachov Grigory[1,2], Otto Florian[1], Richter Klaus[1], Weiss Dieter[1], and Strunk Christoph[1] — [1]Universität Regensburg — [2]Universität Würzburg

We present experimental and theoretical studies of narrow ballistic Josephson weak links in InAs quantum wells contacted by Nb electrodes and subject to an external magnetic field [1]. We find a dramatic magnetic-field suppression of the Andreev reflection amplitude, which occurs even for in-plane field orientation with essentially no magnetic flux through the junction. Our observations demonstrate the presence of a Doppler shift in the energy of the Andreev levels, which results from diamagnetic screening currents in the hybrid Nb/InAs banks. The data for conductance, excess and critical currents can be consistently explained by taking into accout the field- and geometry-dependent phase gradient of the superconducting order parameter and the McMillan energy, characterizing the proximity effect in the Nb/InAs banks. Our analysis suggests that a similar Doppler shift in Andreev reflection should, generally, be expected in other 2D hybrid systems such as, e.g., graphene-superconductor Josephson links [2].

[1] F. Rohlfing et al., Phys. Rev. B **80**(R) (2009).

[2] H. B. Heersche et al., Nature **446**, 56 (2007).

TT 7.3 Mon 14:30 H20

Charge and spin currents in a triplet superconductor-ferromagnet-singlet superconductor Josephson junction — Yasuhiro Asano[1], •Dirk Manske[2], and Philip Brydon[3] — [1]Department of Applied Physics, Hokkaido University — [2]Max Planck Institute for Solid State Research — [3]Institute for Theoretical Physics, TU Dresden

The study of triplet superconductor Josephson junctions with magnetically-active tunneling barriers has revealed an intimate connection between charge and spin supercurrents in these devices [1,2]. Here we generalize this analysis to tunneling between a spin-triplet and a spin-singlet superconductor through a magnetic barrier. Using a tunneling Hamiltonian analysis, we show how spin-flip tunneling processes produce a lowest-order Josephson coupling between the two superconductors, accomplishing both spin- and orbital-parity conversion for the tunneling Cooper pairs. Remarkably, in the triplet superconductor the charge current is accompanied by a phase-dependent spin current. We verify these predictions using a Bogoliubov-de Gennes technique, which reveals the importance of the orbital pairing state of the two superconductors for the appearance of these effects.

[1] P. M. R. Brydon, D. Manske, and M. Sigrist, J. Phys. Soc. Japan 77, 103714 (2008).

[2] P. M. R. Brydon and D. Manske, Phys. Rev. Lett. 103, 147001 (2009).

TT 7.4 Mon 14:45 H20

Spin current due to triplet superconductor - ferromagnet interfaces — •Philip Brydon — Technische Universität Dresden, Dresden, Germany

The interface between a superconductor and a ferromagnet is an ideal setting in which to study the complicated interplay of these two phases. Although the relevant physics is now very well understood for a spin singlet pairing state of the superconductor, qualitatively new phenomena can appear for a spin triplet pairing state due to the intrinsic spin structure of the superconductor. One such surprising result is the existence of a bulk spin supercurrent in the triplet superconductor due to spin-flip reflection of triplet Cooper pairs at the superconductor-ferromagnet interface [1,2]. The resulting spin current displays strong similarities to the spontaneous charge current in a conventional Josephson junction. The dependence of the spin current on a number of relevant parameters is studied e.g. the orbital pairing state of the superconductor and the exchange splitting of the ferromagnet. The possibility of unconventional dynamics of the magnetization of the ferromagnet is discussed.

[1] P. M. R. Brydon and D. Manske, Phys. Rev. Lett. 103, 147001 (2009).

[2] P. M. R. Brydon, cond-mat/0908.4065 (Phys. Rev. B, to be published).

TT 7.5 Mon 15:00 H20

Theory of superconductor-ferromagnet point-contact spectra: the case of strong spin-polarization — •Roland Grein[1], Tomas Löfwander[2], Georgo Metalidis[1], and Matthias Eschrig[3] — [1]Institut für Theoretische Festkörperphysik und DFG-Zentrum für funktionelle Nanostrukturen, Karlsruher Institut für Technologie, D-76128 Karlsruhe — [2]Department of Microtechnology and Nanoscience MC2, Chalmers University of Technology, S-412 96 Göteborg, Sweden — [3]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

We study the effects of spin-active scattering on superconductor-ferromagnet point-contact spectra using the quasiclassical theory of superconductivity. New boundary conditions for the quasiclassical Green's function allow for treating strongly spin-polarized systems with this approach. The theory describes the contact region by a general scattering matrix and various microscopic models of interfacial scattering are studied. We show that the shape of the interface potential plays a crucial role in spin-active scattering and that spin-flip processes can alter the spectra dramatically.

We show that our theory generalizes earlier models for electronic transport across such contacts based on the BTK-approach. They are contained as limiting cases in our formalism.

TT 7.6 Mon 15:15 H20

Re-analysis of experimental point contact Andreev spectra: the case of half-metallic CrO_2 — •Matthias Eschrig[1], Roland Grein[2], and Tomas Löfwander[3] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institut für Theoretische Festkörperphysik und DFG-Zentrum für funktionelle Nanostrukturen, KIT, D-76128 Karlsruhe, Germany — [3]Department of Microtechnology and Nanoscience MC2, Chalmers University of Technology, S-41296 Göteborg, Sweden

Point-contact Andreev spectroscopy has been extensively used to probe the spin-polarization of strong ferromagnets. In this method a nanosized point contact is formed between a superconducting tip and the ferromagnetic material under investigation (or vice versa). The conductance-versus-voltage is recorded at a low temperature. Subsequently, a fitting procedure is undertaken to extract the polarization of the ferromagnet. We re-analyze existing data using a new theoretical treatment that accounts for spin-mixing effects and magnetic inhomogeneities, and that is based on a new formulation of boundary conditions taking into account these effects. We find that for the prominent case of CrO_2 the data are consistent with a spin polarization close to 100%, in agreement with the notion of half-metallic behavior for this material.

TT 7.7 Mon 15:30 H20

High-resolution magnetization profiles in superconducting YBCO and ferromagnetic LCMO hybrid structures at low temperatures. — S. Brück[1], •J. Albrecht[2], S. Soltan[3,4], G. Christiani[4], H.-U. Habermeier[4], P. Audehm[5], S. Macke[5], and E. Goering[5] — [1]Universität Würzburg — [2]Hochschule Aalen — [3]Helwan University, Cairo, Egypt — [4]MPI für Festkörperforschung, Stuttgart — [5]MPI für Metallforschung, Stuttgart

At the interface between ferromagnetic (F) and superconducting (SC) thin films a fascinating competition of ordering parameters takes place. We have investigated a hybrid structure of $SrTiO_3$(substrate), ferromagnetic $La_{0.7}Ca_{0.3}MnO_3$ and superconducting $YBa_2Cu_3O_7$ using X-ray magnetic resonant reflectometry (XRMR) and x-ray magnetic circular dichroism (XMCD). In particular, the XRMR measurements provide element selective magnetic depth profiles of layered samples with an enhanced sensitivity for localized and or interface effects. A

temperature-dependent investigation of the resonant reflectometry at the Mn L edge in the temperature range from T=40K to T=110K was carried out and the magnetic depth profile for Mn was extracted. It can be shown that both the interaction to the adjacent YBCO layer and to the STO substrate influence the magnetization inside the LCMO layer in a particular way which will be presented in detail. The experimental findings give new insight into the physics of multilayered oxidic structures at low temperatures.

15 min. break

Invited Talk TT 7.8 Mon 16:00 H20

Polar Kerr Effect of Unconventional Superconductors — •Aharon Kapitulnik — Stanford University, Stanford, CA, USA

BCS theory of conventional superconductivity can be described by a condensate of Cooper-pairs of time-reversed states. Such superconductors respect time reversal symmetry and are insensitive to nonmagnetic scattering (the Anderson theorem). For unconventional superconductors, sign-changes in different parts of the Fermi surface results is breakdown of Anderson theorem. In addition, the higher angular momentum state gives rise to the possibility of "chiral" order parameter for which time-reversal symmetry (TRS) is broken. A series of recent studies have shown that ultra-sensitive Polar Kerr effect measurements, using a Sagnac interferometer, can detect such TRS breaking effects in unconventional superconductors [1]. For example, Sr_2RuO_4 has been shown to break TRS, and together with other measurements seem to be consistent with some variant of a "p+ip" type order parameter, while ferromagnet/superconductor bilayer structures show signatures of the "inverse proximity effect" which was long sought after following its first theoretical prediction. In this talk we will review measurements on a variety of systems including the heavy fermion URu2Si2 which has mystified researchers since in this system superconductivity occurs deep inside a mysterious "hidden order" state (whose transition temperature is approximately 17.5 K).

[1] For a recent review of our studies see: Aharon Kapitulnik, Jing Xia, Elizabeth Schemm and Alexander Palevski, New J. Phys. 11 (2009) 055060.

TT 7.9 Mon 16:30 H20

Bias-resolved measurements of charge imbalance in superconductors at ultra-low temperatures — •Florian Hübler[1,2], Julien Camirand Lemyre[1], Detlef Beckmann[1], and Hilbert von Löhneysen[2,3] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik — [3]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

In this study we explore charge imbalance in mesoscopic normal-metal/superconductor multiterminal hybrid structures at ultra-low temperatures ($T \ll T_c$). The investigated samples, structured by e-beam lithography and shadow evaporation, consist of a superconducting aluminum bar with several copper fingers forming tunnel contacts at different distances from each other. We measured in detail the local and non-local conductance of these structures as a function of the applied bias voltage V, the applied magnetic field B, the temperature T and the contact distance d. From these data the relaxation length λ_Q^* was derived. The bias-resolved measurements show a transition from dominant elastic scattering close to the gap to inelastic scattering at higher bias. We measured a strong suppression of charge imbalance with magnetic field, which can be directly linked to the pair breaking parameter. In contrast practically no temperature dependence of the charge imbalance signal was observed below 0.5K. These results are relevant for the investigation of other non-local effects such as crossed Andreev reflexion and spin diffusion.

TT 7.10 Mon 16:45 H20

Crossed Andreev Reflection and Charge Imbalance in Diffusive Normal-Superconducting-Normal Structures — •Dmitry Golubev[1], Mikhail Kalenkov[2], and Andrei Zaikin[1] — [1]Karlsruhe Institut für Technologie, Institut für Nanotechnologie, Karlsruhe, Germany — [2]I.E. Tamm Department of Theoretical Physics, P.N. Lebedev Physics Institute, Moscow, Russia

We formulate a microscopic theory of non-local electron transport in three-terminal diffusive normal-superconducting-normal (NSN) structures with arbitrary interface transmissions. At low energies ε we predict strong enhancement of non-local spectral conductance $g_{12} \propto 1/\varepsilon$ due to quantum interference of electrons in disordered N-terminals. In contrast, non-local resistance R_{12} remains smooth at small ε and, furthermore, is found to depend neither on parameters of NS interfaces nor on those of N-terminals. At higher temperatures R_{12} exhibits a peak caused by the trade-off between charge imbalance and Andreev reflection. Our results are in a good agreement with recent experimental observations and can be used for quantitative analysis of future experiments.

TT 7.11 Mon 17:00 H20

Andreev Bound States and Transport in a Kondo Quantum Dot with Superconducting Leads — •Tabea Mandt and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Despite intense theoretical efforts the nature of Andreev bound states and the resulting Josephson current in a Kondo dot coupled to two symmetric s-wave superconductors has remained controversial. We investigate the temperature- and coupling-dependent spectral and transport properties of this system using an extension of the infinite-U non-crossing approximation (NCA) to describe superconducting leads. Using a conserving approximation (generating functional), we extend previous selfconsistent calculations [1] to include multiple Andreev-reflections by summing up the infinite series of ladder diagrams in the relevant anomalous channel (Cooper pair exchange) of the quantum dot Green's function. The *infinite* number of Andreev reflections is necessary to describe true bound states and, hence, to answer the open problems about the number of bound states and, possibly, their spectral width. For the evaluation, the summation is efficiently formulated in terms of coupled Bethe-Salpeter equations for the renormalized pseudoparticle vertices, which can be decoupled due to a separation of energy scales. The phase diagram of the junction and the Josephson current–phase relation are established and related to the phase-dependent position of the subgap bound states.

[1] G. Sellier, Th. Kopp, J. Kroha, Y. S. Barash, Phys. Rev. B **72**, 174502 (2005).

TT 7.12 Mon 17:15 H20

Pure spin current with interacting quantum dots — •David Futterer[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg Essen and CeNIDE, D-47048 Duisburg, Germany — [2]School of Chemical and Physical Sciences, Victoria University of Wellington, PO Box 600, Wellington, New Zealand

We investigate sub-gap transport through an interacting quantum dot tunnel coupled to a superconducting, a ferromagnetic and a normal conducting lead. Despite the tendency of a large charging energy to suppress the equilibrium proximity effect on the dot, a finite Andreev current can be achieved in non-equilibrium situations. Due to the coupling to a ferromagnet, spin can accumulate on the dot. We find situations in which a pure spin current, that is zero charge current together with a finite spin current, occurs in the normal lead. For our calculation we apply a real-time transport theory [1,2].

[1] M. G. Pala, M. Governale, and J. König, New J. Phys. **9**, 278 (2007).

[2] M. Governale, M. G. Pala, and J. König, Phys. Rev. B **77**, 134513 (2008).

TT 7.13 Mon 17:30 H20

Spin-controlled supercurrents in quantum-dot spin valves with a superconducting lead — •Björn Sothmann[1], David Futterer[1], Michele Governale[2], and Jürgen König[1] — [1]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

Quantum dots coupled to ferromagnetic [1] or superconducting [2] electrodes exhibit interesting effects due to an interplay of strong Coulomb interaction, superconducting proximity effect and nonequilibrium spin accumulation as well as spin precession.

Here we investigate a quantum-dot spin valve, i.e., a single-level quantum dot coupled to two ferromagnetic leads with symmetrically applied bias, with an additional superconducting lead at zero chemical potential. Using a real-time diagrammatic approach [1,2] we compute the current taking into account the coupling to the superconductor exactly in the limit of infinite pair potential. For a symmetric coupling to the ferromagnets, the current into the superconductor vanishes in collinear geometries due to a combination of particle-hole and left-right symmetry. A finite supercurrent arises only for noncollinear magnetizations in the intermediate bias regime due to a breaking of the left-right symmetry by the spin accumulation. Due to the presence of an

exchange field, the supercurrent shows a nontrivial bias dependence and can even change sign.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B. **70** (2004).
[2] M. Governale, M. Pala, J. König, Phys. Rev. B. **77** (2008).

TT 7.14 Mon 17:45 H20

The Josephson light-emitting diode — •Patrik Recher[1], Yuli Nazarov[2], and Leo Kouwenhoven[2] — [1]Institut für Theoretische Physik und Astrophysik, University of Würzburg, 97074 Würzburg, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands

We consider an optical quantum dot where an electron level and a hole level are coupled to respective superconducting leads. We find that electrons and holes recombine producing photons at discrete energies as well as a continuous tail. Further, the spectral lines directly probe the induced superconducting correlations on the dot. At energies close to the applied bias voltage $eV_{\rm sd}$, a parameter range exists, where radiation proceeds in pairwise emission of polarization correlated photons. At energies close to $2eV_{\rm sd}$, emitted photons are associated with Cooper pair transfer and are reminiscent of Josephson radiation. We discuss how to probe the coherence of these photons in a SQUID geometry via single photon interference.

TT 8: CE: (General) Theory

Time: Monday 14:00–17:45 Location: H21

TT 8.1 Mon 14:00 H21

Quantum Simulations of Exotic Spin Models — •Hendrik Weimer[1], Markus Müller[2], Igor Lesanovsky[3], Peter Zoller[2], and Hans Peter Büchler[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart — [2]Institut für Theoretische Physik, Universität Innsbruck, und Institut für Quantenoptik und Quanteninformation der Österreichischen Akademie der Wissenschaften, Innsbruck — [3]School of Physics and Astronomy, The University of Nottingham

A universal quantum simulator is a controlled quantum device which efficiently reproduces the dynamics of any other many particle quantum system with short range interactions. Based on a recent proposal for a many-body with cold Rydberg atoms [1], we present an implementation of a digital quantum simulator [2]. Special focus is on the efficient simulation of Hamiltonians with local many-body interactions, including exotic spin models such as Kitaev's toric code, string nets, and lattice gauge theories. In addition, we show that the formalism also provides the simulation of dissipative terms taking the Lindblad form with many-body jump operators. These dissipative terms allow for the efficient ground state cooling and state preparation.

[1] M. Müller et al., Phys. Rev. Lett. **102**, 170502 (2009).
[2] H. Weimer et al., arXiv:0907.1657 (2009).

TT 8.2 Mon 14:15 H21

A model of charge fractionalization on the kagome lattice — •Aroon O'Brien[1], Frank Pollmann[2], Nic Shannon[3], and Peter Fulde[1,4] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [2]University of California, Berkeley, CA94720, USA — [3]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, BS8-1TL, UK — [4]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Geometrically frustrated models exhibit many fascinating physical properties, one of which is the possible existence of fractionally charged excitations [1]. Such excitations may arise here as a consequence of the frustrated electronic interactions [2]. We have investigated a model of spinless fermions on the 2D kagome lattice, for which fractionally charged excitations occur in the limit of strong correlations at 1/3 filling. Here we present results for the dynamical properties of the fractional charges, as revealed by numerically calculated spectral functions. Particular focus is given to the signatures of fractional confined collective excitations observed in these spectra [3]. Recently a scheme for a quantum simulation of this model using cold atoms was proposed; we relate this to numerically calculated quantities that we argue may be measurable in optical lattice experiments [4].

[1] P. Fulde, K. Penc, N. Shannon, Ann. Phys., **11**, 892 (2002).
[2] F. Pollmann and P. Fulde, Europhys. Lett., **75**, 133 (2006).
[3] A. O'Brien, F. Pollmann and P. Fulde, to be submitted.
[4] J. Ruostekoski, Phys. Rev. Lett., **103**, 080406 (2009); J. Ruostekoski and N. Shannon, in preparation.

TT 8.3 Mon 14:30 H21

Groundstatable fermionic wavefunctions and their associated many-body Hamiltonians — •Daniel Charrier[1] and Claudio Chamon[2] — [1]Max Planck Institut für Physikkomplexer Systeme, Nöthnitzer Straße38, 01187 Dresden, Germany — [2]Physics Department, Boston University, Boston, MA

In the vast majority of many-body problems, it is the kinetic energy part of the Hamiltonian that is best known microscopically, and it is the detailed form of the interactions between the particles, the potential energy term, that is harder to determine from first principles. An example is the case of high temperature superconductors: while a tight-binding model captures the kinetic term, it is not clear that there is superconductivity with only an onsite repulsion and, thus, that the problem is accurately described by the Hubbard model alone. Here we pose the question of whether, once the kinetic energy is fixed, a candidate ground state is groundstatable or not. The easiness to answer this question is strongly related to the presence or the absence of a sign problem in the system. When groundstatability is satisfied, it is simple to obtain the potential energy that will lead to such a ground state. As a concrete case study, we apply these ideas to different fermionic wavefunctions with superconductive or spin-density wave correlations.

TT 8.4 Mon 14:45 H21

Instabilities of quadratic band crossing points — •Stefan Uebelacker[1] and Carsten Honerkamp[2] — [1]University of Würzburg — [2]RWTH Aachen

The variation of the orbital composition of bands around band crossing points near the Fermi level can generate interesting effects. In particular, rather simple interactions can give rise to the spontaneous formation of topological insulating phases (S. Raghu et al., Phys. Rev. Lett. **100**, 156401 (2008)). In contrast with Dirac points, quadratic band crossing points offer the advantage of a nonzero density of states at the crossing point, and instabilities occur already at small interaction strengths. Here, we present our results of functional renormalization group calculations for models with one and two quadratic band crossing points and discuss the possibilities for nontrivial insulating phases induced by local interactions.

TT 8.5 Mon 15:00 H21

Electron-plasmon scattering in chiral 1D systems with nonlinear dispersion — Markus Heyl, Stefan Kehrein, Florian Marquardt, and •Clemens Neuenhahn — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics,Center for NanoScience, Ludwig Maximilians Universität München, Munich, Germany

We investigate systems of spinless one dimensional chiral electron systems occuring, e.g., in the arms of electronic Mach-Zehnder interferometers. We take into account both the curvature of the fermionic spectrum and a finite interaction range. The main observation is that due to an interplay of both, an injected high-energy fermion will scatter off plasmons (density variations) leading to an exponential decay of the single particle Green's function (GF) on top of the expected power-law decay even at zero temperature. Remarkably, it turns out that this happens in a coherent fashion, such that a monochromatic sinusoidal density pattern builds up. While one dimensional fermionic systems with linear dispersion relation are described perfectly well by means of bosonizing the system, introducing a finite curvature requires alternative techniques. Here a semiclassical ansatz for the GF is employed whose validity in the low-energy regime was shown earlier [1] and which is extended naturally. Additionally, we make use of a slightly modified version of the method proposed in [2].

[1] C.Neuenhahn and F. Marquardt, PRL 102, 046806 (2009)
[2] M.Pustilnik et al, PRL 96, 196405 (2006)

TT 8.6 Mon 15:15 H21

Fermi-edge singularity in a quantum dot — •Markus Heyl and Stefan Kehrein — Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 München

We investigate the Fermi-edge singularity problem realized in a non-interacting quantum dot. An appropriately tuned laser beam incident on the dot suddenly switches on the hybridization of a dot level with the conduction band electrons. Based on recently developed methods [1], we analytically calculate the exponent of the singularity in the absorption spectrum near the threshold and extend known analytical results [2,3] to the whole parameter regime. Furthermore, we point out that the exponent of the Fermi-edge singularity in the anisotropic Kondo model depends on anisotropy.

[1] N. d'Ambrumenil and B. A. Muzykantskii, Phys. Rev. B **71**, 045326 (2005).

[2] A. Kontani and Y. Toyozawa, J. Phys. Soc. Jpn. **35**, 1073 (1973).

[3] T. Kita, K. Ohtaka and Y. Tanabe, J. Phys. Soc. Jpn. **56**, 4609 (1987).

TT 8.7 Mon 15:30 H21

Dynamical Vertex Approximation for nanosystems — •Angelo Valli, Giorgio Sangiovanni, and Karsten Held — Institut für Festkörperphysik, TU Wien

In the spirit of Dynamical Vertex Approximation (DΓA), we propose a computational approach which assumes the locality of the n-particle fully irreducible vertex to treat nanoscopic systems. To test the reliability of our scheme, we compare it in its simplest version (n=1) to numerically exact Quantum Monte Carlo for a multi-site Anderson Impurity Model when the number of correlated atoms is small. We focus on quantities like electronic spectra and double occupancies and compare them to alternative methods [1]. The nanoscopic DΓA has the advantage that the simulation of a much larger number of coupled nanosystems is possible than for the exact solution, e.g., an ensemble of coupled quantum dots, macromolecules, or a cluster of ad atoms on surfaces.

[1] S. Florens, PRL99, 046402 (2007)

15 min. break

TT 8.8 Mon 16:00 H21

Critical exponents and phase diagram of the Hubbard model — •Karsten Held[1], Alessandro Toschi[1], Georg Rohringer[1], and Andrey Katanin[2,3] — [1]Institute of solid state physics, Vienna University of Technology — [2]Max-Planck-Insitut für Festkörperphysik, Stuttgart — [3]Institute of metal physics, Ekaterinburg

Despite being the prototype for strongly correlated electron systems, an accurate calculation of the critical behavior of the Hubbard model was hitherto not possible. With the recently developed dynamical vertex approximation (DΓA) [1], we are finally able to include non-local correlations beyond dynamical mean field theory (DMFT) in a systematic way - on all length scales. In two dimensions, this results in a reduction of the antiferromagnetic transition temperature to $T_N = 0$ [2], in agreement with the Mermin-Wagner theorem. In three dimensions, we get a non-mean-field critical behavior, in contrast to DMFT. It agrees, at least for half filling and large Coulomb repulsion, with the Heisenberg critical exponents.

By means of DΓA, we are also able to estimate the error of DMFT. In particular, we will discuss in which regions of the phase diagram a DMFT treatment is sufficient and where non-local correlations necessarily need to be included.

[1] A. Toschi, A. A. Katanin, K. Held, Phys. Rev. B 75, 045118 (2007).

[2] A. A. Katanin, A. Toschi, K. Held, Phys. Rev. B 80, 075104 (2009).

TT 8.9 Mon 16:15 H21

Vertex Function and Dynamical Spin-Susceptibilities from DMFT — •Andreas Dolfen and Erik Koch — German Research School for Simulation Sciences and RWTH Aachen University, Germany

DMFT providing a local approximation to the electronic self-energy readily gives one-body quantities such as the Green's function. Two-body quantities like general dynamical susceptibilities are significantly harder to obtain.

Here we describe how to evaluate spin susceptibilities from an exact diagonalization impurity solver. First we construct the two-particle Green's function of the impurity model and the corresponding local irreducible vertex function. Inserting the vertex and interacting electron propagator for the lattice model into the Bethe-Salpeter equation we obtain dynamical susceptibilities. This technique allows the direct calculation of the susceptibility on the real axis.

As example, we present results for the Periodic Anderson Model.

TT 8.10 Mon 16:30 H21

LSDA+DMFT calculations of electron phonon coupling and its combination with one step model of photoemission — •Jan Minar[1], J. Braun[1], S. Mankovskyy[1], H. Ebert[1], R. Ovsyannikov[2], H. A. Duerr[2], and J. Fink[2] — [1]Dep. Chemie und Biochemie, LMU University of Munich, Germany — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

Recent developments and improvements in the resolution of angle-resolved UPS and XPS photoemission experiments require an improved (or revised) theoretical description of the photoemission process in the framework of the one-step model. In particular, the combination of the KKR band structure method with the dynamical mean field theory (DMFT) provides a quantitative interpretation of photoemission data including all matrix elements effects. Here, we present a formalism that allows to include lattice vibrations into the one-step model. In the UPS regime electron-phonon interaction is reflected by kinks and related phenomena. Calculation of the force-constant tensor within the KKR Green's function method gives access to the k-resolved Eliashberg function and an electron-phonon self-energy. This quantity can be included into the photoemission formalism. The method has been applied to angle-resolved photoemission from Ni(111) and is compared to corresponding experimental data. In contrary to the standard interpretations we found a considerable impact on the electron-phonon self-energy due to spin-flip processes that are induced by spin-orbit coupling. We also show that inclusion of correlations effects is crucial in order to describe electron phonon coupling in Ni.

TT 8.11 Mon 16:45 H21

Influence of Coulomb repulsion on the electron-phonon interaction in high-temperature superconducting copper oxides — •Giorgio Sangiovanni[1] and Olle Gunnarsson[2] — [1]Institut für Festkörperphysik, TU Wien — [2]Max-Planck Institut für Festkörperforschung, Stuttgart

The issue of how strong is the electron-phonon interaction in cuprates and how much it influences their properties is not yet settled [1-2]. Whether or not the coupling to, for instance, oxygen bond-stretching modes is sizable cannot be established with standard tools, like those based on plain Local Density Approximation, as this neglects most of the correlation effects. As several sophisticated methods for many-body calculations are now available, it turns out instead that dynamical self-energy effects strongly influence not only the interplay between an instantaneous Coulomb repulsion and a phonon-mediated retarded attraction, but also the very bare estimate of the electron-phonon matrix elements. Using Cluster Dynamical Mean Field Theory and realistic methods beyond Local Density Approximation we can study the electron-phonon interaction in cuprates in an unbiased way.

[1] R. Heid, *et al.*, PRL **100**, 137001 (2008)

[2] D. Reznik, *el al*, Nature **455**, E6 (2008)

TT 8.12 Mon 17:00 H21

Bilayer Hubbard model for ^{3}He: a cluster dynamical mean-field calculation — K.S.D. Beach[1] and •F.F. Assaad[2] — [1]Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7 — [2]Institut für theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Inspired by recent experiments on bilayer ^{3}He, we consider a bilayer Hubbard model on a triangular lattice. For appropriate model parameters, we observe a band-selective Mott transition at a critical chemical potential, μ_c, corresponding to the solidification of the fermions in the first layer. The growth of the effective mass on the metallic side ($\mu < \mu_c$) is cut off by a first order transition in which the first layer fermions drop out of the Luttinger volume and their spin degrees of freedom become locked in a spin singlet state. These results are obtained from a cluster dynamical mean-field calculation on an eight-site cluster with a quantum Monte Carlo cluster solver.
http://xxx.lanl.gov/abs/0905.1127

TT 8.13 Mon 17:15 H21

Two-particle response functions for multi-band Hubbard models — •Ernst von Oelsen[1], Jörg Bünemann[2], and Götz Seibold[1] — [1]BTU Cottbus, Lehrstuhl für Theoretische Physik, Cottbus — [2]Philipps Universität Marburg, Fakultät für Physik, Marburg

In various studies on single-band Hubbard models, see, e.g., Ref. [1,2], the time-dependent Gutzwiller theory has been shown to be a valuable tool for the investigation of frequency and wave-vector dependent two-particle response functions. We have successfully generalised this approach for the study of arbitrary multi-band Hubbard models. With our new approach it is now possible to investigate such response functions, as e.g., the magnetic susceptibility for realistic three-dimensional multi-band models. This opens the way for a better understanding of various experimental results on systems with medium or strong Coulomb-interaction effects. In our presentation, we give a brief introduction to our theoretical approach and outline its prospects for future studies of real materials. As a first application, we show results for the magnetic susceptibility and the spin-wave properties of a two-band Hubbard model. We compare our findings with those of a Hartree-Fock based random-phase approximation, which is the standard textbook method for the calculation of two-particle response functions.

[1] G. Seibold, J. Lorenzana, PRL **94**, 107006 (2005)
[2] G. Seibold, F. Becca, J. Lorenzana, PRL **100**, 016405 (2008)

TT 8.14 Mon 17:30 H21

Lattice Density Functional Theory of the inhomogeneous Hubbard model. — •Matthieu Saubanère and G. M. Pastor — Institut für Theoretische Physik, Universität Kassel, Kassel, Germany

The inhomogeneous Hubbard Hamiltonian is investigated in the framework of lattice density functional theory (LDFT). The single-particle density-matrix γ_{ij} with respect to the lattice sites is considered as the basic variable of the many-body problem. Two new approximations to the interaction-energy functional $W[\gamma_{ij}]$ are proposed. The first one is based on the scaling properties of $W[\gamma_{ij}]$. It allows to recover the exact limit of strong correlations for the homogeneous Hubbard Hamiltonian at half band-filling. The second one is obtained by projecting the many-body ground-state on the different states with defined occupations of the atomic sites. A system of equations is then derived, from which $W[\gamma_{ij}]$ is obtained. As examples of applications we present results for the kinetic, Coulomb and total ground-state energy, charge excitation gap, and charge susceptibility of the inhomogeneous Hubbard model in one, two and three dimensional periodic lattices, as well as in small clusters. The accuracy of the method is demonstrated by comparison with available analytical and numerical exact solutions.

TT 9: SC: Poster Session

Time: Monday 14:00–18:00 Location: Poster A

TT 9.1 Mon 14:00 Poster A

Calorimetry of high-T_c superconductors at different doping levels obtained with ultrafast spectroscopy — •Martin Scheuch[1,3], Luca Perfetti[2], Tobias Kampfrath[3], Christian Frischkorn[1], and Martin Wolf[1,3] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Laboratoire des Solides Irradiés, Ecole polytechnique, 91128 Palaiseau cedex, France — [3]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

A new approach for obtaining the electronic part of the heat capacity of highly correlated electron systems is discussed. When energy is absorbed from an incident femtosecond laser pulse, it is first deposited in the electronic system of a solid and, subsequently, tranferred to the lattice. Using a THz probe pulse directly after optical excitation, before energy is transferred to the lattice, one can determine the instantaneous temperature of the electrons. This has been done for the high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$. In combination with time-domain THz spectroscopy at different sample temperatures, the equivalence of photo- and heat-induced conductivity-changes, especially regarding the phase transition, was shown. With this the electronic heat capacity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ was extracted for different doping levels δ.

TT 9.2 Mon 14:00 Poster A

Angle resolved photoemission spectroscopy (ARPES) studies on Bi2201 and Bi2223 high temperature superconductors — •Jia Wei[1,2], Martin Aeschlimann[1], and Donglai Feng[2] — [1]Department of Physics, University of Kaiserslautern, Fachbereich Physik, Erwin Sch€oodinger Str. 46, 67663 Kaiserslautern, Germany — [2]1Department of Physics, Surface Physics Laboratory (National Key Laboratory) and Advanced Materials Laboratory, Fudan University, Shanghai 200433, P. R. China

The Bismuth-family of high temperature superconductors has played a vital role in the understanding of high temperature superconductivity. For the single layer system Bi2201, We observed the symbolic superconducting coherence peak in antinodal region for the first time. The 19 meV peak dip separation seriously challenges models based on electron*phonon interactions. Meanwhile, this energy scale and temperature dependence intriguingly correlate with the behaviors of spin fluctuations. For the trilayer Bi2223 system, its underdoped (UD) regime has been largely inaccessible so far. With elaborate vacuum annealing, we have succeeded in obtaining a series of UD samples for the first time. And we have identified a new experimental energy scale in the trilayer material, caused by trilayer band splitting, which shows very different behavior for bilayer band splitting in Bi2212.

TT 9.3 Mon 14:00 Poster A

Double Photoemission from LSCO and BiSCO — •Deborah Schneider[1], Robert Wallauer[1], Stefan Voss[1], Tobias Bauer[1], Birte Ulrich[1], Markus Waitz[1], Dawiet Haile[1], Till Jahnke[1], Götz Berner[2], Amit Kanigel[3], Markus Schöffler[4], Horst Schmidt-Böcking[1], and Reinhard Dörner[1] — [1]IKF, Universität Frankfurt — [2]EP4, Universität Würzburg — [3]Technion, Haifa, Israel — [4]ALS, Berkeley, USA

We investigate the emission of two electrons by a single photon from LSCO and BiSCO surfaces. Photon energy used was between 20 and 40 eV. The experiment took place at Bessy, the synchrotron in Berlin (single bunch mode). The detection method [1] was a time of flight spectrometer with a position sensitive detector, so that we are able to calculate the full momentum of each electron.

The theory [2] predicts that the back to back correlation of Cooper pairs should be conserved in the final state. Therefore we expect to be able to distinguish the pairs from the isotropic background of scattered electron pairs. We will show a comparison of spectra obtained in the superconducting state and the normal state.

[1] M. Hattass et. al, Rev. Sci. Instr. 75, 2373 (2004)
[2] K. A. Kouzakov and J. Berakdar, Phys. Rev. Lett. 91, 257007 (2003)

TT 9.4 Mon 14:00 Poster A

Abnormal Temperature Dependence of the Itinerant Hole Density of Bi(Pb)-2201 by X-ray Absorption Spectroscopy (XAS) — •Aliakbar Ghafari, Ahmad Kamal Ariffin, Beate Müller, Rüdiger Mitdank, Helmut Dwelk, Alica Krapf, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

It has been reported recently that in $YBa_2Cu_3O_{7-\delta}$, $La_{2-x}Sr_xCuO_4$ and also double layer $Bi_2Sr_2CaCu_2O_{8-\delta}$ some ordering of charges and followed by the formation of Cooper pairs in the CuO_2 plane takes place at $T>>T_c$. In view of this, a polarized X-ray absorption study is made on single layer $Bi_{2-y}Pb_ySr_{2-x}La_xCuO_{6+\delta}$ [Bi(Pb)-2201] single crystals to investigate the temperature dependence of the itinerant hole density within the ab plane on Bi(Pb)-2201 single crystals as well. The XAS measurements were made at the CuL_3 edges by changing the temperature from room temperature (RT) to ∼10K using a liquid helium cryostat. It has been established that there is a strong dependence of itinerant hole density on temperature. This contribution will discuss the results and the possible causes of the abnormal temperature dependence of the itinerant hole density.

TT 9.5 Mon 14:00 Poster A

Static stripe ordering in underdoped Bi2201 and Bi(Pb)2201 single crystals — •Valentina Scherer, Christoph Janowitz, Beate Müller, Lenart Dudy, Alica Krapf, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

Underdoped Bi2201 and Bi(Pb)2201 single crystals with a nominal hole doping of $n_h = 1/10$ and $n_h = 1/8$ were investigated using high resolution photoemission and transport measurements. By photoemis-

sion measurements spectral functions, dispersions, and Fermi surfaces were detected that correspond to calculations of the site centered stripe model. The resistivity curves exhibit typical transitions due to spin ordering as already found in other stripe phase materials as LSCO (cite Tranquada, Phys. Rev. B 78, 174529 (2008)). Close correspondence between changes of Fermi surface features and resistivity curves is found. Thus a static site centered stripe phase ordering of charge and spin degrees of freedom is the most plausible explanation for the findings, establishing stripes as playing an important role in another class of HTC materials, namely the Bi-cuprates.

TT 9.6 Mon 14:00 Poster A

Nanostripe structures in as-grown light-rare-earth-based high-T_c superconductors — •Michael R Koblischka[1], Anjela Koblischka-Veneva[2], Miryala Muralidhar[3], Thomas Wolf[4], Nadendla Hari BAbu[5], and Uwe Hartmann[1] — [1]Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Functional Materials, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [3]Superconductivity Research Laboratory ISTEC, 1-10-13, Shinonome, Koto-ku, Tokyo, 135-0062, Japan — [4]Forschungszentrum Karlsruhe GmbH, Institute of Solid State Physics, D-76021 Karlsruhe, Germany — [5]IRC in Superconductivity, University of Cambridge, Madingley Road, Cambridge, CB3 0HE, U. K.

Nanostripes are visualized on as-grown light-rare-earth-based high-T_c superconductors by means of atomic force microscopy (AFM) and scanning tunnelling microscopy (STM) at ambient conditions. The samples investigated are non-superconducting, and hence, twin-free. Our observations of nanostripe structures in these samples directly proof that the nanostripes are formed during the growth of the 123-phase itself, whereas the twin boundaries appear in a second step during the required oxygenation of the samples. This explains the often observed features that the nanostripes are curved towards or away from the twins. Due to the different length scales, the nanostripes in the LRE-materials are filling effectively the space between the twin boundaries and provide flux pinning sites much closer to the size of the coherence length, ξ.

TT 9.7 Mon 14:00 Poster A

Relaxation behaviour of levitation forces of various thin high-T_c superconductor samples — •Michael R Koblischka, Michael Becker, Jerome Meiser, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany

We present the construction of a so-called levitation balance which is capable of measuring the levitation forces between a permanent magnet and a superconducting high-T_c thin film sample. Using this setup, we measure the relaxation behaviour of the levitation forces of different thin high-T_c samples: YBCO thin films as well as a commercial YBCO coated conductor and a piece of an Ag-sheathed Bi-2223 tape. From the relaxation curves, we obtain the pinning energies, which correspond well to the data of conventional relaxation measurements. We further show that a small movement of the sample prior to the relaxation measurement influences the relaxation behaviour drastically, so a situation with practically no relaxation effects can be generated.

TT 9.8 Mon 14:00 Poster A

Charge order in $La_{2-x}Ba_xCuO_4$ studied by resonant soft x-ray diffraction — •Eugen Weschke[1], Victor Soltwisch[1], Enrico Schierle[1], Stuart P. Wilkins[2], Jochen Geck[3], John P. Hill[2], John M. Tranquada[2], and Jörg Fink[1,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Brookhaven National Laboratory, Upton, New York, USA — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

$La_{2-x}Ba_xCuO_4$ (x = 0.125 and x = 0.115) was studied by x-ray diffraction at the O-K and the Cu-L_3 resonances, in this way focussing on the O-2p and Cu-3d electronic structure. In both cases, pronounced charge-order superstructure peaks are observed directly below the temperature of the structural transition from the LTO into the LTT phase. This is in contrast to the case of $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$, where charge order occurs at a lower temperature than the structural phase transition. Further differences between the materials are observed in the coherence lengths of the charge order, which is significantly larger in case of $La_{2-x}Ba_xCuO_4$. For the two resonances indications for a different evolution with temperature of the superstructure peaks in $La_{2-x}Ba_xCuO_4$ are found.

TT 9.9 Mon 14:00 Poster A

Out-of-plane transport properties of $YBa_2Cu_3O_7/PrBa_2Cu_3O_7$ superlattices — •Ayman El Tahan[1], Fabrizio Porrati[2], Michael Huth[2], Hermann Adrian[1], and Gerhard Jakob[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz — [2]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt

The aim is to show how a change in superlattice modulation effects the transport properties in the c-axis direction, and whether a coherent Josephson coupling between $YBa_2Cu_3O_7$ layers separated by $PrBa_2Cu_3O_7$ sheets can appear or not. The I(V)-characteristic and differential conductivity G(V)=dI(V)/dV at different temperature will be measured. For this purpose we prepared the samples by two methods. The first one by wiring a mesa structure with holes of quadratic shape and dimensions of 30μm × 30μm and 20μm × 20μm, respectively. The second one by focused-ion beam cutting of a bridge with a width 1μm. In these cases the current J will flow vertically through the $YBa_2Cu_3O_7/PrBa_2Cu_3O_7$ multilayers.

TT 9.10 Mon 14:00 Poster A

Modification of high-T_c superconducting thin films by light-ion irradiation — •Marius-Aurel Bodea[1], Johannes D. Pedarnig[1], Bernd Steiger[2], Wilhelm Markowitsch[2], and Wolfgang Lang[2] — [1]Institute of Applied Physics, Johannes Kepler University, A-4040 Linz, Austria — [2]Faculty of Physics, University of Vienna, A-1090 Vienna, Austria

Irradiation of high-temperature superconducting (HTS) $YBa_2Cu_3O_7$ (Y-123) thin films by light ions of low energy modifies the electrical and superconducting properties of layers without destroying the lattice structure of the HTS material. In situ electrical measurements reveal a strong and non-linear increase of film resistance with employed Helium ion dose (ion energy 75 keV) and a relaxation of resistance after irradiation is stopped. The resistance increase during irradiation is described by a simple resistor network model. Ex situ measurements show a substantial decrease of critical temperature T_c with increasing applied dose and a relaxation of T_c and normal state resistivity that continues for several weeks after the ion irradiation. The modification of defect density and charge carrier density of Y-123 films by light-ion irradiation is discussed. Masked ion irradiation enables to pattern Y-123 films into high-T_c superconducting and non-superconducting regions and to produce tracks of high critical current density (3 MA/cm^2 at 77 K) without removal of HTS material.

TT 9.11 Mon 14:00 Poster A

Suppression of the critical current at grain boundaries of high-temperature superconductors — •Siegfried Graser[1], Thilo Kopp[1], Jochen Mannhart[1], Raphael Gutser[1], Peter Hirschfeld[2], and Brian M. Andersen[3] — [1]Zentrum für Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg — [2]Department of Physics, University of Florida, Gainesville, FL (USA) — [3]Niels Bohr Institute, University of Copenhagen, Copenhagen (Denmark)

The interface properties of high-temperature cuprate superconductors (HTS) have been of interest for many years, and play essential roles in Josephson junctions, superconducting cables, and microwave electronics. In particular, the maximum critical current achievable in HTS wires and tapes is well known to usually be limited by the presence of grain boundaries, regions of mismatch between crystallites with misoriented crystalline axes. In studies of single, artificially fabricated grain boundaries the striking observation has been made that in a variety of HTS materials, the critical current J_c of a grain boundary junction depends exponentially on the misorientation angle. Until now microscopic understanding of this apparently universal behavior has been lacking. We present here the results of microscopic evaluations in which we construct fully 3D YBCO grain boundaries by molecular dynamics. With these structures the critical current in a *d*-wave superconductor is shown to follow an exponential reduction with grain boundary angle. We identify the build up of charge inhomogeneities to be the dominant mechanism for the suppression of the supercurrent.

TT 9.12 Mon 14:00 Poster A

Consistent description of magnetic excitations and phase diagram of high-T_c cuprates within a strong-coupling approach — Sascha Brehm[1], •Enrico Arrigoni[2], Markus Aichhorn[3], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Theoretical Physics and Computational Physics,

Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

Poster has been moved to TT 27.84.

TT 9.13 Mon 14:00 Poster A

Fabrication of MgB_2 thin films by co-sputtering — •Savio Fabretti, Patrick Thomas, Günter Reiss, and Andy Thomas — Thin Films and Physics of Nanostructures, Bielefeld University, Bielefeld, Germany

MgB_2 is an intermetallic compound with a high critical temperature of T_c=40K. The simple cristall structure, large coherence lengh and the high critical current density makes thin magnesium diboride films attractive for superconducting applications like Josephson junctions. To fabricate thin MgB_2 films, we used a magnetron co-sputtering system with a Mg and a B target respectively. The films were deposited by dc-magnetron sputtering of Mg and rf-magnetron sputtering of B at a low substrate temperature between 210°C and 260°C without a post annealing process. The differences in vacuum pressure between Mg and B make it essential that the composition ratio is controlled by different sputtering power of each target. The crystal structure was measured by X-ray diffraction and transport investigations at low temperatures were performed.

TT 9.14 Mon 14:00 Poster A

Mechanically alloyed MgB_2: Effect of the Preparation on the Properties of PIT Wires and Tapes — •Marko Herrmann[1], Wolfgang Hässler[1], Christian Rodig[1], Margitta Schubert[1], Ania Kario[1], Konstantin Nenkov[1], Bernhard Holzapfel[1], Ludwig Schultz[1], Ludwig Schmolinga[2], André Aubele[2], Bernd Sailer[2], and Klaus Schlenga[3] — [1]IFW Dresden, Dresden, Germany — [2]Bruker HTS GmbH, Development HTS, Alzenau, Germany — [3]Bruker EAS GmbH, Hanau, Germany

To face the challenge of introducing MgB_2 wires and tapes into low temperature applications, it is essential to adapt its preparation to the industrial scale. Only a reasonable interplay of ampacity and an appropriate preparation route, will lead to a widespread use of MgB_2 conductors. Mechanical alloying is an excellent technique to adjust the microstructure of the precursor powder and allows for high critical current densities in MgB_2. Due to the milling, the morphology and flowability of the powder is affected. To allow for an easy and reliable production of MgB_2 wires on the kilometre scale, it is essential to make use of a precursor which can be deformed properly within the sophisticated architecture of a conductor as required for the application. In this paper, the influence of different milling parameters on the microstructure and the superconducting properties of MgB_2 is discussed. With increasing milling energy, a refined microstructure and improved homogeneity of the powder and subsequently improved critical current densities are observed. At the same time the changing flowability of the precursor requires an appropriate wire processing.

TT 9.15 Mon 14:00 Poster A

Texture Development of Single Phase (R=Y,Ho,Lu) Rare Earth Nickel Borocarbide Thin Films onto MgO Substrates of Different Orientation and Mixed Phase ($Ho_xLu_{1-x}Ni_2B_2C$) Thin Films on MgO(110) — •Tim Niemeier, Karolin Tscharntke, Ruben Hühne, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, PF 270116, D-01171 Dresden

Epitaxial thin films of $LuNi_2B_2C$ were deposited on MgO single crystal substrates using Pulsed Laser Deposition from a stoichiometric target. For optimized deposition parameters, a sharp c-axis texture and a high quality of the superconducting phase were achieved on MgO(100) [T_c = 15.6 K] as well as on MgO(110) [T_c = 15.8 K] substrates. Residual resistivity ratios are about 12 – 13 in the unstructured samples. Before this investigation, these properties are have not been reached independently from the substrate orientation. A far higher in-plane order is observed in the MgO(110) case for the chosen deposition parameters. To understand this behaviour, comprehensive texture investigations of the grown films on both substrate types were performed to reveal the differences in the growth processes. It is assumed that the growth mode of the rare earth oxide layer, forming *in situ* at the substrate interface is responsible for the different growth characteristics. Therefore, a detailed investigation of the texture of the oxide interface is performed as well. Finally, the texture formation of epitaxially grown mixed phase films $Ho_xLu_{1-x}Ni_2B_2C$ [see TT.598] is analyzed in dependence on their deposition parameters.

TT 9.16 Mon 14:00 Poster A

Calorimetric investigations of $HoNi_2B_2C$ — •R. Beyer[1], T. Herrmannsdörfer[1], O. Ignatchik[1], D. Souptel[2], G. Behr[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institut für Festkörperforschung, IFW Dresden, 01069 Dresden, Germany

The rare-earth nickel borocarbides show an intriguing competition between magnetism and superconductivity. For $HoNi_2B_2C$, this leads to a rich phase diagram with superconducting and magnetic phase transitions. Besides these competing electronic interactions, also the nuclear magnetic moment of Holmium may influence the superconducting state due to a strong hyperfine-enhanced nuclear polarisation. In order to study this in more detail, we have performed high-resolution specific-heat measurements by use of a continuous relaxation-time method. While the superconducting transition at about 8 K results in a very small, but resolvable specific-heat feature, at lower temperatures there are at least three independent magnetic-ordering transitions. One shows a lambda-like anomaly with a small hysteresis indicating a first-order phase transition. Additionally, susceptibility measurements performed below 1K fully agree with specific heat data indicating a possible re-entrant phase transition driven by hyperfine enhanced nuclear magnetism. This work has been partially supported by EuroMagNET II.

TT 9.17 Mon 14:00 Poster A

Superconductivity in $Na_{1-x}CoO_2{\cdot}yH_2O$ thin films — •Sandra Hildebrandt[1], Philipp Komissinkiy[1], Ingo Fritsch[2], Hanns-Ulrich Habermeier[2], Peter Lemmens[3], and Lambert Alff[1] — [1]Institute for Materials Science, TU Darmstadt — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Institute for Condensed Matter Physics, TU Braunschweig

Sodium cobaltate ($Na_{1-x}CoO_2$) is a novel material with thermoelectric behavior, charge and spin ordered states dependent on the sodium content in the composition. A superconducting phase was found in water intercalated sodium cobaltate ($Na_{1-x}CoO_2{\cdot}yH_2O$) with x = 0.65 - 0.7 and y = 0.9 - 1.3. The pairing state is still under debate, but there are some indications for a spin-triplet or p-wave superconducting pairing state. First films of $Na_{1-x}CoO_2{\cdot}yH_2O$ with a superconducting transition temperature near 5 K have been successfully grown. Here we report on thin films of $Na_{1-x}CoO_2$ grown by pulsed laser deposition technique. The deposition parameters, sodium deintercalation and water intercalation conditions are tuned in order to obtain the superconducting phase. The instability of this phase might be an indication for triplet superconductivity, which is known to be affected strongly by impurities and defects.This observation is in agreement with the fact that so far also no superconducting thin films of the most famous triplet superconductor Sr_2RuO_4 have been reported.

TT 9.18 Mon 14:00 Poster A

Thin Film Deposition of the Pnictide Superconductors $LaO_{1-x}NiBi$ and $LaO_{1-x}CuBi$ using Reactive Molecular Beam Epitaxy — •Alexander Buckow, Jose Kurian, and Lambert Alff — Institut für Materialwissenschaft, TU Darmstadt, Germany

The discovery of iron-based superconductors with T_C above 50 K [1,2] has renewed the interest in the area of high-temperature superconductors. To establish the mechanism of superconductivity in this new group of superconductors, one needs high quality single crystalline and/or epitaxial thin film samples. Most attempts to grow epitaxial thin films of iron-based superconductors were by Pulsed Laser Deposition (PLD) with limited success.

Reactive Molecular Beam Epitaxy (RMBE) is not only a powerful and flexible tool for the synthesis of thin films, but also an ideal technique for the study of composition dependent properties or in the search for new compounds. Since arsenic is toxic we have grown films of the similar compounds $LaO_{1-x}NiBi$ and $LaO_{1-x}CuBi$ [3] from elemental sources on (100) MgO substrates by RMBE. Thin films were characterized by XRD, ρ – T and ICP-OES. The superconducting transition temperature of $LaO_{1-x}NiBi$ thin film is about 6 K compared to 4.4 K as reported for bulk.

[1] Kamihara *et al.*, J. Am. Chem. Soc. 130, 3296 (2008).
[2] Wang *et al.*, EPL 83, 67006 (2008).
[3] Kozhevnikov *et al.*, JETP Lett. 87, 649 (2008).

TT 9.19 Mon 14:00 Poster A

Preparation and investigation of tunnel junctions based on

ironpnictide superconductors — •Stefan Schmidt[1], Sebastian Döring[1], Veit Grosse[1], Frank Schmidl[1], Paul Seidel[1], Martin Kidszun[2], Silvia Haindl[2], Bernhard Holzapfel[2], and Ingolf Mönch[2] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

Examination of superconductor tunnel structures allows experimental proof of theoretical predictions about their superconducting properties. Especially for the new iron arsenide based superconductors those examinations are of great importance, because they lead to basic understanding of physical processes in those materials, such as determination of the energy gap and its temperature dependence.

Based on $LaO_{1-x}F_xFeAs$ thin films grown via pulsed laser deposition (PLD) on $LaAlO_3$ substrates, we prepared superconductor - normal conductor - superconductor (S-N-S) tunnel structures by using photolithography, ion beam etching as well as insulating SiO_2 layers. We present first measuring of a $LaO_{1-x}F_xFeAs$ / Au / PbIn system and discuss possibilities for further examinations, including variation of the barrier respectively covering electrode materials on this basis.

TT 9.20 Mon 14:00 Poster A

Investigation on ironarsenide superconductors for their application in Josephson junctions — •Sebastian Döring[1], Stefan Schmidt[1], Veit Grosse[1], Frank Schmidl[1], Paul Seidel[1], Martin Kidszun[2], Silvia Haindl[2], Bernhard Holzapfel[2], and Ingolf Mönch[2] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden. Germany

We investigate the possibility to produce and characterize Josephson junctions, based on new ironarsenide superconductors. Starting with $LaO_{1-x}F_xFeAs$ thin films, which were produced by pulsed laser deposition (PLD), we present structures, in which Josephson effects can be studied. Because of the technological requirements, tunnel-like structures with natural or artificial barriers seems to be best suited for such investigations. Therefore the ironarsenide base electrode and subsequently the tunnel area were structured by ion beam etching. Sputtered SiO_2 thin films were used as insulating materials. For the counter electrode, conventional superconductors (e.g. Pb, Nb) can be used. We present the first measurement on such systems.

TT 9.21 Mon 14:00 Poster A

Nernst Effect in $LaFeAsO_{1-x}F_x$ — •Agnieszka Kondrat[1], Jorge Enrique Hamann-Borrero[1], Norman Leps[1], Martin Kosmala[2], Olaf Schumann[2], Jochen Werner[1], Guenter Behr[1], Markus Braden[2], Ruediger Klingeler[1], Christian Hess[1], and Bernd Buechner[1] — [1]IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]II. Physikalisches Institut, Universitaet zu Koeln, 50937 Koeln, Germany

We report a study on electrical resistivity, thermoelectric power, Hall effect and Nernst coefficient of polycrystalline $LaFeAsO_{1-x}F_x$ in the temperature range 5-300 K and magnetic field 14 T. We show the evolution of transport properties with electron doping (F content x=0, 0.05, 0.1). The parent compound undergoes two phase transitions at the temperature around 150 K: magnetic to antiferromagnetically ordered spin density wave state and structural - from tetragonal to orthorombic crystal structure. The presence of phase transitions gives rise to changes in charge carrier scattering processes, which is reflected as profound anomalies in investigated transport properties. In the superconducting samples these two transitions are not present, nevertheless in the underdoped compound (x=0.05) we observe features reminiscent of the transitions, in particular change of slope in electrical resistivity and Nernst signal. We discuss the possibility of presence of spin fluctations, which lead to formation of SDW state in parent compound and to anomalies in transport properties in underdoped superconducting samples. At the same time the optimally doped sample (x=0.1) does not show any of these characteristic features.

TT 9.22 Mon 14:00 Poster A

Universal normal state susceptibility in iron pnictides — •Rüdiger Klingeler, Norman Leps, Christian Hess, Ulrike Stockert, Hans-Joachim Grafe, Franziska Hammerath, Guillaume Lang, Mahmoud Abdel-Hafez, Luminita Harnagea, Surjeet Singh, Sabine Wurmehl, Günter Behr, Vladislav Kataev, Igor Morozov, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany

The normal state magnetisation of iron pnctides exhibits a universal increase upon heating. In $LaFeAsO_{1-x}F_x$, both the slope and the absolute value of the susceptibility at elevated temperatures are independent on doping, irrespectively whether long range antiferromagnetic order or the non-magnetic superconducting ground state appears. Our data on LiFeAs, NaFeAs, Ba- and $Ca(Fe_{1-x}Co_x)_2As_2$ single crystals imply the generic nature of this feature. Remarkably, there is quantitative agreement of the slope well above the ground states. We present a scenario of robust local antiferromagnetic correlations persisting even in the superconducting regime of the phase diagram. In addition, we present the phase diagrams based on our specific heat, thermal expansion, μSR, magnetisation and resistivity data. In particular, our data allow to assessing the size of renormalisation effects and we discuss the particular case of LiFeAs.

TT 9.23 Mon 14:00 Poster A

Magnetic properties of $CeFeAs_{1-x}P_xO$ iron pnictides studied by muon spin relaxation — •Johannes Spehling[1], Hans-Henning Klauss[1], Hemke Maeter[1], Til Dellmann[1], Hubertus Luetkens[2], Alex Amato[2], Anton Jesche[3], Cornelius Krellner[3], and Christoph Geibel[3] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Max-Planck-Institut fürChemische Physik fester Stoffe Dresden, Germany

We have investigated the electronic phase diagram of the 1111 Fe-pnictide $CeFeAs_{1-x}P_xO$ by means of muon spin relaxation (μSR). From resistivity and magnetic susceptibility a rich variety of electronic ground states including antiferromagnetism, ferromagnetism and superconductivity is inferred. We find that the examined compounds show a strong polarization of the rare earth moments by the long range ordered iron sublattice for x <= 0.4 and independent order of the Cerium-4f moments and short range ordered iron moments for x > 0.4. The peculiar interplay of the rare earth and iron magnetic order as a function of chemical pressure is examined. We further investigated the ground state properties of the heavy fermion system CeFePO.

TT 9.24 Mon 14:00 Poster A

Electrodynamics of electron doped iron-pnictide superconductors $Ba(Fe_{1-x}M_x)_2As_2$ — •Dan Wu[1], Neven Barisic[1], Natalia Drichko[1], Boris Gorshunov[1], Philipp Kallina[1], Martin Dressel[1], Linjun Li[2], Xiao Lin[2], Guanghan Cao[2], and Zhu-an Xu[2] — [1]1. Physikalisches Institut, Universiät Stuttgart, Germany — [2]Department of Physics, Zhejiang University, People's Republic of China

The temperature dependence of the *ab*-plane optical reflectivity of $Ba(Fe_{0.92}Co_{0.08})_2As_2$ and $Ba(Fe_{0.95}Ni_{0.05})_2As_2$ single crystals is measured in a wide spectral range. In the metallic state, the optical conductivity consists of a broad incoherent background and a narrow Drude-like component which determines the transport properties; only the latter contribution strongly depends on the composition and temperature. Upon entering the superconducting regime, the conductivity below 100 cm^{-1} drops due to the complete opening a gap in the density of states at $2\Delta/k_BT_c \approx 2.5-3$. From the analysis of the complex conductivity spectra we obtain the penetration depth $\lambda = (3500 \pm 350)$ Å for $Ba(Fe_{0.92}Co_{0.08})_2As_2$ and (3000 ± 300) Å for $Ba(Fe_{0.95}Ni_{0.05})_2As_2$. The calculated superfluid density ρ_s of both compounds nicely fits the scaling relation $\rho_s = (125 \pm 25)\sigma_{dc}T_c$.

TT 9.25 Mon 14:00 Poster A

Investiagtion of $A Fe_2As_2$ – compounds by means of x-ray spectroscopy — •Anna Buling[1], Ernst Kurmaev[2], J. A. McLeod[3], Alexander Moewes[3], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]Institute of Metal Physics, Russian Academy of Sciences-Ural Division, 620219 Yekaterinburg, Russia — [3]Department of Physics and Engineering Physics, University of Saskatchewan, 116 Science Place, Saskatoon, Saskatchewan, Canada S7N 5E2

The discovery of superconductivity in FeAs – compounds gives rise to a high advance in the research of high – temperature superconductors. Shortly after finding superconductivity in the rare – earth compounds (*RE*OFeAs, *RE*=rare-earth) further compounds with Fe_2As_2 layers were discribed.

Different compounds of the new superconductor family AFe_2As_2 (A= Ba, Ca) were investigated by means of x-ray spectroscopy. On the basis of XPS Fe 2*p* core level spectra of doped and undoped compounds

we discuss the Fe 3*d* electrons to be not strongly but weakly or at most moderatly correlated. The valence band spectra show that the Fermi level is dominated by the Fe 3*d* states. The influence of doping of the host material with different metals is determined and offers new results in the superconducting behavior of these compounds.

TT 9.26 Mon 14:00 Poster A

Phase diagram of $Ca(Fe_{1-x}Co_x)_2As_2$ single crystals — •Mahmoud Abdel-Hafez, Luminita Harnagea, Surjeet Singh, Norman Leps, Liran Wang, Gerd Friemel, Ulrike Stockert, Sabine Wurmehl, Günter Behr, Christian Hess, Rüdiger Klingeler, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany

We present specific heat, thermal expansion and magnetization data on $Ca(Fe_{1-x}Co_x)_2As_2$ single crystals grown from Sn-flux with $0 \leq x \leq 0.2$. From our measurements we determine the phase diagram depicting the doping dependence of the structural/magnetic and superconducting transition temperatures. With increasing Co doping, the simultaneous first-order structural/magnetic transition at $T_0 = 170$ K of pristine $CaFe_2As_2$ is suppressed and superconductivity for $x \geq 0.045$ emerges. The optimal doping level was found to be $x_0 \sim 0.065$. Below and above this value, the superconducting volume fraction diminishes rapidly. In contrast, the onset T_c remains rather unchanged for $x < x_0$ but decreases slowly to 10 K in the overdoped region of the phase diagram. These observations are discussed in the light of recent studies which show extreme pressure sensitivity of $CaFe_2As_2$ with a pressure induced T_c of 10 K.

TT 9.27 Mon 14:00 Poster A

Local visualization of the disordered vortex lattice in overdoped $BaFe_{2-x}Co_xAs_2$ superconductor — •Henry Stopfel[1], Tetyana Shapoval[1], Dmytro S. Inosov[2], Volker Neu[1], Ulrike Wolff[1], Silvia Haindl[1], Konstantin Nenkov[1], Bernhard Holzapfel[1], Ji Tae Park[2], Dunlu L. Sun[2], Chengtian T. Lin[2], Vladimir Hinkov[2], and Ludwig Schultz[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Using low temperature magnetic force microscopy (MFM) we imaged the vortex distribution in a slightly overdoped $BaFe_{2-x}Co_xAs_2$ ($x = 0.19, T_c = 23$ K) superconducting single crystal [1]. Our local method reveals that at low fields (3 mT und 6 mT) the superconducting flux lines arrange in a vortex glass phase with only a short-range order. This denotes a presence of pinning centres which prohibit a formation of the ordered Abrikosov lattice. From the statistical processing of MFM data we have extracted the radial correlation length ζ of the vortex lattice and have established the hexagonal local lattice symmetry. It reveals that the visualized vortex distribution can be treated as a disordered triangular lattice. Moreover, the isothermal magnetization loops measured at various temperatures in a wide field range up to 14 T exhibit the "fishtail" effect that is known to be related to the vortex pinning and to the crossover between two different regimes of the vortex lattice.

[1] D. S. Inosov, T. Shapoval, V. Neu, *et al.*, arXiv:0911.1971v1 (2009).

TT 9.28 Mon 14:00 Poster A

Transport studies on 122 Iron Arsenide superconductors — •Gerd Friemel, Saicharan Aswartham, Luminita Harnagea, Surjeet Singh, Norman Leps, Mahmoud Abdel-Hafez, Ulrike Stockert, Günter Behr, Christian Hess, Rüdiger Klingeler, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Germany

We present the transport properties of $Ca(Fe_{1-x}Co_x)_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals. In particular, we develop an electronic phase diagram for $Ca(Fe_{1-x}Co_x)_2As_2$, supported by measurements of magnetization and heat capacity. Our data reveal, that bulk superconductivity exists only in a very narrow doping range. Furthermore, we discuss the impact of different doping schemes on the electronic transport in pnictide superconductors.

TT 9.29 Mon 14:00 Poster A

Superconductivity and magnetism in $Eu_{1-x}K_xFe_2(As_{1-y}P_y)_2$ — •Jannis Maiwald, Hirale S. Jeevan, and Philipp Gegenwart — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany

We report on a detailed investigation of superconductivity and magnetism in $EuFe_2As_2$ by doping of K and P. In this new class of FeAs-based superconductors it is found that superconductivity appears close to a magnetic instability, suggesting a possible unconventional pairing mechanism.

We have synthesized single crystals and powder samples of both doped and undoped samples of $EuFe_2As_2$ and investigated their physical properties, by means of heat capacity, resistivity, magnetization, thermal conductivity and seebeck-coefficient measurements. The parent compound shows an antiferromagnetic spin-density-wave accompanied by a structural transition (T_{SDW}) at $\approx$ 190K related to the Fe_2As_2 layers and magnetic ordering of Eu^{2+} (T_N) moments at $\approx$ 20K. Upon doping Eu with K >30%, T_{SDW} and T_N get suppressed and superconductivity appears at $\approx$ 32K. On the other hand P doping to the As site also suppresses the SDW transition and leads to a superconducting phase. However in the latter case the Eu transition temperature remains undisturbed. With further increased P doping the Eu order changes from AFM to FM. We will mainly discuss the thermal conductivity measurements of P and K doped samples.

TT 9.30 Mon 14:00 Poster A

Possible Mechanism of Small Magnetic Moment in Iron Pnictides — Hunpyo Lee, •Yu-Zhong Zhang, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The experimentally observed small iron magnetic moment in undoped iron pnictides at low temperatures is still not well understood. We propose that the interplay between frustrated and non-frustrated bands could be the origin for the antiferromagnetic metallic state with small magnetization. Our theory is free of assumptions, like, negative U, effective pressure or localization. The proposal is verified by using dynamical mean field theory combined with the continuous time quantum Monte Carlo method to solve a two-band frustrated Hubbard model without artificially ignoring the antiferromagnetic solution. Furthermore, interesting phenomena, like orbital selective metal-to-insulator transitions, are carefully investigated.

TT 9.31 Mon 14:00 Poster A

Electronic dispersion anomalies in Fe-pnictide superconductors — •Andreas Heimes[1], Roland Grein[1,2], Matthias Eschrig[1,2,3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]DFG Forschungszentrum Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [3]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We investigate anomalies in the electronic band dispersion in Fe-pnictides that result from a coupling of electrons to spin fluctuations. It is known from inelastic neutron scattering experiments that a magnetic resonance feature appears in the dynamical spin susceptibility when entering the superconducting state, both in Fe-pnictides and in cuprates. This raises the question, if similar mechanisms are at work. An important question related to this is to which extend the dispersion of the electronic bands is modified by the interaction between electrons and this resonant spin excitation, similarly as it is the case for cuprate superconductors. We present a theoretical study of this problem.

TT 9.32 Mon 14:00 Poster A

Gauge modes in non-centrosymmetric superconductors — •Ludwig Klam[1], Dietrich Einzel[2], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, D-8548 Garching

It is well-known, that the broken gauge symmetry characterizing the ground state of conventional BCS-superconductors is reflected in the existence of a gapless collective mode, the so-called Anderson-Bogoliubov or *gauge mode*. Besides other possible collective mode excitations, it is the gauge mode, that exists also in unconventional superconductors, which can be described by order parameters with more than two components. In this contribution, we investigate the structure and the role of the gauge mode in a class of superconductors without inversion center. In these so-called non-centrosymmetric superconductors (NCS), a parity violating antisymmetric spin-orbit coupling (ASOC) gives rise to a band splitting and causes the possible coexistence of singlet and triplet contributions to the superconducting order parameter. Using the Nambu kinetic equation approach, we

present a comprehensive analysis of the gauge mode in NCS. Particular emphasis will be on (i) its ultimate necessity for the existence of the charge conservation law and (ii) the prediction of a splitting of the gauge mode into two branches, located on the two bands, with increasing strength of the ASOC.

TT 9.33 Mon 14:00 Poster A

Transition to a single-sheet Fermi surface in bulk nickelates and in $LaNiO_3/LaAlO_3$ Heterostructures — Philipp Hansmann[1,2], •Alessandro Toschi[1], Xiaoping Yang[2], Giniyat Khaliullin[2], Ryotaro Arita[3], Ole K. Andersen[2], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Department of Applied Physics, Universtity of Tokyo

The possibility of finding bulk nickelates with an electronic structure analogous to that of high temperature cuprate superconductors was considered a while ago [1]. For the systems available at that time the results were not encouraging so the idea was discarded. However, nowadays, due to new experimental techniques, heterostructures can be engineered offering new possibilities for actual material design. Using the local density approximation and its combination with dynamical mean field theory (LDA+DMFT), we compare the transition to a single sheet (cuprate-like) Fermi surface induced by the strong electronic correlation in bulk nickelates and in $LaNiO_3/LaAlO_3$ Heterostructures [2].

[1] V.I. Anisimov et al., Phys. Rev.B **59**, 7901 (1999).
[2] P. Hansmann et al., Phys. Rev. Lett. **103**, 016401 (2009).

TT 9.34 Mon 14:00 Poster A

De Haas-van Alphen (dHvA) study of the isostructural compounds $YbCoIn_5$ and $LuCoIn_5$ — •A. Polyakov[1], O. Ignatchik[1], M. Bartkowiak[1], A. Bianchi[2], B. Prevost[2], G. Seyfarth[2], Z. Fisk[3], D. Hurt[3], R.G. Goodrich[4], E.S. Choi[5], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, Dresden, Germany — [2]Department of Physics, University of Montreal, Canada — [3]Department of Physics and Astronomy, University of California, Irvine (CA), USA — [4]Department of Physics, George Washington University, Washington (DC), USA — [5]National High Magnetic Field Laboratory, Tallahassee (FL), USA

The intermetallic compounds $R\mathrm{In}_3$ and $RT\mathrm{In}_5$ (R = rare earth, T = transition metal) have attracted great interest for their large variety of anomalous ground states. Among these are the well-known heavy-fermion superconductors $CeCoIn_5$ and $CeIrIn_5$. We present here a dHvA study of $YbCoIn_5$ and $LuCoIn_5$, performed by use of a capacitive torque cantilever technique at temperatures down to 0.4 K in magnetic fields up to 13 T. In addition, one single crystal of $LuCoIn_5$ has been measured in magnetic field up to 34 T. Besides their angular-dependent Fermi-surface topologies, we have also determined the effective masses of the different bands by following the temperature-dependent amplitude changes of the dHvA oscillations. A large number of different dHvA frequencies has been observed for the main crystallographic directions. In contrast to $CeCoIn_5$ and $CeIrIn_5$, the cyclotron effective masses for these compounds are in the range from 0.7 to 2.0 m_0.
Work supported in part by EuroMagNET, EU contract No. 228043.

TT 9.35 Mon 14:00 Poster A

Low-temperature thermal expansion of URhGe — •Sebastian Zaum[1,2], Frédéric Hardy[1], Kai Grube[1], Roland Schäfer[1], Christoph Meingast[1], Hilbert v. Löhneysen[1,2], Dai Aoki[3], and Jacques Flouquet[3] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe, Germany — [3]Commissariat à l'Énergie Atomique, INAC, SPSMS, 17 rue des Martyrs, 38054 Grenoble, France

URhGe is one of the few ferromagnetic superconductors. At ambient pressure, it exhibits superconductivity with an upper critical field of $B_{c2}^{\parallel b} \approx 2$ T. A characteristic feature of these superconductors is their strong magnetic anisotropy. In URhGe, the magnetic field can be used to tune the system to a metamagnetic transition where the magnetic moment reveals a sudden rotation in the crystallographic bc plane and superconductivity reappears at a magnetic field of $B \approx 12$ T with $B \parallel b$. To study the anisotropic coupling of ferromagnetism and superconductivity to the crystal lattice, we performed thermal expansion measurements of a URhGe crystal in the temperature range 30 mK $< T <$ 15 K and in magnetic fields up to 14 T. At $B = 0$, the measurements show the ferromagnetic transition at $T_C \approx 10$ K and confirm bulk superconductivity below $T_{sc} \approx 0.2$ K. The field dependence of the thermal expansion and first results of the uniaxial pressure dependences of T_{sc} will be presented and discussed in comparison with related U-based superconductors.

TT 9.36 Mon 14:00 Poster A

Superconducting Phase Diagram of $Rh_{17}S_{15}$ — •M. Uhlarz[1], O. Ignatchik[1], J. Wosnitza[1,3], R. Daou[2], M. Doerr[3], A. Haase[1,3], H.R. Naren[4], A. Thamizhavel[4], and S. Ramakrishnan[4] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, 01314 Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [4]Tata Institute of Fundamental Research, Mumbai-400005, India

$Rh_{17}S_{15}$ is a 4*d*-electron metal which becomes superconducting below $T_c = 5.4$ K at zero field. The upper critical field is 19.2 T at $T = 0.07$ K. Above T_c, $Rh_{17}S_{15}$ is a paramagnet. The crystallographic structure (Pm3m) of $Rh_{17}S_{15}$ features a nearest-neighbor Rh-Rh distance even less than in elementary (fcc) Rh, possibly resulting in a high density of 4*d*-electron states at the Fermi level.

Using a polycrystalline sample, we measured the specific heat, resistivity, magnetisation, and magnetostriction in fields up to 14 T as well as the magnetic susceptibility in fields up to 20 T. Our data allow us to present the complete superconducting phase diagram. The assumption of narrow 4*d* band states (and thus of strong electronic correlations not providing magnetic correlations) is supported by the moderately enhanced electronic contribution to the specific heat of 107 mJ/molK^2 and favors the existence of a strong superconducting interaction. Together with the remarkably high upper critical field (exceeding the Pauli limit by a factor of two), our findings make $Rh_{17}S_{15}$ a likely candidate for unconventional superconductivity.

TT 9.37 Mon 14:00 Poster A

Surface induced superconductivity of Bi nanowires? — T. Kaupp[1,2], T.W. Cornelius[3], R. Neumann[3], •T. Peichl[1], and G. Weiss[1,2] — [1]Physikalisches Institut — [2]Centrum für funktionelle Nanostrukturen, KIT 76128 Karlsruhe — [3]GSI Darmstadt

Owing to its large Fermi wavelength and very long mean free paths, Bi is a fascinating metal for studies of transport phenomena in samples of reduced dimensions. Previous experiments explored the influence of the wire diameter on the resistance and the magnetoresistance in a wide temperature range above 1 K. Here, we present to our knowledge for the first time transport measurements below 1 K of crystalline Bi wires with diameters in the 100 nm range. At temperatures below about 0.3 K we find a remarkable decrease of the sample resistances and related effects of an external magnetic field. At first glance, some of our measurements are reminiscent of weak localization. By considering the observed conductance variations of up to 600 e^2/h this can be ruled out after all. Although the measurements suggest that the band structure of our wires are close to that of bulk crystalline Bi, which is not superconducting, one might speculate whether surface states can change the electronic structure in favor of superconductivity.

TT 9.38 Mon 14:00 Poster A

Charge Transport through One-dimensional Arrays of Small Capacitance Josephson Junctions — •Jochen Zimmer, Hannes Rotzinger, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology

We investigate one-dimensional arrays of small capacitance Josephson junctions fabricated by conventional e-beam lithography techniques. The arrays are designed to operate in the vicinity of the Coulomb blockade regime. It has been suggested that charges propagate though these arrays in a form similar to solitary waves, following the sine-Gordon model. This system is dual to a long Josephson junction, in which magnetic flux solitons have been thoroughly investigated in the past. Localized charge excitations are of metrological interest because they might offer access to very accurate frequency-to-current conversion. Although previous experiments appear consistent with the existence of solitary charge transport, conclusive evidence is still missing. We present our recent fabrication and measurement results obtained at millikelvin temperatures.

TT 9.39 Mon 14:00 Poster A

Numerical analysis of small charge solitons in 1D arrays of Josephson junctions — •Jens Homfeld, Alexander Shnirman, and Ivan Protopopov — Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruhe Insti-

tute of Technology, 76128 Karlsruhe, Deutschland

We investigate numerically a one-dimensional array of Josephson junctions in the regime of small charge solitons, $\Lambda E_J > E_C > E_J$. Here E_C and E_J are the charging and the Josephson energies of the junction, respectivly, and Λ is the bare screening length (measured in number of junctions). Our investigation is based on the many-body tight binding approach developed in Ref. [1]. We have developed an efficient algebraic method which allowed us to take into account many charge states and confirm the observations of Ref. [1], namely i) the flattening of the dispersion relation in the outer region of the Brillouin zone; ii) the broadening of the soliton in the flat band regime.

[1] S. Rachel and A. Shnirman, Phys. Rev. B 80, 180508(R) (2009).

TT 9.40 Mon 14:00 Poster A

Simulation of the I-V characteristics of short arrays of small Josephson junctions — •Felix Maibaum and Alexander Zorin — Physikalisch-Technische Bundesanstalt Braunschweig

Small single Josephson junctions and short serial arrays of these elements whith comparable charging- and Josephson energies can exhibit constant-current steps in their I-V characteristics when an AC signal is applied. This effect is due to phase locking of the Bloch oscillations associated with coherent tunneling of single Cooper pairs and is in many ways dual to the Shapiro steps, which appear at a constant voltage in arrays of larger junctions. To observe the current steps, the circuit needs to be embedded in a high-impedance environment, with an impedance significantly larger than the resistance quantum at the characteristic frequencies of the system. Such an impedance can be provided by high-ohmic on-chip thin-film resistors. Stray capacitances of these resistors will in reality result in a frequency-dependent impedance of the environment. We have performed circuit simulations to evaluate the influence of different electromagnetic environments on the step size as well as optimized the delivery of the AC drive. We have also examined the influence of noise in the on-chip resistors on the shape of the steps which can be observed in this system.

TT 9.41 Mon 14:00 Poster A

Critical disorder effects in Josephson-coupled quasi-one-dimensional superconductors — •Enver Nakhmedov and Reinhold Oppermann — Institut für Theoretische Physik, Universität Würzburg, D-97074 Würzburg, Germany

Effects of non-magnetic randomness on the critical temperature T_c and diamagnetism are studied in a class of quasi-one dimensional superconductors. The energy of Josephson-coupling between wires is considered to be random, which is typical for dirty organic superconductors. We show that this randomness destroys phase coherence between the wires and T_c vanishes discontinuously when the randomness reaches a critical value. The parallel and transverse components of the penetration depth are found to diverge at different critical temperatures $T_c^{(1)}$ and T_c, which correspond to pair-breaking and phase-coherence breaking. The interplay between disorder and quantum phase fluctuations results in quantum critical behavior at $T = 0$, manifesting itself as a superconducting-normal metal phase transition of first-order at a critical disorder strength.

TT 9.42 Mon 14:00 Poster A

Surface superconductivity controlled by electric field — •Klaus Morawetz[1,2], Pavel Lipavský[3,4], and Jan Kolaček[4] — [1]University of Applied Science Münster, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Center for Condensed Matter Physics, Universidade de Brasília, 70904-910, Brasília-DF, Brazil — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic

We discuss an effect of the electrostatic field on superconductivity near the surface. First, we use the microscopic theory of de Gennes to show that the electric field changes the boundary condition for the Ginzburg-Landau function. Second, the effect of the electric field is evaluated in the vicinity of H_{c3}, where the boundary condition plays a crucial role.We predict that the field effect on the surface superconductivity leads to a discontinuity of the magnetocapacitance. We estimate that the predicted discontinuity is accessible for nowadays experimental tools and materials. It is shown that the magnitude of this discontinuity can be used to predict the dependence of the critical temperature on the charge carrier density which can be tailored by doping.

TT 9.43 Mon 14:00 Poster A

Measurement of Dielectric Losses in Amorphous Thin Films at GHz Frequencies Using Superconducting Resonators — •Sebastian Skacel[1], Christoph Kaiser[1], Stefan Wünsch[1,2], Michael Siegel[1,2], Ralf Dolata[3], Brigitte Mackrodt[3], and Alexander Zorin[3] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie — [2]Center for Functional Nanostructures, Karlsruher Institut für Technologie — [3]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

Josephson junctions (JJs) are employed for many applications involving microwave signals, so that low microwave losses in the structures are desirable. We have developed a reliable method for the direct measurement of dielectric losses in thin films. Thus we obtain quantitative values for the losses in the film volume as well as the metal/dielectric interfaces. Using different resonator geometries we studied the losses in dielectric thin films usually used for JJ fabrication, such as Nb_2O_5, SiO, SiO_2 and SiN_x, at 4.2K and low GHz frequencies. The results show that for such amorphous materials, the bulk losses clearly exceed the interface losses. Furthermore, the frequency dependence of the losses in this working regime was studied for the first time. Our results are in good agreement with the universal law and suggest that the losses are due to many-body interacting dipoles, which is an important fact for the theoretical modelling of two-level-fluctuators. Further investigations of dielectric multi-layer films are in good agreement with the theoretical expectations, which allows the optimisation of such multi-layers usually used in JJ and qubit fabrication.

TT 9.44 Mon 14:00 Poster A

Dc SQUIDs with sub-micron-sized Nb/HfTi/Nb Josephson junctions for operation in high magnetic fields — •Joachim Nagel[1], Oliver Kieler[2], Konstantin Konovalenko[1], Johannes Kohlmann[2], Alexander Zorin[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut – Experimentalphysik II and Center for Collective Quantum Phenomena and their Applications, Universität Tübingen, Auf der Morgenstelle 14, D-72076, Germany — [2]Fachbereich 2.4 "Quantenelektronik", Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

We investigate the suitability of dc superconducting quantum interference devices (SQUIDs) for operation in high magnetic fields (up to $B \approx 100\,\mathrm{mT}$) at temperature $T = 4.2\,\mathrm{K}$. The micro SQUIDs with superconductor (S) - normal metal (N) - superconductor (S) submicrometer Josephson junctions were realized using Nb electrodes and HfTi for the normal interlayer. Our fabrication technology combines e-beam lithography and chemical-mechanical polishing which enables junction sizes down to $200\,\mathrm{nm} \times 200\,\mathrm{nm}$, integrated into small superconductor rings with inner dimensions down to $0.5\,\mu\mathrm{m} \times 0.5\,\mu\mathrm{m}$. The characteristic voltage of the SNS junctions is typically $30 - 40\,\mu\mathrm{V}$ with a McCumber parameter $\beta_C < 0.1$, and a screening parameter of the SQUIDs $\beta_L \approx 0.2$. The SQUIDs where characterized by measurements of electric transport and noise (using a Nb dc SQUID amplifier) in a magnetically shielded environment as well as in high magnetic fields. The SQUIDs show very low flux noise which is a major prerequisite for their application as detectors for magnetic properties of nanoparticles.

TT 9.45 Mon 14:00 Poster A

Experimental Test for "Münchhausen Effect" in an Asymmetric dc-SQUID — •Susanne Butz, Kirill G. Fedorov, Alexey K. Feofanov, and Alexey V. Ustinov — Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We will report experiments aimed at observation of the so called "Münchhausen effect" - a coupling of one classical and one quantum mechanical degree of freedom. It has been theoretically predicted in [1] that this effect can be realised in an asymmetric dc-SQUID. The two junctions in the superconducting loop are made to have the same critical current but different capacitances. This creates a system with strongly asymmetric dynamical parameters. The capacitively shunted junction behaves classically and thus cannot tunnel out of a metastable state. In turn, the quantum mechanical junction can leave its metastable minimum via macroscopic quantum tunneling. This process distorts the potential for the classical junction resulting in an effective decrease of the potential barrier height. If the coupling between the juntions is strong enough this distortion is sufficient to turn the metastable minimum into an inflection point of the classical junction.

We will report switching current histograms taken and investigated for different dc-SQUID parameters, temperatures and flux biases. In

addition we performed numerical simulations using classical noise and compared the results with experimental data.

[1] A.U. Thomann, V.B. Geshkenbein and G. Blatter, Phys. Rev. B **79**, 184515 (2009).

TT 9.46 Mon 14:00 Poster A

Microwave Fluxon Readout for Superconducting Qubits — •Kirill G. Fedorov and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

We are experimentally investigating a new type of detector for very fast and weakly perturbing readout of superconducting qubits. The detection principle is based on measuring the delay time of a ballistic magnetic fluxon moving in a Josephson transmission line when passing by a qubit [1,2]. Due to magnetic perturbation the fluxon propagation delay depends on the state of the qubit. On the way towards experimental realization of fluxon detector, we report measurements of such fluxon radiation from annular Josephson junctions using a cryogenic microwave amplifier. We have measured fine structure of fluxon step on current-voltage characteristic by detecting fluxon radiation frequency. The fluxon delay by an external magnetic perturbation of 0.1 nT induces fluxon oscillations frequency shift of 1.9 MHz. This suggest that a phase shift of fluxon oscillator can be used for non-destructive repetitive measurements of the qubit state.

[1] D.V. Averin, K. Rabenstein, and V. K. Semenov, Phys. Rev. B **73**, 094504 (2006).

[2] A. Fedorov, A. Shnirman, G. Schön, and A. Kidiyarova-Shevchenko, Phys. Rev. B **75**, 224504 (2007).

TT 9.47 Mon 14:00 Poster A

Experiments with phase qubits and two-level-fluctuators — •Grigorij J. Grabovskij, Pavel Bushev, Juergen Lisenfeld, Alexander Lukashenko, and Alexey V. Ustinov — KIT, Physikalisches Institut, Wolfgang-Gaede-Strasse 1, 76131 Karlsruhe

We explore the complexity of the dynamical behaviour of a system consisting of a Josephson phase qubit and several two-level-fluctuators (TLF) coupled to it. Coherent driving of a qubit at the resonance with a TLF results in formation of a hybrid system consisting of 4 levels [1]. In our study we aim at a more detailed understanding of the physical nature of TLFs and their interaction with the qubit and electromagnetic environment. The presence of TLFs clearly appears in excitation spectrum of the qubit as avoided level crossings. The measured relaxation dynamics of individual TLFs yields the value for decay time T_1 and decoherence time T_2. Surprisingly, the measured T_1 and T_2 of some of TLFs exceed those of the qubit ($\sim$ 100 ns). We show that quantum beating between qubit and TLF reveals the presence of weak fluctuators which are hardly detectable in a standard spectroscopy. We will report new data on swap-spectroscopy, in which a microwave pulse and population swap between qubit and fluctuator is followed by the qubit readout. Using this method, it becomes possible to study direct interaction of microwave excitation. [1] J. Lisenfeld et al., arXiv:0909.3425

TT 9.48 Mon 14:00 Poster A

The influence of magnetic stray field on the critical current in NbN/$SmCo_5$-bilayers — •Jan Engelmann, Silvia Haindl, Ingolf Moench, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P. O. Box 27 01 16, 01171 Dresden, Germany

The coexistence of superconductivity (sc) and ferromagnetism (fm) in artificially grown heterostructures, sc/fm-bilayers in the simplest case, leads to new interesting phenomena like field compensation- and stray field effects. The intermetallic permanent magnet $SmCo_5$ is especially known for its large magnetic anisotropy energy. Thin films of $SmCo_5$ have been prepared with extremely high coercivity fields up to 3 T (at room temperature) and up to 5 T at 10 K. To investigate the influence of the magnetic stray field on a conventional superconductor, 50 nm NbN layers have been grown on $SmCo_5$ thin films using pulsed laser deposition (PLD). The magnetic properties were determined by VSM and MFM measurements. Critical current measurements were made by a standard four-probe technique. The angular-dependent critical current has been investigated.

TT 9.49 Mon 14:00 Poster A

Inverse Proximity Effect in FSF Heterostructures — Christian Wagner[1], Roland Grein[1], Matthias Eschrig[1,2], and •Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany. — [2]Fachbereich Physik, Universität Konstanz

We employ the quasiclassical theory of superconductivity to study the inverse proximity effect in FSF trilayer structures, where F is a strongly spin-polarized ferromagnet and S a singlet superconductor. In particular, we focus on effects induced by spin-dependent scattering phases at the S/F-interfaces. The resulting triplet pairing component will lead to a suppression of the superconducting gap. This enables us to investigate the influence of the relative magnetization orientation of the two ferromagnetic layers on the superconducting transition temperature.

TT 9.50 Mon 14:00 Poster A

Planar S-(S/F)-S Josephson junctions induced by inverse proximity effect — •Andreas Pfeffer[1], Ondrej Vavra[1], Wolfgang Pfaff[1], Marco Aprili[2], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]CSNSM-CNRS, Université Paris-Sud, 91405 Orsay Cedex, France

We investigate Josephson contacts made from crossed Nb and Fe strips. The weak link is created by the inverse proximity effect in the contact area between superconductor and ferromagnet. If we vary the width of the ferromagnetic strip and the ferromagnetic material, we observe a reduction of the critical current with increasing Fe strip width, which can be explained qualitatively by a reduced coupling between the superconducting reservoirs. A more detailed investigation has been performed on a sample with a 200 nm wide Fe strip and strong coupling between the superconducting leads. A quasiparticle current injected via the Fe strip has a strong impact on the critical current I_c. For comparison, samples with pure Pd instead of Fe were studied. This enables us to compare the effect of charge imbalance, spin injection and electron heating.

TT 9.51 Mon 14:00 Poster A

Investigation of nanoscale superconductor-ferromagnet hybrids using very low temperature STS — •Michael Wolz and Elke Scheer — Fachberich Physik, Universität Konstanz, 78457 Konstanz

We investigate laterally structured superconductor-ferromagnet hybrids using a very low temperature STM. A STM is the ideal instrument to investigate the quasiparticle density of states (DOS) with high lateral resolution.The DOS in the superconductor is influenced by proximity effect as well as by the electromagnetic interaction with the ferromagnet. In an external magnetic field B, this can lead to interesting effects such as the oscillatory dependence of the critical temperature on B or the nonuniform nucleation of superconductivity. For a review see [1]. The proximity effect can be suppressed by spatial separation of the superconductor from the ferromagnet using an insulating layer. We present first results obtained on arrays of ferromagnetic Co dots covered by Al as a superconductor.

[1] A. Y. Aladyshkin, A. V. Silhanek, W. Gillijns, and V. V. Moshchalkov, Superconductor Science and Technology 22, 053001 (2009).

TT 9.52 Mon 14:00 Poster A

Ferromagnet-superconductor hybrids with perpendicular magnetization: current-perpendicular-to-plane measurements — •Richard Montbrun[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, D-76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76131 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 perpendicular magnetization of the F electrodes was confirmed by measurements of the anomalous Hall effect. The sample layout was developed to allow for four-point resistivity measurements with the current perpendicular to the F/S interface. In the normal state (temperature T = 10 K) the magnetoresistance $R(H)$ shows a spin-valve effect due to the different coercivities of the top and bottom F electrode arising from different Co-layer thicknesses and deposition temperatures. At lower temperatures we investigate the resistance $R(H,T)$ of the superconducting spin-valve for different S-layer thicknesses and transport currents. Preliminary data demonstrate a current dependence of the transition temperature T_c in the magnetically saturated state but only a minor influence of the relative orientation of the two F-layer magnetizations on T_c. Effects of the magnetic stray fields arising from the nanostructured F electrodes and the spin-dependent

scattering on the superconducting properties are discussed.

TT 9.53 Mon 14:00 Poster A

Supercurrents through carbon nanotubes with Nb contacts — •Thomas Geiger — Institute for Experimental and Applied Physics, University of Regensburg

Based on previous work in our group, proximity induced supercurrents through a MWCNT of length 1.3 μm and diameter about 15 nm was measured. The sample was connected in 3-point geometry using a Pd/Nb 2.5/45 nm bilayer as direct contact material. Since Nb is the strongest elementary superconductor, it promises advantages over other materials like Al. Contact separation was about 300 nm, exceeding the typical scattering length in the tube. An elaborate on-chip RC-environment consisting of high-Ohmic leads and large bonding pads made of AuPd was used to ensure good electrical filtering in direct vicinity of the structure. In addition to thorough electrical filtering of the measurement lines this enabled us to perform sensitive measurements of the critical current.

The sample was covered with 50 nm Al_2O_3 and a local 2.6 μm wide and 55 nm thick Pd-topgate directly above the nanotube. This gate showed very effective and reliable operation. Despite the coverage of the nanotube, supercurrent was still detectable.

We found a peculiar subgap structure in the dI/dV- and IV-characteristics and investigated its temperature and gate voltage dependence.

TT 9.54 Mon 14:00 Poster A

Spatially Resolved Photoresponse of NbN Nanowires — •Philipp Jung[1], Alexander Lukashenko[1], Alexander P. Zhuravel[2], Stefan Wuensch[1], Matthias Hofherr[1], Konstantin Ilin[1], Michael Siegel[1], and Alexey V. Ustinov[1] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]B. Verkin Institute for Low Temperature Physics & Engineering, Kharkov Ukraine

We are investigating optical response of superconducting nanowires patterned from thin NbN films deposited on sapphire and Si substrates. These structures are often used for radiation detectors like single-photon detectors and hot-electron bolometer mixers. In our experiments, we precisely position a focused laser beam on the detector to correlate the response to a local excitation. Scanning the laser spot over the sample surface allows us to obtain response maps of the investigated wires.

We have found spatially localized weak areas in case of NbN films on sapphire substrates, which can be attributed to grain boundaries with suppressed superconducting properties. In opposite, the strongest response of NbN bridges on Si substrates was obtained at the edges of bridges. We are going to present and analyze the dependence of response of NbN thin film bridges on light intensity and operation temperature.

TT 9.55 Mon 14:00 Poster A

Progress in the development of large-scale MMC detector arrays — •Sebastian Kempf, Andreas Fleischmann, Loredana Gastaldo, Thomas Wolf, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany.

During the last decade low-temperature particle detectors like metallic magnetic calorimeters (MMCs) became interesting instruments for numerous experiments in atomic and nuclear physics, material science and x-ray astronomy. Since large detection areas, high count rates or especially imaging capabilities are often required, significant effort is put into the development of large detector arrays. To accommodate constraints on cryogenic wiring and to reduce parasitic heat load, sophisticated techniques for reading out large arrays with a small number of wires have to be designed.

We discuss possible multiplexing techniques for MMCs and present recent results of the development of a frequency-domain multiplexed MMC detector array based on a dissipationless microwave SQUID multiplexer. This includes a systematic study of the properties of the fabricated superconducting CPW microwave resonators, a full characterization of the microwave setup and a preliminary design of a microwave rf-SQUID. We present performance tests of a single pixel MMC optimized for high-resolution x-ray spectroscopy and outline the properties of a room-temperature microwave electronics needed to read out a fully working MMC detector array.

TT 9.56 Mon 14:00 Poster A

Micro-fabrication of metallic magnetic calorimeters — •S. Schäfer, S. Kempf, A. Pabinger, C. Pies, J-P. Porst, F. v. Seggern, T. Wolf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff Institut für Physik, INF 227, 69120 Heidelberg

Metallic magnetic calorimeters (MMC) are energy dispersive particle detectors with very high resolving power that are operated at temperatures below 100 mK. Our presently fabricated MMCs consist of a particle absorber made of electroplated gold, in tight thermal contact to a temperature sensor. The sensor is made of the paramagnetic alloy Au:Er and placed in a weak magnetic field. A temperature rise upon the absorption of a particle is detected via the change of the sensor's magnetization monitored by a dc-SQUID. A planar meander shaped coil made of niobium underneath the sensor is used to generate the necessary bias magnetic field and to pick-up the change of magnetization. An on-chip persistent current switch with Au:Pd heater is used to inject the field generating current. We describe the fabrication steps for the Au:Er sputter target and the co-sputter process for the deposition of the sensor material. We discuss the challenge of electroplating high quality gold into a mold of photo resist to fabricate overhanging absorbers on top of the sensors and present the processes for the sputter deposition and micro-structuring of niobium, SiO_x and Au:Pd. We report on measurements of all relevant material properties at low temperatures, e.g. the critical current density of the niobium structures as well as the specific heat and the magnetization of the sensor material, and compare them to those of the corresponding bulk materials.

TT 9.57 Mon 14:00 Poster A

Metallic magnetic calorimeters for high-precission QED tests at GSI/FAIR — •Christian Pies, Andreas Pabinger, Sebastian Kempf, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany.

Quantum electrodynamics belongs to the best tested and established theories in modern physics. However, the evaluation of high order processes, as necessary in strong fields, is still demanding. A precission test of QED in strong fields is the comparison of the calculated and measured Lamb-shift of the ground state in hydrogen-like heavy ions.

For the spectroscopy of hydrogen-like Uranium at GSI/FAIR, we recently started the development of a detector for hard x-rays emitted during the transition into the ground state. The detector consists of four independent, gradiometric metallic magnetic calorimeters (MMCs) forming a linear 8-pixel array and is completely microfabricated. Each pixel covers an area of 1 mm^2 and is equipped with a 200 μm thick electrodeposited gold absorber. The detectors are designed to provide an energy resolution better than 30 eV in the relevant energy range up to 100 keV with a stopping power larger than 85 %.

We present the considerations which lead to our present detector design, the methods used for the fabrication of the MMC array as well as first characterization measurements.

TT 9.58 Mon 14:00 Poster A

Low temperature detectors for direct neutrino mass measurements — •Jan-Patrick Porst, Falk v. Seggern, Andrea Kirsch, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, INF 227, 69120 Heidelberg

Presently one of the great challenges in neutrino physics is to determine the mass hierarchy of the neutrino mass eigenstates as well as the absolute values of the masses. The spectrum of a beta decay or an electron capture decay contains the mass information and is thus a main focus of studies in this field. Besides the already well established examination of the shape of the tritium beta spectrum with large scale spectrometers also other isotopes and experimental methods are under investigation. We present two promising experiments studying the beta decay of ^{187}Re and the electron capture decay of ^{163}Ho. Both isotopes have low Q-values and are therefore well suited for neutrino mass investigations. In both experiments the decay spectrum is measured calorimetrically with an energy resolution as high as $\Delta_{\mathrm{FWHM}} = 2\,\mathrm{eV}$. Low temperature metallic magnetic calorimeters were developed and fabricated for these applications.
We present currently developed detector prototypes and results of characterization measurements. Furthermore, we discuss the sensitivity of future mid- or large-scale experiments on the neutrino mass assuming the presently achieved detector performance.

TT 9.59 Mon 14:00 Poster A

Investigation of superconductors as particle absorbers of metallic magnetic calorimeters — •Jan-Patrick Porst, Andrea Kirsch, Philipp Ranitzsch, Richard Weldle, Loredana

Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut for Physics, INF 227, 69120 Heidelberg

The choice of an absorber material for low temperature calorimeters is a crucial one. Generally, the absorber should possess high stopping power for incoming energetic particles or photons and have low heat capacity. Currently mostly gold and bismuth are used for this purpose. The very small specific heat of superconductors far below their T_c makes them very promising candidates as absorber material. However, these materials show different thermalization behaviour, of which the underlying thermalization processes are so far not understood. In superconducting rhenium this thermalization is of particular interest with regard to the development of detectors for neutrino mass measurements. We investigated three different superconducting materials (Re, Al and Al:Mn) as absorbers of metallic magnetic calorimeters (MMCs). MMCs are low temperature energy dispersive detectors composed of an energy absorber well thermally connected to a paramagnetic temperature sensor which resides in a small magnetic field. The change of magnetization following the absorption of energy is measured as a change of flux in a low noise high bandwidth dc-SQUID. We present the observed dependence of the energy thermalization on temperature and geometry for all three materials and discuss the importance of the diffusive transport of heat as well as of quasiparticle recombination.

TT 9.60 Mon 14:00 Poster A

Inductance of thin metal strips in broadband Corbino microwave spectroscopy — •Katrin Steinberg, Marc Scheffler, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Broadband microwave spectroscopy is a emerging technique to study the electronic properties of different materials in a huge range of frequency. Using a Corbino setup, where the sample is pressed against an open end of a coaxial cable, we investigate a broad range of samples from semiconducting crystals to metallic or superconducting thin films. To increase the measurement sensitivity for the metallic and superconducting samples, one can use a strip-shaped sample geometry instead of samples covering the complete Corbino probe. This geometry increases sample impedance but also leads to additional effects in the measured sample impedance, which have to be taken into account. We present the analysis of the strip-shaped film inductance for different geometric film parameters like thickness, width and length. The frequency and temperature dependence of these effects was investigated for different materials. We compare the theoretical predictions with our experimental data covering a broad frequency range (45 MHz - 40 GHz) and varying sample geometries and materials, including metals and superconductors at temperatures between 1 K and 300 K. Our results apply to conductive strips at microwave frequencies in general.

TT 10: Measuring Devices, Cryotechnique: Poster Session

Time: Monday 14:00–18:00 Location: Poster A

TT 10.1 Mon 14:00 Poster A

Broadband cw THz spectroscopy at low temperatures and high magnetic fields — •A. Janssen[1], K. Thirunavukkuarasu[1], H. Schmitz[1], A. Roggenbuck[1,2], A. Deninger[2], I. Cámara Mayorga[3], J. Hemberger[1], R. Güsten[3], and M. Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]TOPTICA Photonics AG, Lochhamer Schlag 19, D-82166 Gräfelfing, Germany — [3]Max-Planck-Institute for Radio Astronomy, Auf dem Hügel 69, D-53121 Bonn, Germany

THz spectroscopy has been of great interest lately as it reveals the low-energy electronic phenomena in several materials like high-Tc superconductors, heavy fermion compounds and more recently multiferroic materials. While in particular time-domain THz-spectroscopy meanwhile has become a common tool, we use an optical homodyne method to generate a continuous-wave (cw) THz-Signal: A photomixer is illuminated by the light of two tunable DFB IR-lasers with adjacent frequencies and emits an electromagnetic wave through a silicon lens with the difference frequency in the THz-frequency range. A wide bandwidth, high spectral resolution and frequency stability are the benefits of this technique. For investigations at low temperatures and high magnetic fields, an integrated photomixer face-to-face assembly was set up circumventing the need of intensity diminishing optical components as lenses, mirrors, or windows. We will present the development and testing of a fiber-based cw broadband THz spectrometer in the frequency range of 60 GHz to 1.8 THz for the use within conventional 4He magneto-cryostat systems.

TT 10.2 Mon 14:00 Poster A

Coherent broadband cw THz spectroscopy on solid-state samples: recent improvements — •H. Schmitz[1], A. Roggenbuck[1,2], K. Thirunavukkuarasu[1], A. Janssen[1], A. Deninger[2], I. Cámara Mayorga[3], J. Hemberger[1], R. Güsten[3], and M. Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]TOPTICA Photonics AG, Lochhamer Schlag 19, D-82166 Gräfelfing, Germany — [3]Max-Planck-Institute for Radio Astronomy, Auf dem Hügel 69, D-53121 Bonn, Germany

We aim at the precise determination of the complex dielectric function $\varepsilon(\omega)$ of solid state samples in the THz range. Our spectrometer employs photomixing of two NIR lasers. The photomixer efficiently converts the laser beat into THz radiation from 60 GHz to 1.8 THz. The signal is coherently detected using a second photomixer which preserves the THz phase information. In order to determine $\varepsilon(\omega)$, we either sweep the frequency in small steps ($\sim$ 30 MHz) or we modulate the phase of the laser beat. This can be achieved using a fiber stretcher which modulates faster than a mechanical delay stage. In addition, we implement a photocurrent correction to account for drifts in the THz intensity using the dc photocurrents measured at the photomixers. We demonstrate the excellent performance of the spectrometer for different solid state samples.

TT 10.3 Mon 14:00 Poster A

A 300 mK, 9 T, UHV scanning tunneling microscope — •Danny Baumann[1], Juliana Brunzlaff[1], Torben Hänke[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

We present the results of first measurements with a 300 mK 9 T ultra high vacuum (UHV) scanning tunneling microscope (STM). This home build STM is equipped with a coarse xy-sample positioning system, in-situ tip exchange as well as a three chamber UHV system to prepare, store and analyze samples.

Furthermore, we show the design of the new home build coarse xy-sample positioning system which is directly mounted on the STM head and works at very low temperatures, high magnetic fields and UHV conditions.

TT 10.4 Mon 14:00 Poster A

Design of a dip stick 4 K scanning tunneling microscope — •Ronny Schlegel[1], Torben Hänke[1], Danny Baumann[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperorperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

To study electronic and surface structures with scanning tunneling spectroscopy (STS) we designed a STM for temperatures from 300 K down to 4 K. The microscope will be placed in a ^{4}He cryogenic system with a superconducting coil (up to 17 Tesla) or in a standard lab Dewar for zero field measurements. An implemented cleaving mechanism allows sample preparation at low temperatures.

TT 10.5 Mon 14:00 Poster A

Broadband magnetodielectric spectroscopy in the millikelvin-regime — •Christoph Grams, Tim Steinmetzer, Florian Waschkowski, Daniel Niermann, and Joachim Hemberger — 2. Physikalisches Institut, Universiät zu Köln, Deutschland

Broadband dielectric spectroscopy provides a wealth of information on the polarization dynamics in condensed matter. Our goal is to measure the complex permittivity from 1 Hz to 20 GHz inside a top loading dilution refrigerator at temperatures down to 20 mK and magnetic

fields up to 13 T. We use a frequency response analyzer for frequencies up to 10 MHz with shielded coax cables for measurements of the complex impedance. From 10 MHz to 20 GHz we realize coaxial reflection measurements employing a network analyzer and a microstrip sample-holder. One of the major problems with this setup is the calibration due to the temperature dependent internal reflections. The broad frequency range of the network analyzer allows the use of time-domain-gating as a secondary error correction. We present our calibration results and first reference measurements, e.g. on $SrTiO_3$ and the spin-ice $Dy_2Ti_2O_7$.

TT 10.6 Mon 14:00 Poster A

SQUID submicroemu ferromagnetic and superconducting signals embedded in much larger diamagnetic ones — •Ana Ballestar[1,2], Annette Setzer[2], Pablo Esquinazi[2], and Nicolas Garcia[1] — [1]Laboratorio de Fisica de Sistemas Pequeños (LFSPyN), Consejo Superior de Investigaciones Científicas (CSIC), Serrano 144, 28006 Madrid, Spain — [2]Division of Superconductivity and Magnetism Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany

Commercial superconducting quantum interferometer devices (SQUID) are widely used to measure small magnetic signals. In general, the SQUID signal is taken as a proof for the existence of ferromagnetic or superconducting phases in the samples. When magnetic moment signals below 1 μemu are present the situation is complicated due to the intrinsic resolution limits of the magnetometer. Measuring the response of a superconducting Pb-thin film on the surface of a graphite sample we were able to show that the sub-μemu signals of the ferromagnetic (from graphite) and superconducting (from Pb) phases are very well measured even when they are embedded in diamagnetic signals in the range of 4 to 30 μemu. Our work proves that it is possible to work with a commercial SQUID down to sub-μemu region after the subtraction of a large background signal coming from the same sample.

TT 10.7 Mon 14:00 Poster A

Multipurpose filter for high-resolution electronic measurements at very low temperatures — •Hans-Fridtjof Pernau[1], Christian Schirm[1], Christian Debuschewitz[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Attocube Systems, Munich, Germany

Low-temperature transport measurements with high energy resolution require effective filtering of high-frequency input and an optimized thermal link between the electronic system and the thermal bath. Standard RC filters built from SMD or other discrete electronic elements provide a very sharp filtering characteristic. However, with those devices it is difficult to hinder crosstalk between in- and output. Their high dc resistance and restricted contact area results in considerable heat input. Furthermore the elevated dc resistance hampers measurements with high currents or voltages. We developed compact and reliable filters based on the filter concept presented by Martinis, Devoret and Clarke in 1987 [1] which we adapted to various purposes and shapes and to fit into almost every cryostat system. We present the manufacturing procedure, the filtering properties together with examples of implementations of our homemade copper and stainless steel powder filters which are used down to 10 mK.

[1] J.M. Martinis, M.H. Devoret and J. Clarke, Phys. Rev. B **35**, 4682 (1987)

TT 11: CE: Low-dimensional Systems - Materials 2

Time: Tuesday 9:30–12:45 Location: H18

TT 11.1 Tue 9:30 H18

Electron Energy-Loss Spectroscopy on the Transition-Metal Dichalchogenide $2H$-$TaSe_2$ — •Andreas König[1], Roman Schuster[1], Helmuth Berger[2], Martin Knupfer[1], and Bernd Büchner[1] — [1]Institute for Solid State Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Insitut de Physique de la Matière Complexe, EPFL, CH-1051 Lausanne, Switzerland

$2H$-$TaSe_2$ is one of the various polytypes of the transition-metal dichalchogenide (TMDC) $TaSe_2$. It consists of hexagonal layers with weak interlayer van-der-Waals bonding. It shows phase transitions to a charge-density wave (CDW) and to a superconducting state. Although there is strong evidence for the competition of these two ordering effects as well as for a Peierls transition scenario for the origin of the CDW, a theoretical understanding of the mechanism leading to the phase transitions is still subject of discussions. What is already proved for $2H$-$TaSe_2$ and a few other TMDCs is a negative dispersion of the bulk plasmon in the normal state and an even larger bandwidth of this negative dispersion in the CDW state, which is altogether not a common metal behavior [1]. We performed Electron Energy-Loss Spectroscopy in transmission on thin films of $2H$-$TaSe_2$ for different temperatures above and below the CDW transition temperature to investigate the connection of the CDW phase transition to the plasmon dispersion.

[1] Schuster et al., Phys. Rev. B. **79**, 045134 (2009)

TT 11.2 Tue 9:45 H18

Raman scattering evidence for a cascade-like evolution of the charge-density-wave collective amplitude mode — •Hans-Martin Eiter[1], Michela Lavagnini[2], Leonardo Tassini[1], Bernhard Muschler[1], Jiun-Haw Chu[3], Nancy Ru[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, CA 94304, USA

We report results of Raman scattering experiments as a function of temperature on the charge-density-wave (CDW) systems $DyTe_3$ and on $LaTe_3$ at 6 GPa applied pressure. We clearly identify the unidirectional collective CDW amplitude excitation and follow their temperature dependence in the range from 6 K to 311 K. Surprisingly, we discover that the amplitude mode develops as a succession of two mean-field, BCS-like transitions at two different temperatures.

Tri-tellurides with heavier rare-earth atoms (i.e. Tm, Er, Ho, Dy) undergo another phase transition to a bidirectional CDW at low temperatures. In $DyTe_3$ we find spectroscopic evidence for the amplitude mode excitation associated with the bidirectional CDW occuring below 50 K.

This work is supported by the DFG under Grant No. Ha2071/5-1.

TT 11.3 Tue 10:00 H18

LDA+Slave-boson mean-field theory: a powerful low-energy tool for realistic strongly correlated systems — •Christoph Piefke and Frank Lechermann — I. Institut fuer Theoretische Physik, Universitaet Hamburg, Jungiusstrasse 9, 20355 Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) has proven to be a powerful tool to investigate large parameter spaces of arbitrary strongly interacting systems [1,2]. In this approach, complex fermionic interactions are described by means of an electon-operator decoupling into a quasiparticle part and localized bosonic degrees of freedom. A set of constraints ensures that this mapping does not leave the Hilbert space of the original problem. At saddle-point, a self-consistent mean-field solution is obtained.

As an efficent method for demanding problems, RISB is used to investigate LDA-based models for realistic materials with strong electronic correlations. Resulting physical quantities like the quasiparticle weight or the local spin correlations for, e.g., the Na_xCoO_2 system [3], are in very good agreement with more accurate many-body approaches. Moreover the additionally extracted multiplet weights for atoms and clusters in the strongly correlated regime provide further important insight into the competition between itinerancy and localization.

[1] T. Li, P. Wölfle, and P. J. Hirschfeld, Phys. Rev. B **40**, 6817 (1989).

[2] F. Lechermann, A. Georges, G. Kotliar and O. Parcollet, Phys. Rev. B **76**, 155102 (2007).

[3] F. Lechermann, Phys. Rev. Lett. **102**, 046403 (2009).

TT 11.4 Tue 10:15 H18

Ground state description of $BiCu_2PO_6$ and $BiCu_2AsO_6$ — •Deepa Kasinathan, Alexander Tsirlin, Oleg Janson, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Low dimensional spin systems have always been of interest to the physics community due to their inherent exotic magnetic properties.

A further impetus for the study of low-dimensional spin systems was given by the discovery of spin-ladder materials, due to the fact that they are intermediate objects between 1D and 2D systems. Recent experiments by two groups [1,2] on a spin-ladder material $BiCu_2PO_6$ exhibited a gapped singlet ground state with a spin gap of about 34 K, though the strength of the spin-exchange interactions have remained controversial. No consensus has been reached on the correct spin-ladder model to describe this compound. We will report on our re-investigations of $BiCu_2PO_6$ and the related material $BiCu_2AsO_6$ using density functional theory based electronic structure calculations and as well as Transfer Matrix Renormalization Group (TMRG) calculations. Our results necessitate the inclusion of previously neglected exchange couplings to describe the spin-ladder model more appropriately.

[1] B. Koteswararao, *et. al.*, Phys. Rev. B **76**, 052402 (2007).
[2] O. Mentré, *et. al.*, Phys. Rev. B **80**, 180413 (2009).

TT 11.5 Tue 10:30 H18

Unraveling the 1/2 magnetization plateau: a new microscopic magnetic model for $CdCu_2(BO_3)_2$ — •Oleg Janson[1], Alexander Tsirlin[1], Johannes Richter[2], Yurii Skourski[3], and Helge Rosner[1] — [1]MPI CPfS Dresden — [2]University of Magdeburg — [3]Dresden High Magnetic Field Laboratory (HLD)

Copper(II) cadmium borate $CdCu_2(BO_3)_2$ is a spin-1/2 Heisenberg system showing a remarkable 1/2 plateau in the magnetization curve. Based on experimental studies of this compound ($\chi(T)$, $C_p(T)$, $M(H)$), a phenomenological model for its magnetism has been suggested [1]. According to this model, the system can be described as consisting of spin chains and dimers, formed by structurally different atoms Cu1 and Cu2, respectively. However, recent neutron diffraction experiments [2] evidence an inconsistency of this simple chain-dimer model, since both Cu positions show sizable magnetic moments in the ordered state.

We have studied this system using DFT calculations. Typically for Cu^{2+} materials, the magnetism of $CdCu_2(BO_3)_2$ can be described by an effective one-orbital approach. Based on the tight-binding fit of the relevant LDA bands, we estimate the antiferromagnetic contribution to the magnetic exchange. The total exchange is obtained by LSDA+U supercell calculations. Exact diagonalization studies of the parameterized Heisenberg model evidence that the new microscopic model consistently describes all existing thermodynamical data. The results of new $M(H)$ measurements and NMR experiments will be briefly discussed.

[1] Hase et al., Phys. Rev. B **72** 172412 (2005).
[2] Hase et al., Phys. Rev. B **80** 104405 (2009).

TT 11.6 Tue 10:45 H18

Magnetic properties of the spin chain compound Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R.O. Kuzian[2], W.-D. Stein[3], N. Wizent[1], G. Behr[1], A. Hiess[4], W. Schmidt[5], S. Petit[6], K. Nenkov[1], M. Loewenhaupt[3], R. Klingeler[1], and B. Büchner[1] — [1]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Inst. f. Problems of Materials Science, Kiev, Ukraine — [3]Inst. f. Festkörperphysik, TU Dresden — [4]Inst. Laue Langevin, Grenoble, France — [5]Jülich Centre f. Neutron Science — [6]Laboratoire Léon Brillouin, Saclay, France

We report recent experiments on Li_2CuO_2 single crystals. The magnetic phase diagram we have derived from magnetization, specific heat, thermal expansion and magnetostriction data is discussed in view of a new detailed inelastic neutron scattering study [1]. Li_2CuO_2 represents a simple, strongly frustrated spin chain material close to the 3D ferromagnetic (FM)-helical critical point. At low temperatures weak antiferromagnetic inter-chain exchange interactions are found to cause FM in-chain ordering. Above the ground state low-lying helical excitations are observed. Implications - esp. of the relatively large nearest neighbor exchange interaction - for the frustrated akin ferromagnetic spin chain compound $Ca_2Y_2Cu_5O_{10}$ and the helical system Li_2ZrCuO_4 are pointed out.

[1] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).

15 min. break

TT 11.7 Tue 11:15 H18

Spectroscopic ellipsometry study of the edge-sharing CuO_4 chain cuprate Li_2CuO_2 — •Yulia Matiks[1], A.V. Boris[1], J. Malek[2], S. Nishimoto[2], S.-L. Drechsler[2], P. Horsch[1], N. Wizent[2], G. Behr[2], M. Knupfer[2], B. Buchner[2], and B. Keimer[1] — [1]Max-Planck-Inst. f. Festkörperforschung, Stuttgart, Germany — [2]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany

Motivated by observation of a double-peak structure in the edge-sharing chain cuprate $LiCuVO_4$, assigned to the Zhang-Rice exciton states [1], we report detailed ellipsometric measurements on Li_2CuO_2. This compound is characterized by different ratio between the near-neighbor J_1 and the next-near-neighbor J_2 exchange integrals, $\alpha = -J_2/J_1 = 0.33$ [2]. Temperature dependence of the interband transition peaked at 3.7 eV in the optical conductivity along the chains follows spin correlations and becomes apparent below $T_N \approx 9K$. This excitation is assigned to the Zhang-Rice singlet excitation and modelled within a five band Cu 3d O2 p extended Hubbard model including long range Coulomb interactions. Applying exact diagonalization and DMRG studies to Cu_nO_{2n+2} chains and corresponding rings a strong intersite Coulomb interaction of about V_{pd}=2.2 eV is found. The main in-chain exchange integrals obtained from a mapping onto a spin-1/2 Hamiltonian are in agreement with the spin wave analysis of the new detailed inelastic neutron scattering study [2].

[1] Y. Matiks *et al.*, Phys. Rev. Lett. **103**, 187401 (2009).
[2] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).

TT 11.8 Tue 11:30 H18

Longitudinal magnon in the AF chain system $KCuF_3$ — Vladimir Gnezdilov[1], •Peter Lemmens[2], Dirk Wulferding[2], Paolo Ghigna[3], and Joachim Deisenhofer[4] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DCF, Univ. Pavia, Italy — [4]Exp. Phys. V, CECM, Univ. Augsburg

The low energy longitudinal magnon in $KCuF_3$ was observed and studied for the first time in Raman scattering at temperatures below the Neel temperature. The observation of a spinon continuum and this longitudinal mode reveals the coexistence of antiferromagnetic ordering and quantum fluctuations in $KCuF_3$ for T<T_N. Work supported by DFG.

TT 11.9 Tue 11:45 H18

Ballistic heat transport of quantum spin excitations — •Nikolai Hlubek[1], Patrick Ribeiro[1], Romuald Saint-Martin[2], Surjeet Singh[1], Alexandre Revcolevschi[2], Georg Roth[3], Günter Behr[1], Bernd Büchner[1], and Christian Hess[1] — [1]IFW-Dresden, Germany — [2]Université Paris-Sud, Orsay, France — [3]RWTH Aachen, Germany

We provide experimental evidence for ballistic heat transport in the spin chain material $SrCuO_2$. In particular, we investigate high purity samples of this double chain cuprate and observe a huge magnetic heat conductivity κ_{mag}. An extremely large spinon mean free path of more than a micrometer demonstrates that κ_{mag} is only limited by extrinsic scattering processes which is a clear signature of ballistic transport in the underlying spin model. Furthermore we study the influence of magnetic Ni and non-magnetic Mg impurities on κ_{mag} of $SrCuO_2$. While Ni-doping has a large impact on the magnetic thermal conductivity, Mg-doping shows no influence. In order to clarify this surprising behavior we compare κ_{mag} to measurements of the single chain compound Sr_2CuO_3.

TT 11.10 Tue 12:00 H18

Ferromagnetic zigzag chains in $CdVO_3$: the role of cadmium — •Alexander Tsirlin and Helge Rosner — Max-Planck Institute CPfS, Dresden, Germany

Most of the low-dimensional spin systems show antiferromagnetic ground states or ground states with low net magnetization due to a weak asymmetry of the exchange couplings. Low-dimensional ferromagnets are rare, yet they show interesting low-temperature properties. These properties can be affected by quantum fluctuations, although entirely ferromagnetic systems with isotropic exchange couplings are not subject to the magnetic frustration. In this contribution, we present a band structure-based microscopic model for the low-dimensional spin-$\frac{1}{2}$ compound $CdVO_3$. The crystal structure of $CdVO_3$ shows zigzag chains of VO_5 square pyramids. These chains can be considered as spin chains with nearest-neighbor (J_1) and next-nearest-neighbor (J_2) couplings, both being ferromagnetic: $J_1 \simeq J_2 \simeq -50$ K. Moreover, the interchain couplings are also ferromagnetic and lead to ferromagnetic ordering at $T_C = 24$ K. From the structural point of view, the exclusively ferromagnetic couplings in $CdVO_3$ are highly counter-intuitive. However, band structure calculations explain these couplings by an effect of low-lying Cd 5s states that mix with V 3d states and mediate hoppings between the half-filled V d_{xy} and the empty V d_{xz}, d_{yz} orbitals. The severe violation

of the conventional superexchange scenario should be a general feature of Cd-containing compounds and can be used for the design of new low-dimensional magnets.

TT 11.11 Tue 12:15 H18

Quantum evolution from spin-gap to AF state in a low-dimensional spin system — Vladimir Gnezdilov[1], •Peter Lemmens[2], Dirk Wulferding[2], Reinhard Kremer[3], Collin Broholm[4], and Helmuth Berger[5] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]MPI-FKF, Stuttgart — [4]DPA, Johns Hopkins Univ., Baltimore, USA — [5]EPFL Lausanne

The low-dimensional spin systems α- and β-$TeVO_4$ share the same monoclinic crystal symmetry while having a different connectivity of VO_4 octahedra and long range order vs. a quantum disordered ground state, respectively. We report a rich magnetic Raman spectrum and phonon anomalies that evidence strong spin-lattice coupling in both systems. Work supported by DFG.

TT 11.12 Tue 12:30 H18

Spin-Jahn-Teller Effect in the Antiferromagnetic Molecular Wheel $CsFe_8$ — •Johannes Lotze[1], Oliver Waldmann[1], Anne-Christine Chamayou[2], Christoph Janiak[2], Ayuk M. Ako[3], Annie K. Powell[3], and Ilya Sheikin[4] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany — [3]Institut für Anorganische Chemie, Universität Karlsruhe, Germany — [4]Grenoble High Magnetic Field Laboratory, CNRS Grenoble, France

Antiferromagnetic molecular wheels are ring-like arrangements of exchange-coupled magnetic metal ions. As a function of a magnetic field, the Zeeman splitting leads to a series of level-crossings (LCs) at characteristic fields, where the ground state changes from total spin $S = 0$ to $S = 1$, $S = 2$, and so on. Previous magnetic torque and ^{1}H-NMR measurements on $CsFe_8$ single crystals demonstrated phase transitions at the LCs at low temperatures [PRL 96, 027206 (2006), PRL 99, 087201 (2007)]. They were explained by a field-induced spin-Jahn-Teller effect (JTE) due to a magneto-elastic coupling between the spins in the wheel and the lattice. Some models for this process were developed, but a full microscopic understanding is lacking. New high-field torque data were recorded, which provide a comprehensive picture of the angular as well as temperature dependence of the phase transition. A strong angle dependence of the critical fields and temperatures with two qualitatively different regimes was observed, which allows us to distinguish the relative contributions of zero-field splitting and Dzyaloshinsky-Moriya interactions to the spin-JTE.

TT 12: CE: Metal-Insulator Transition 1

Time: Tuesday 9:30–13:00 Location: H19

TT 12.1 Tue 9:30 H19

Nonequilibrium Mott-Hubbard Systems Driven by External Laser Fields — •Andreas Lubatsch and Johann Kroha — Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany

Mott-Hubbard insulating materials have the potential for use as ultrafast electric switches, driven by an external laser field, due to the short relaxation times characteristic for strongly correlated systems. We consider the Hubbard model at half filling, driven out of equilibrium by an external, time-periodic laser field. The vector nature of the external field and a gauge where the electric field couples to the dipole monent of the charge distribution, different from the "Peierls substitution" of previous authors' work, is essential for obtaining the correct infrared behavior. We generalize the dynamical mean-field theory (DMFT) to nonequilibrium in a time-periodic driving field, using a Floquet mode representation and the Keldysh formalism. We calculate the nonequilibrium electron distribution function, the spectral density, nonequilibrium relaxation times and the DC conductivity in the presence of the external laser field for the metallic and for the insulating phase of the Hubbard model. In the metallic pseudo-gap phase, enhanced quantum coherence due to a polariton-like coupling of electronic excitations to the discrete electromagnetic mode is predicted. This leads to a revival of the many-particle resonance at the Fermi energy at resonant laser frequencies. In the Mott insulating (equilibrium) phase, an insulator-metal transition occurs as a function of the laser frequency, while the Mott-Hubbard gap remains rubust. This corresponds to nonequilibrium pumping into the upper Hubbard band.

TT 12.2 Tue 9:45 H19

Efficient treatment of frequency dependent interactions in DMFT — •Philipp Werner[1] and Andrew Millis[2] — [1]Theoretische Physik, ETH Zurich, 8093 Zurich — [2]Department of Physics, Columbia University, New York 10027

First principles calculations of screened Coulomb interaction parameters lead in some materials to a strongly frequency dependent $U(\omega)$ [1]. The recently developed diagrammatic impurity solvers [2,3] enable a very efficient treatment of the resulting retarded interactions within the framework of dynamical mean field theory (DMFT). I will explain the main algorithmic ideas in the context of a DMFT simulation of the Holstein-Hubbard model [4] and show how this method can be adapted to models with arbitrary $U(\omega)$.

[1] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B **70**, 195104 (2004).

[2] A. N. Rubtsov, V. V. Savkin, A. I. Lichtenstein, Phys. Rev. B **72** 035122 (2005).

[3] P. Werner, A. Comanac, L. De Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

[4] P. Werner and A. J. Millis, Phys. Rev. Lett. **99**, 146404 (2007).

TT 12.3 Tue 10:00 H19

Electronic correlations in vanadium chalcogenides: $BaVS_3$ vs $BaVSe_3$ — •Daniel Grieger, Lewin Boehnke, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

As opposed to its structurally and electronically very similar selenide counterpart $BaVSe_3$, the vanadium sulfide $BaVS_3$ shows a metal-to-insulator transition at $T\sim$70K, which can be attributed to the correlation-induced formation of a charge-density wave [1]. The underlying subtle electronical differences cannot be resolved by pure density functional theory (DFT) in local density approximation (LDA), but require its combination with an explicit many-particle method such as dynamical mean-field theory (DMFT). In this presentation, we will discuss the correlated electronic structure of the named vanadium chalcogenides in view of the apparently different physics at low temperature. Thereby, special methodological attention is addressed to the interface between LDA and DMFT through a comparision of different interfacing techniques, namely maximally-localized Wannier functions and projected local orbitals.

[1] F. Lechermann, S. Biermann, and A. Georges, Phys. Rev. B **76**, 085101 (2007).

TT 12.4 Tue 10:15 H19

Inequivalent routes across the metal-to-insulator transition in V_2O_3 — •Alessandro Toschi[1], Philipp Hansmann[1,2], Giorgio Sangiovanni[1], Maurits Haverkort[2], Tanusri Saha-Dasgupta[3], Ole K. Andersen[2], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]S.N. Bose Centre for Basic Sciences, Kolkata (India)

The equivalence between the doping-driven and the pressure-driven metal-to-insulator transition, which was hitherto assumed in studies on Cr-doped V_2O_3, has been recently questioned by the results of novel optical and X-ray absorption spectroscopy experiments. Theoretical calculations, combining full multiplet cluster calculations and the merger of the local density approximation with the dynamical mean field theory (LDA+DMFT), shed light on the differences in the ground states of the two metallic phases obtained by reducing the Cr-doping or by applying pressure, and how these differences reflect in the results of different spectroscopic techniques[1].

[1] F. Rodolakis, P. Hansmann, J.-P. Rueff, A. Toschi, *et al.*, submitted.

TT 12.5 Tue 10:30 H19

Insulator-to-Insulator Transition in TiOCl upon Doping —

•Yu-Zhong Zhang[1], Kateryna Foyevtsova[1], Harald Jeschke[1], Martin Schmidt[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt am Main, Germany

By applying Car-Parrinello molecular dynamics with a projector augmented-wave basis, we investigate the effect of sodium doping in the layered Mott insulator TiOCl and predict the lattice structure under doping. We find that the system remains insulating at all doping concentrations in agreement with recent photoemission spectroscopy experiments and propose that the behavior of Na-doped TiOCl can be understood on the basis of a multi-orbital ionic extended Hubbard model. We extend our study to alternative doping routes like substitutions of Cl, O, and Ti by S, F, V/Sc, respectively and discuss the possibility to metallize TiOCl.

TT 12.6 Tue 10:45 H19

Disorder enhanced fluctuations in κ-(D_8-ET)$_2$Cu[N(CN)$_2$]Br — •Jens Brandenburg[1], Jens Müller[2], Steffen Wirth[1], and John A. Schlueter[3] — [1]Max-Planck-Insitut für Chemische Physik feste Stoffe, Dresden — [2]Goethe-Universität Frankfurt am Main — [3]Argonne National Laboratory, Argonne, IL, USA

The way in which disorder influences the electronic properties in strongly correlated systems is an intriguing question in modern condensed matter physics. Here, we report on fluctuation spectroscopy studies of the organic charge transfer salt κ-(D_8-ET)$_2$Cu[N(CN)$_2$]Br. The degree of intrinsic disorder in this quasi-2D conductor can be tuned by varying the cooling rate at the structural glass-like transition around $T_g \simeq 75\,\mathrm{K}$ [1]. We compare data taken after slow ($0.05\,\mathrm{K/min}$) and fast ($5\,\mathrm{K/min}$) cooling. Larger cooling rates increase the amount of disorder and therefore enhance the resistance fluctuations. The total noise power originating from the vibrational degrees of freedom of the ET molecules [2] is about 25% higher for the faster cooling rate. In addition, our experiments reveal another contribution to the resistance noise. Since κ-(D_8-ET)$_2$Cu[N(CN)$_2$]Br is very close to a Mott metal-to-insulator transition the coexistence of electronic correlations and disorder may result in the formation of a so-called soft Hubbard gap in the DOS due to localization effects.

[1] N. Toyota, M. Lang, and J. Müller, Low-Dimensional Molecular Metals, Springer (2007)

[2] J. Müller et al., Phys. Rev. B 79, 214521 (2009)

15 min. break

TT 12.7 Tue 11:15 H19

Universal critical conductivity at the metal-insulator transition in the two-dimensional Anderson-Hubbard model — •Prabuddha Chakraborty[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135, Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, Warszawa, Poland

We demonstrate, through extensive quantum Monte-Carlo simulations, the existence of a universal critical conductivity at an Anderson insulator-metal transition in two dimensions.The universality of the critical conductivity across various models of disorder is presented, thus pointing to the existence of a quantum critical point with universal properties. We also present results for the compressibility and magnetic susceptibilities across the phase transition and compare them to experimental data and analytical renormalization group predictions. This research is supported through SFB 484 of the Deutsche Forschungsgemeinschaft.

TT 12.8 Tue 11:30 H19

Real-Space Renormalization Group for Anderson Localization of Interacting Electrons in the Hubbard-Anderson Model — •Roman Katzer, Peter Henseler, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Anderson localization of interacting fermions remains a controversial issue even for short-range interaction. We construct a real-space renormalization group (RG) approach for the disordered Hubbard model with random onsite single-particle energies ε_i. The Hubbard interaction U leads to a non-trivial random distribution of many-body energy levels. In the atomic limit (hopping $t \to 0$ adiabatically, while keeping the chemical potential equal on all sites) this distribution can be calculated exactly, depending on ε_i, U and the filling fraction, and can be expressed in terms of a modified ("screened") single-particle level distribution [1]. Switching on hopping ($t \neq 0$), successively increasing the real-space cluster size and mapping a cluster onto a single site generates an RG flow in the space of disordered many-body Hamiltonians. Restricting the flow to low energies and observing the spin structure, the Fock space may be decimated in each RG step to keep only three Fock-space sectors with consecutive cluster occupation numbers and in each sector the lowest energy state. This leads to an RG flow of disordered Hubbard models, where the flow of the random distribution of energy levels serves as indicator for localization or delocalization. The evaluation of this scheme in $d = 1$ agrees with previous results.

[1] P. Henseler, J. Kroha and B. Shapiro, Phys. Rev. B **77**, 075101 (2008); **78**, 235116 (2008).

TT 12.9 Tue 11:45 H19

Microdomain Formation near the First-Order Metal-Insulator Transition of the Hubbard Model — •Qinyong Liu and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Since the metal-insulator transition (MIT) in Mott-Hubbard systems at finite temperature is of first order, there must be a region in the vicinity of the transition where metallic and insulating phases coexist. Thus, in this region insulating microdomains are thermally excited within the thermodynamically stable metallic phase or vice versa. The existence of such microdomains has recently been demonstrated experimentally in VO_2. We calculate the size distribution of microdomains as a function of temperature and Hubbard repulsion U. The electronic spectra and the free energy per site are calculated in metallic and in insulating regions as well as across a metal-insulator domain wall, using the generalization of dynamical mean field theory (DMFT) for inhomogeneous systems, with the non-crossing approximation (NCA) as impurity solver. The domain-size distribution is obtained from the resulting free energy difference, including volume and domain wall energies, and exhibits non-trivial, non-monotonic behavior. The first-order MIT of Mott-Hubbard systems may, hence, be viewed as a percolation problem with an anomalous resistivity due to self-generated domain disorder.

TT 12.10 Tue 12:00 H19

Interplay of thermal and quantum spin fluctuations on the Kagome lattice — •Dirk Wulferding[1,2], Patric Scheib[1], Peter Lemmens[1,2], Jens Röder[3], Philippe Mendels[4], Young Lee[5], Wing-Ho Ko[5], and Mark de Vries[6] — [1]IPKM, TU-BS, Braunschweig — [2]IGSM, TU-BS, Braunschweig — [3]IPTC, TU-BS, Braunschweig — [4]Univ. Paris Sud, France — [5]MIT, Cambridge, MA, USA — [6]CSEC and SC, Univ. Edinburgh, UK

Raman scattering in the Herbertsmithite $ZnCu_3(OH)_6Cl_2$, the first realization of a Heisenberg spin 1/2 AF on a kagome lattice, shows two components, a high temperature quasi elastic signal and a low temperature, broad maximum, extending to high energy. We have investigated the temperature dependence and symmetry properties of both signals in this highly frustrated material. Work supported by ESF-HFM and DFG.

TT 12.11 Tue 12:15 H19

Quantum magnetism of the Hubbard model on the Triangular Lattice — •Hong-Yu Yang[1], Andreas Läuchli[2], Frederic Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany — [2]Max Planck Institut für Physik komplexer Systeme, Nöthnitzerstrasse 38, 01187 Dresden, Germany — [3]Institute for Theoretical Physics, EPF Lausanne, 1015 Lausanne, Switzerland

The organic compound κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ exhibits strong evidence for a spin liquid phase at low temperatures. To study this possible spin liquid phase we investigate the quantum magnetism of the Hubbard model on the isotropic and anisotropic triangular lattice at half filling. First, we quantitatively derive effective quantum spin models using perturbative continuous unitary transformations. The accuracy of this spin model is determined by comparing it with exact diagonalizations (ED) on the original Hubbard model. In the second step we use ED to analyze the properties of the spin model on larger clusters. We find clear evidence for the existence of a spin liquid phase located between the long-range ordered antiferromagnet and the metallic phase. Finally, the anisotropic case is tackled which is expected to give further insights into the quantum magnetism of the organic compound.

TT 12.12 Tue 12:30 H19

Quantum spin-liquid state emerging in two-dimensional correlated Dirac fermions — Zi Yang Meng[1], •Thomas C. Lang[2], Stefan Wessel[1], Fakher F. Assaad[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We analyze the ground-state of the Hubbard model of spin-$\frac{1}{2}$ Dirac fermions on the honeycomb lattice at half-filling, using large-scale quantum Monte Carlo simulations. We find that the weak coupling semimetal and the antiferromagnetic Mott insulator at strong interactions are separated by an extended gapped phase in an intermediate coupling regime. Exploring excitation gaps, correlation functions as well as probing for flux quantization, we conclude that a spin liquid, lacking any conventional order (i.e. symmetry breaking), emerges in the vicinity of the Mott transition with local correlations best described by resonating valence bonds.

TT 12.13 Tue 12:45 H19

Competing interactions and symmetry breaking in the Hubbard-Holstein model — •Johannes Bauer — Max-Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

This contribution has been withdrawn.

TT 13: FS: Topological Defects in Electronic Systems

Time: Tuesday 9:30–13:45 Location: H20

Invited Talk TT 13.1 Tue 9:30 H20

Skyrmions in Chiral Magnets — •Ulrich K. Rössler, Andrei A. Leonov, Anna B. Butenko, and Alexei N. Bogdanov — IFW Dresden

In non-centrosymmetric magnets the chiral Dzyaloshinskii-Moriya (DM) exchange stabilizes tubular baby-Skyrmions. These are topologically non-trivial localized, but smooth and static textures of a spin system. Chiral Skyrmionic states may exist in various magnetic systems as the chiral DM-couplings stem from the leading spin-orbit effect, if they are allowed by crystal symmetry. Extended Skyrmionic textures are determined by the stability of the localized solitonic Skyrmion cores and their geometrical incompatibility, which frustrates a homogeneous space-filling. Two-dimensional models for these inhomogeneous magnetic states bear strong similarity with Abrikosov-lattices. Just as cylindrical vortices arrange into regular arrays in type-II superconductors, Skyrmions may form ordered arrays in chiral magnets. Basic phenomenological continuum theory suggests that a cornucopia of unexpected effects can be found in these chiral magnets. The isolated particle-like Skyrmion excitations may undergo confinement near the magnetic transition, and these molecular units may finally condense into extended mesophases. This magnetic 'Skyrmionic matter' strongly resembles chiral nematic liquid crystal textures. The underlying theoretical ideas shed new light on more fundamental question about the appearance of countable units in a continuum, and mechanisms for the formation of self-generated amorphous states.

Invited Talk TT 13.2 Tue 10:00 H20

Dirac Strings and Magnetic Monopoles in the Spin Ice, $Dy_2Ti_2O_7$ — •David Jonathan Pryce Morris[1], Alan Tennant[1,2], Santiago Grigera[3], Bastian Klemke[1,2], Claudio Castelnovo[4], Roderich Moessner[5], Clemens Czternasty[1], Michael Meissner[1], Kirrily Rule[1], Jens-Uwe Hoffmann[1], Klaus Kiefer[1], Damien Slobinsky[6], and Robin Perry[7] — [1]Helmholtz Center Berlin for Materials and Energy, Berlin, Germany — [2]Technische Universität Berlin, Germany — [3]Instituto de Fisica de Liquidos y Sistemas Biologicos, La Plata, Argentina — [4]University of Oxford, United Kingdom — [5]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [6]St. Andrews University, United Kingdom — [7]University of Edinburgh, Scotland

Recent proposals in condensed matter physics that magnetic monopoles can appear as emergent quasiparticles have attracted wide levels of interest. Dirac's original picture of magnetic monopoles had them connected to strings through which magnetic flux flowed. Here we report studies into a system called Spin Ice, where spins obey "ice rules" of 2 spins into and 2 spins out of their tetrahedron. In these materials it has been predicted that strings of spins form via a 3D Kasteleyn transition [1]. The geometry of spin-ice allows for net magnetic charge (magnetic monopoles) to form where "ice rules" are broken at the tips of the strings [2]. Here we present three experimental pieces of evidence for these strings and magnetic monopoles [3].

[1] Phys Rev. Lett. 100, 067207 (2008)
[2] Nature 451, 42 (2008)
[3] Science 326, 411 (2009)

Topical Talk TT 13.3 Tue 10:30 H20

Manifestations of monopole physics in spin ice materials — •Claudio Castelnovo[1], Roderich Moessner[2], and Shivaji Sondhi[3] — [1]University of Oxford, Oxford, UK — [2]MPI-PKS, Dresden, Germany — [3]Princeton University, Princeton, USA

Spin ice materials such as $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ provide a rare instance of fractionalisation in three dimensions: their elementary excitations carry a fraction of the magnetic moment of the microscopic spin degrees of freedom, and they can be thought of as magnetic monopoles.

The peculiar nature of these excitations leads to unique signatures in the equilibrium and response properties. These include unusual neutron scattering structure factors, dynamical arrest and long lived non-equilibrium metastable states, as well as a response to external magnetic fields that promotes spin ice as a magnetic analogue of an electrolyte. In this talk, we review several of these striking phenomena.

The formulation of the low-temperature phase in terms of an emergent gauge field permits an unusual degree of analytical progress in the modelling of these materials.

Invited Talk TT 13.4 Tue 11:00 H20

Skyrmion Lattices in Pure Metals and Strongly Doped Semiconductors — •Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85748 Garching, Germany

For a long time it was anticipated theoretically, that chiral magnets may support topological defects with the characteristics of skyrmions. We used neutron scattering and measurements of the Hall effect to identify the formation of two-dimensional lattices of skyrmion lines, a new form of magnetic order, in metallic and semiconducting B20 compounds, namely MnSi [1,2], $Mn_{1-x}Co_xSi$, $Mn_{1-x}Fe_xSi$ and $Fe_{1-x}Co_xSi$ [3]. The skyrmion lattices share remarkable similarities with vortex lattices in type II superconductors. For instance, they may exhibit domain formation and complex morphologies as seen, e.g., in ultrapure Nb [4]. Moreover, the pinning of the skyrmion lattices to the crystal lattice is extremely weak. In fact, they may be viewed as a spin crystal that is essentially disconnected from the atomic lattice. Our study establishes magnetic materials lacking inversion symmetry as an arena for new forms of order composed of topologically stable spin configurations.

[1] S. Mühlbauer, et al. , Science **323**, 915 (2009).
[2] A. Neubauer, et al., Phys. Rev. Lett. **102**, 186602 (2009).
[3] W. Münzer, et al., arXiv/0902.2587.
[4] S. Mühlbauer, et al., Phys. Rev. Lett. **102**, 136409 (2009).

15 min. break

Topical Talk TT 13.5 Tue 11:45 H20

Skyrmion lattice in MnSi — •Achim Rosch — Institute of Theoretical Physics, University of Cologne, 50937 Cologne, Germany

A magnetic skyrmion is a topologically stable vortex-like spin configuration. Similarly to a vortex lattice of a superconductor, a lattice of skyrmion lines is found [1] in the metallic magnet MnSi in a small magnetic field for a small range of temperatures. This state of matter is stabilized by weak spin-orbit interactions and thermal fluctuations. The topological winding number of the skyrmions implies that moving electrons pick up a Berry phase which leads to a characteristic contribution to the Hall constant [2] and an efficient coupling of currents to the magnetic structure. We therefore also investigate how spin-torque effects can lead to modifications of the magnetic structure when electric currents are applied.

[1] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A.

Neubauer, R. Georgii, P. Böni, Science **323**, 915 (2009).

[2] A. Neubauer, C. Pfleiderer, B. Binz, A. Rosch, R. Ritz, P. G. Niklowitz, P. Böni , Phys. Rev. Lett. **102**, 186602 (2009).

Invited Talk TT 13.6 Tue 12:15 H20

Topological Insulators in Applied Fields: Magnetoelectric Effects and Exciton Condensation — •Joel Moore — University of California, Berkeley CA USA

"Topological insulators" are insulating in bulk but have protected metallic surface states as a result of topological properties of the electron wavefunctions. Several examples have been discovered recently in ARPES experiments that directly probe the surface state, including its spin structure. One way to characterize the topological insulator is through its magnetoelectric response in a weak applied field: it generates an electrical polarization in response to an applied magnetic field, and a magnetization in response to an applied electrical field. This talk first reviews the origin of this response and its generalization to other insulators and topological states. A strong applied electrical field can combine with Coulomb interactions to generate an unusual "exciton condensate" involving both surfaces of a thin film of topological insulator. This exciton condensate has several topological features that distinguish it from an ordinary superfluid; the most significant is that vortices support midgap localized states ("zero modes" in the particle-hole symmetric case) with effective fractional charge $\pm e/2$.

Topical Talk TT 13.7 Tue 12:45 H20

Probing non-Abelian statistics with quasiparticle interferometry — •Kirill Shtengel — University of California, Riverside, USA

States of matter are conventionally classified according to broken symmetries. Topologically ordered phases fall outside of this paradigm: with no local order parameter, they nevertheless have many peculiar properties setting them apart from disordered phases. In 2D, such phases may support anyons - quasiparticles that are neither bosons nor fermions. Moreover, anyons with non-Abelian statistics can occur, particularly in the fractional quantum Hall regime.

In this talk, I will focus on solid state interferometers designed to detect such exotic statistics. I will discuss Recent experiments in the the quantum Hall regime at 5/2 filling where the evidence for the existence of non-Abelian anyons may have in fact been observed for the first time. I will also mention potential applications of such interferometeric schemes for topological quantum computation.

Topical Talk TT 13.8 Tue 13:15 H20

Spin Hall effects in HgTe Quantum Well Structures — •Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Recently, it was pointed out that inverted HgTe structures are topologically non-trivial insulators, in which the quantum spin Hall insulator state should occur. In this novel quantum state of matter, a pair of spin polarized helical edge channels develops when the bulk of the material is insulating, leading to a quantized conductance. I will present transport data provide very direct evidence for the existence of this third quantum Hall effect: when the bulk of the material is insulating, we observe a quantized electrical conductance. Further experiments, using non-local transport measurements, show that the charge transport occurs through helical edge channels. The spin polarization of the edge channels can be demonstrated in split gate devices that are partially in the insulting and partly in the metallic regime, making use of the occurrence of the non-quantized metallic spin Hall effect to convert the magnetic spin signal into an electrical one.

TT 14: TR: Graphene 2

Time: Tuesday 9:30–12:45 Location: H21

TT 14.1 Tue 9:30 H21

Relativistic quantum Corbino effect in graphene — •Adam Rycerz — Institut für Theoretische Physik, Universität Regensburg, D–93040, Germany — Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, PL–30059 Kraków, Poland

Electron transport through the Corbino disk in graphene is studied in the presence of uniform magnetic fields. At the Dirac point, we observe conductance oscillations with the flux piercing the disk area Φ_d, characterized by the period $\Phi_0 = (2h/e)\ln(R_o/R_i)$, where R_o (R_i) is the outer (inner) disk radius. The oscillations magnitude increase with the radii ratio and exceed 10% of the average conductance for $R_o/R_i \geqslant 5$ in the case of the normal Corbino setup, or for $R_o/R_i \geqslant 2.2$ in the case of the Andreev-Corbino setup. At a finite but weak doping, the oscillations still appear in a limited range of $|\Phi_d| \leqslant \Phi_d^{max}$, away from which the conductance is strongly suppressed. At large dopings and weak fields we identify the crossover to a ballistic transport regime.

[1] A. Rycerz, arXiv:0909.3018 (unpublished).

TT 14.2 Tue 9:45 H21

Electrical transport and low-temperature scanning tunneling microscopy of microsoldered graphene — •Viktor Geringer[1], Dinesh Subramaniam[1], Ann-Kathrin Michel[1], Bart Szafranek[2], Daniel Schall[2], Alexander Georgi[1], Torge Mashoff[1], Daniel Neumaier[2], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

Using the recently developed technique of microsoldering [1], we perform a systematic transport study of the influence of PMMA on graphene flakes revealing a doping effect of up to $\Delta n = 3.8{\times}10^{12}\,\mathrm{cm}^{-2}$, but a negligible influence on mobility and gate voltage induced hysteresis. Moreover, we show that the microsoldered graphene is free of contamination and exhibits a very similar intrinsic rippling as has been found for lithographically contacted flakes. Finally, we demonstrate a current induced closing of the previously found phonon gap appearing in scanning tunneling spectroscopy experiments, strongly non-linear features at higher bias probably caused by vibrations of the flake and a B-field induced double peak attributed to the 0. Landau level of graphene.

[1] Ç. Ö. Girit and A. Zettl, Appl. Phys. Lett. 91, 193512 (2007).

TT 14.3 Tue 10:00 H21

Spin injection in graphene spin valve devices via thin MgO barriers — •Tsung-Yeh Yang[1], Julia Samm[1], Marc Drögeler[1], Sebastian Blaeser[1], Frank Volmer[1], Mihaita Popinciuc[1], Jayakumar Balakrishnan[2], Ahmet Avsar[2], Manu Jaiswal[2], Mingang Zheng[2], Bernd Beschoten[1], Barbaros Oezyilmaz[2], and Gernot Güntherodt[1] — [1]II. Physikalisches Institut, RWTH Aachen University, Templergraben 55, 52056 Aachen, Germany — [2]Department of Physics, National University of Singapore, 2 Science Drive 3 Singapore 117542

We report all-electrical spin transport measurements in non-local spin valve structures on graphene at room temperature. The graphene flakes were deposited on Si/SiO_2 substrates by mechanical exfoliation. The application of a back gate voltage allows for continuous control of the charge carrier type and density. Using ferromagnetic Co electrodes, efficient spin injection/detection was realized via thin MgO layers introduced between Co and graphene. Spin valve and Hanle spin precession measurements were performed for various charge carrier densities. The measurements at room temperature reveal the charge carrier mobilities of 4-5x10^3 cm^2/Vs and spin relaxation lengths of about 3 micrometers in the metallic conduction regime. Temperature dependent measurements of the Co/MgO/graphene contacts resistances indicate that the thin MgO layers behave as tunnel barriers.

This work is supported by DFG through FOR 912.

TT 14.4 Tue 10:15 H21

Direct measurement of the electron mean free path in few layer graphene samples — •Srujana Dusari, Jose Barzola-Quiquia, and Pablo Esquinazi — Division of Superconductivity and magnetism, Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany

The large coherence length of the electrons in graphite is expected to lead to a long electronic mean free path and to a large spin-diffusion length even at room temperature [1]. The aim of this work is the direct measurement of the electron mean free path, Fermi wavelength and mobility and their temperature dependence in multigraphene sam-

ples, i.e. micrometer large few layer graphene (FLG) samples with thickness below 100 nm. This is possible by studying the electronic transport through constrictions using specific design and nanostructuring of the sample. By measuring the resistance before and after making constrictions of different size it is possible to obtain the necessary parameters [1]. We developed a new method to avoid Ga+ ion contamination while making the constriction on the samples. First results on the temperature dependence of the mean free path in FLG samples obtained without free parameters will be presented.

[1]. N García, P. Esquinazi, J. Barzola-Quiquia, B. Ming, and D. Spoddig, Phys. Rev. B 78, 035413 (2008).

TT 14.5 Tue 10:30 H21

Electronic properties of graphene nanoribbons under gate electric fields — •Tobias Burnus[1], Daniel Wortmann[1], Yuriy Mokrousov[1], Gustav Bihlmayer[1], Stefan Blügel[1], and Klaus Michael Indlekofer[2] — [1]Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Hochschule RheinMain, Unter den Eichen 5, 65195 Wiesbaden, Germany

Graphene nanoribbons (GNR) hold great future promise for field-effect transistor and quantum dot (QD) devices. The gate electrodes and the electric field distribution play a crucial role. For a realistic description of a quantum dot, the many-body interaction of the few electrons in the quantum dot have to be described properly. The QD itself is formed by the vast number of electrons in a many nanometer long ribbon under the presence of a gate. As a first step, the GNR is calculated using density-functional theory (DFT), where the gate electrode is simulated by an inhomogeneous charge-sheet placed atop of the ribbon. Hereby, all electrons in the GNR are taken into account and one can directly calculate the dielectric constant ε and changes in the charge density due to the applied voltage on the gates. Using this technique, adatoms or different ribbon terminations can be taken into account. Based on the resulting matrix elements, the few electron problem of the GNR QD is treated within a relevant many-body subspace by means of configuration interaction (CI). In the presentation, the first result along this line will be shown. The work is supported by the DFG Research Unit 912 "Coherence and Relaxation Properties of Electron Spins".

TT 14.6 Tue 10:45 H21

How Graphene-like is Epitaxial Graphene? Quantum Oscillations and Quantum Hall Effect — •Johannes Jobst[1], Daniel Waldmann[1], Florian Speck[2], Roland Hirner[2], Duncan K. Maude[3], Thomas Seyller[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Laboratoire des Champs Magnétiques Intenses, 25 Avenue des Martyrs, 38042 Grenoble, France

We report on the transport properties – in particular charge carrier density, mobility, conductivity and magnetoconductance – of high-quality single-layer graphene. Graphene was epitaxially grown on the silicon terminated face of a semi-insulating 6H silicon carbide substrate and then patterned into devices of different geometry and size. Large samples as well as submicrometer-sized Hall bars which are entirely lying on atomically flat substrate terraces yield similar transport properties confirming the uniformity of the epitaxial process. In high magnetic fields Shubnikov-de Haas oscillations with the distinct Landau level spectrum of single-layer graphene are clearly visible in samples with different charge carrier densities. When gated close to the Dirac point, the mobility increases substantially, and the graphene-like quantum Hall effect occurs. This proves that epitaxial graphene is ruled by the same pseudo-relativistic physics observed previously in exfoliated graphene.

15 min. break

TT 14.7 Tue 11:15 H21

Top and bottom gated field effect devices on epitaxial graphene — •Daniel Waldmann[1], Johannes Jobst[1], Florian Speck[2], Thomas Seyller[2] und Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universtität Erlangen-Nürnberg, Erlangen, Germany — [2]Lehrstuhl für Technische Physik, Universtität Erlangen-Nürnberg, Erlangen, Germany

We fabricate high-quality epitaxial graphene devices (Hall bars) for electrical transport measurements. In order to tune the charge density in the graphene layer, we developed different gating schemes (top gate and bottom gate). As a top gate we either used an electrochemical gate employing an ionic liquid or a solid state gate using aluminium oxide. A bottom gate has the advantage of leaving the graphene layer open. We have opted for an implanted conducting layer buried in the semi-insulating silicon carbide substrate. Hence, the SiC above the implanted gate serves both as substrate and gate dielectric. We present experimental data from low temperatures to room temperature which cover a broad range of charge densities including the electron hole transition at the Dirac point. Advantages and limitations of each method are discussed.

TT 14.8 Tue 11:30 H21

Giant Rashba splitting in Au-intercalated graphene — •Dmitry Marchenko[1], Andrei Varykhalov[1], Markus R. Scholz[1], Oliver Rader[1], Gustav Bihlmayer[2], and Emmanuel I. Rashba[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie — [2]Institut für Festkörperforschung, Forschungszentrum Jülich — [3]Department of Physics and Center for Nanoscale Systems, Harvard University

The use of graphene for spin transport [1] is generally connected to the small size of its intrinsic spin-orbit coupling leading to a splitting of the order of 0.01 to 0.1 meV [2]. This small value can be enhanced by a Rashba effect from a substrate [3] which couples graphene spin and pseudospin [4]. For the graphene-Au interface created by intercalation of a Au monolayer between graphene and Ni(111) a spin-orbit splitting of $\Delta_{so} \sim 13$ meV was measured [3]. By optimized sample preparation, we obtain now Δ_{so} values of the order of 100 meV near the Fermi energy by spin- and angle-resolved photoelectron spectroscopy, i. e., an enhancement by 3 to 4 orders of magnitude relative to the intrinsic values. We discuss the origin of this large splitting with the help of ab initio density functional calculations using the generalized gradient approximation.

[1] N. Tombros et al., Nature 448, 571 (2007)
[2] J. C. Boettger and S. B. Trickey, Phys. Rev. B 75, 121402(R) (2007); C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005)
[3] A. Varykhalov et al., Phys. Rev. Lett. 101, 157601 (2008)
[4] E. I. Rashba, Phys. Rev. B 79, 161409(R) (2009)

TT 14.9 Tue 11:45 H21

Spin relaxation of conduction electrons in Graphene induced by impurities — Martin Gradhand[1], •Dmitry Fedorov[2], Sergey Ostanin[1], Igor Maznichenko[2], Arthur Ernst[1], Peter Zahn[2], and Ingrid Mertig[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Martin-Luther-Universität Halle, Institut für Physik, D-06099 Halle, Germany

Graphene is a very attractive system for future spintronics applications. Experiments [1,2] have shown unexpected fast spin relaxation of conduction electrons in Graphene. A probable explanation is based on the dominance of the Elliott-Yafet spin relaxation mechanism.
Recently, we have developed a fully relativistic ab initio approach, based on the Korringa-Kohn-Rostoker method, for a theoretical study of the Elliott-Yafet mechanism caused by impurities [3]. Here we present our calculations of the spin-flip scattering time in Graphene via the Elliott-Yafet mechanism and estimate the Dyakonov-Perel spin relaxation time.

[1] N. Tombros et al., Nature 448, 571 (2007)
[2] N. Tombros et al., Phys. Rev. Lett. 101, 046601 (2008)
[3] M. Gradhand et al., submitted to Phys. Rev. B (2009)

TT 14.10 Tue 12:00 H21

The x-ray edge problem in graphene — Georg Röder[1], Grigory Tkachov[2], and •Martina Hentschel[1] — [1]MPI für Physik komplexer Systeme, Dresden — [2]Julius-Maximilians-Universität Würzburg

The excitation of a core electron to the conduction band by an x ray leads to the sudden creation of a localized, attractive potential and triggers the many-body responses that contribute to the x-ray edge problem, namely Anderson orthogonality catastrophe and Mahan's exciton (Mahan-Nozieres-DeDominicis response). We study them in mesoscopic systems, in particular for graphene, where the discrete level structure, boundary effects, and the filling-dependent variations in the density of states cause characteristic deviations from the well-understood bulk (metallic) behavior. The vanishing of the density of states at the Dirac points suppresses the orthogonality catastrophe. In the photoabsorption cross section, and for fillings smaller than

half-filling, an additional Fermi-edge singularity develops at the Dirac point, similar to the behavior that, in metals, is known as the opening of a second band. We furthermore discuss the role of edge states that occur on zig-zag edges and their influence on the photoabsorption cross section.

TT 14.11 Tue 12:15 H21

Analog of graphene using microwave photonic crystals — •Maksim Miski-Oglu[1], Stefan Bittner[1], Barbara Dietz[1], Pedro Oria Iriarte[1], Achim Richter[1,2], and Florian Schaefer[3] — [1]Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany — [2]ECT*, Villa Tambosi, I-38100 Villazzano (Trento), Italy — [3]LENS, University of Florence, I-50019 Sesto-Fiorentino (Firenze), Italy

A Dirac spectrum has been measured in a microwave photonic crystal consisting of a triangular lattice of metallic cylinders placed between two metallic plates. Up to a certain excitation frequency the wave propagation in this structure is governed by the 2D Helmholz equation with Dirichlet conditions at the boundaries of the cylinders. Microwave power is coupled into the periodioc structure via one dipole antenna and the reflected power is measured. It is proportional to the local density of states at the position of the antenna. In a Dirac spectrum the local density of states tends to zero linearly with the frequency at the Dirac point where two bands approach each other as a pair of cones. This linear character of the dispersion relation is clearly seen in the measured reflection spectra. These and measured wave functions are presented in the talk. It is argued, that these experiments offer the possibility to study a variety of phenomena connected with graphene as well as with QED in the table top experiments in photonic crystals with well controlled parameters.

This work has been supported within the DFG grant SFB634.

TT 14.12 Tue 12:30 H21

Time-resolved spectroscopy of graphene — •Tim Botzem[1], Tobias Plötzing[1], Bart Szafranek[2], Daniel Schall[2], Daniel Neumaier[2], and Heinrich Kurz[1] — [1]Institut für Halbleitertechnik, RWTH Aachen, Gemany — [2]AMICA, AMO GmbH, Aachen, Gemany

In graphene the coupling of various quasi particles accounts for the ultrafast temporal evolution of nonequilibrium carrier distributions. Hence understanding of the relaxation processes is crucial for designing high speed electronic and photonic devices. For investigating the involved quasi particle interactions we apply femtosecond pump-probe spectroscopy (17 fs temporal resolution) on exfoliated graphene mono- and bilayer flakes prepared on transparent sapphire substrates. Relaxation of hot carriers takes place within the first few tens of femtoseconds after excitation, revealing the strong coupling between the different quasi particles involved. A detailed analysis of the dependence on excitation fluence, carrier concentration and fabrication method will be given.

TT 15: MLT: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 1

Time: Tuesday 14:00–16:15 Location: H18

TT 15.1 Tue 14:00 H18

Transport and scale invariance in the unitary Fermi gas — •Tilman Enss and Wilhelm Zwerger — Technische Universität München, Germany

The string theory conjecture of a universal lower bound on the shear viscosity to entropy ratio, characterizing a perfect fluid, has stimulated work from nuclear physics to ultracold atoms. We compute the bulk and shear viscosities of a strongly interacting Fermi gas in three dimensions above the superfluid transition temperature using a diagrammatic technique. It is shown that vertex corrections and the associated Aslamazov-Larkin contributions are crucial to reproduce the correct high-temperature limit and the vanishing of the bulk viscosity due to scale invariance. The resulting shear viscosity to entropy ratio has a minimum value above the superfluid transition that is a factor of five above the string theory bound. The results are compared to recent experimental data on the damping of collective modes of a trapped unitary Fermi gas.

TT 15.2 Tue 14:15 H18

Ward identities and skeleton equations in the functional renormalization group approach to the BCS-BEC crossover — •Lorenz Bartosch[1], Peter Kopietz[1], and Alvaro Ferraz[2] — [1]Institut für Theoretische Physik, Universität Frankfurt, Germany — [2]International Center for Condensed Matter Physics, Universidade de Brasília, Brazil

We use the functional renormalization group approach with partial bosonization in the particle-particle channel to study the effect of order parameter fluctuations on the BCS-BEC crossover of superfluid fermions in three dimensions. Our approach is based on a new truncation of the vertex expansion where the renormalization group flow of bosonic two-point functions is closed by means of skeleton equations (Dyson-Schwinger equations) and the superfluid order parameter is related to the single particle gap via a Ward identity. We explicitly calculate the chemical potential, the single-particle gap, and the superfluid order parameter at the unitary point and compare our results with experiments and previous calculations.

TT 15.3 Tue 14:30 H18

Elastic anomalies at the field-induced quantum-critical point in the quasi 2D-antiferromagnet Cs_2CuCl_4 — •P. T. Cong, B. Wolf, S. Belz, N. Krüger, F. Ritter, W. Assmus, and M. Lang — Physikalisches Institut, Goethe- Universität, SFB/TR 49, D-60438 Frankfurt(M).

The quasi-2D antiferromagnet Cs_2CuCl_4 is one of the prime examples where the phenomenon of Bose-Einstein condensation (BEC) of magnetic excitations has been discussed [1]. The long-range antiferromagnetic order can be suppressed to $T_N = 0$ in a magnetic field $B_c \sim 8.5$ T (B//a), which constitutes a quantum critical point (QCP). At B_c, quantum-critical fluctuations are expected to give rise to anomalous physical properties at finite temperatures. Here we present a detailed investigation of the elastic constants and ultrasonic attenuation near the B-induced QCP. Distinct anomalies were found at $B_c \sim 8.5$ T, which are particularly strongly pronounced in the ultrasonic attenuation. Around B_c below 0.2 K the ultrasonic attenuation of the c_11 mode exhibits a pronounced double structure, reminiscent of two anomalies of different origin. One is very sharp, strongly temperature dependent and is located at $T_N(B)$ and the other one is distinctly broader at slightly higher fields. [1] T. Radu *et al.*,PRL 95, 127202, (2005)

Invited Talk TT 15.4 Tue 14:45 H18

Superconductivity vs. Superinsulation in TiN Thin Films — •Christoph Strunk — Universität Regensburg, D-93040 Regensburg, Germany

TiN thin films display a very sharp superconductor-insulator transition both vs. degree of disorder and vs. magnetic field. In the insulating phase an abrupt drop of the already low, thermally activated conductance is observed below certain threshold voltages V_{th}, which has been interpreted as the transition to a novel 'superinsulating' state at very low temperatures [1]. Subsequently, similar experiments on InO_x have been interpreted in terms of electron heating of an insulator with a strongly temperature-dependent conductance [2]. The experiments on the insulating side of the transition are complemented by a study of the IV-characteristics on the superconducting side, which demonstrates a striking duality between the transport characteristics on both sides of the transition. Our results are discussed in the light of recent experimental and theoretical developments.

[1] V. Vinokur *et al.*, Nature **452**, 613 (2008).

[2] M. Ovadia, B. Sacepe and D. Shahar, PRL **102**, 176802 (2009).

TT 15.5 Tue 15:15 H18

Bogoliubov excitations in correlated disorder potentials — •Christopher Gaul and Cord A. Müller — Physikalisches Institut, Universität Bayreuth, Deutschland

Bogoliubov excitations carry precious information about the properties of disordered Bose-Einstein condensates. By a saddle-point expansion of the Gross-Pitaevskii energy functional around the disorder-modified ground state, we derive the effective Hamiltonian for the Bogoliubov excitations [1]. Expectation values of physically interesting quantities

are obtained by weak-disorder perturbation theory in the Nambu formalism. We extend previous work in the hydrodynamic regime [2] and compute the disorder-broadened dispersion relation for arbitrary condensate healing length, disorder correlation length and excitation wavelength. Observable disorder-induced effects are predicted for the excitation lifetime and localization length, their speed of sound and average density of states.

[1] Gaul and Müller, Europhys. Lett., 83, 10006 (2008)
[2] Gaul, Renner and Müller, Phys. Rev. A, 80, 053620 (2009)

TT 15.6 Tue 15:30 H18

Impurities in the hardcore Bose-Hubbard model and the xxz model on the triangular lattice — •Xuefeng Zhang[1,2], Yuchuan Wen[3], and Sebastian Eggert[2] — [1]Institute of theoretical physics of Chinese Academy of Science, Beijing, China — [2]Department of Physics of Univ. Kaiserslautern, Ksierslautern,Germany — [3]Capital Normal university, Beijing, China

The ferromagnetic-antiferromagnetic xxz model is equivalent to the hardcore Bose-Hubbard model. On a triangular lattice frustration effects give rise to interesting physical behavior, including a realization of a supersolid phase. We now consider vacancies in this model using a combination of numerical Monte Carlo simulations and analytic calculations. The solid order and the superfluid density show characteristic changes locally around the impurity depending on the phase. In some cases a single impurity can affect the physical behavior of the entire system. The results show an interesting competition of the different order parameters and illustrate the nature of the excitations in the different phases.

TT 15.7 Tue 15:45 H18

Numerical analysis of dissipation-induced correlations in 1D bosonic systems — •Martin Kiffner and Michael Hartmann — Technische Universität München, Physik-Department I, James-Franck-Straße, 85748 Garching, Germany

In one-dimensional systems, bosons can behave with respect to many observables as if they were fermions. This strongly correlated regime of a Tonks-Girardeau (TG) gas regime can be reached for strong repulsive interactions between the particles. Recently, an experiment [1] with cold molecules showed that not only elastic interactions, but even two-particle losses alone are able to create a TG gas. Theoretical work [2] suggests that a dissipation induced TG gas could also be realized with polaritons. The molecular and the polariton system are both described by a master equation for bosons in a one-dimensional setting that experience inelastic two-particle interactions.

Here we present a numerical analysis of this master equation via a time-evolving block-decimation (TEBD) algorithm. In particular, we address the preparation of the strongly correlated regime starting from an uncorrelated state and discuss the time evolution of local as well as non-local observables.

[1] N. Syassen, D. M. Bauer, M. Lettner, T. Volz, D. Dietze, J. J. Garcia-Ripoll, J. I. Cirac, G. Rempe, S. Dürr, Science **320**, 1329 (2009).
[2] M. Kiffner and M. J. Hartmann, arXiv:0908.2055.

TT 15.8 Tue 16:00 H18

ac-driven atomic quantum motor — •Sergey Denisov, Alexey V. Ponomarev, and Peter Hanggi — Institute of Physics, University of Augsburg, Germany

Our ac-driven quantum motor [1,2,3] consists of only two different, interacting ultracold atoms placed into a ring-shaped optical lattice. In this setup, while the first atom driven by an external magnetic field carries a current, the second one serves as a quantum starter. We demonstrate that (i) for zero-momentum initial conditions the asymptotic carrier velocity converges to a unique non-zero value, and (ii) the atomic quantum motor is able to perform a work against a constant load.

[1] A. V. Ponomarev, S. Denisov, and P. Hanggi, Phys. Rev. Lett. **102**, 230601 (2009);
[2] A. V. Ponomarev, S. Denisov, and P. Hanggi, arXiv:0909.2813 (in press)
[3] Adrian Cho, feature in Science, web-link:
http://sciencenow.sciencemag.org/cgi/content/full/2009/609/1

TT 16: CE: Quantum-Critical Phenomena 1

Time: Tuesday 14:00–16:15 Location: H19

TT 16.1 Tue 14:00 H19

Specific heat and magnetocaloric effect at the field-induced quantum-critical point in $CeCu_{5.7}Au_{0.3}$ — •Michael J. Wolf, Gernot Goll, Veronika Fritsch, and Hilbert v. Löhneysen — Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

The heavy-fermion system $CeCu_{6-x}Au_x$ can be tuned to a quantum critical point by application of different tuning parameters such as pressure or magnetic field. We present specific heat measurements on single crystalline $CeCu_{5.7}Au_{0.3}$ in the temperature range from 70 mK to 1.5 K and in magnetic fields up to 4 T with $B \parallel c$. In addition, the magnetocaloric effect was measured in the temperature range from 70 mK to 1 K and in magnetic fields up to 2 T. The critical magnetic field B_c was determined to be $B_c = 0.95 \pm 0.1$ T. At the critical magnetic field the specific heat data can be well described by the self-consistent spin-fluctuation model of Moriya and Takimoto [1]. The magnetocaloric data at low temperatures show a jump of the magnetic Grüneisen ratio at the phase boundary for $B < B_c$ as well as a monotonic increase towards the lowest measured temperatures for $B > B_c$. These results are compared to previous magnetization measurements and discussed within the framework of theoretical models.

[1] T. Moriya and T. Takimoto, J. Phys. Soc. Japan 64 (1995), 960.

TT 16.2 Tue 14:15 H19

Magnetocaloric effect in $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ — •Alexander Steppke, Niels Oeschler, Cornelius Krellner, Manuel Brando, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Str. 40, 01187 Dresden, Germany

The magnetic Grüneisen ratio is defined as $\Gamma_H = -(dM/dT)_H/C_H = 1/T(dT/dH)_S$. Investigation of the magnetocaloric effect (MCE) therefore provides a direct measure of Γ_H. At a field-induced quantum critical point (QCP) the critical part of Γ_H, Γ_H^{cr}, is expected to diverge and to change its sign across the QCP, indicating the accumulation of entropy [1]. The heavy-fermion compound $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ is a prototype system which allows us to study a field-induced QCP [2]. In zero field this compound exhibits two antiferromagnetic transitions at $T_N = 0.4$ K and $T_L = 0.07$ K, which can be continuously suppressed by small magnetic fields $\mu_0 H_N = 0.24$ T and $\mu_0 H_L = 0.05$ T, respectively. At these fields a maximum in $S(H)$, i.e. a minimum in $dT/dH(H)$, is anticipated. We measured the MCE and the specific heat of $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ down to 0.025 K. Across both T_N and T_L, Γ_H^{cr} changes sign, since dT/dH shows a kink or a minimum. The kink at T_N follows the phase boundary $T_N(H)$ and disappears for $T \to 0$. However, the minimum at T_L is more pronounced in dT/dH, indicating a significant change in entropy. This change in entropy seems to be located near to but not at the phase boundary $T_L(H)$.

[1] L. Zhu *et al.*, PRL **91** (2003) 066404; M. Garst and A. Rosch, PRB **72** (2005) 205129
[2] S. Friedemann *et al.*, Nat. Phys. **5** (2009) 465.

TT 16.3 Tue 14:30 H19

Magnetocaloric effect of $YbRh_2Si_2$ at field-induced QCP — •Y. Tokiwa — I. Physik. Institut, Georg-August Universität Gottingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We develop a system to measure a magneto-caloric effect, dT/dH, at low temperatures down to ∼50 mK to study the field-induced QCP of $YbRh_2Si_2$. The key quantity for a study of field-induced QCP called magnetic Grüneisen ratio, $\Gamma_{mag}=1/T(dT/dH)=1/T(dT/dH)=-(dM/dT)/C$ (M: magnetization, C: specific heat), for this compound was previously obtained by measuring both M and C at the critical field H_{cr}=0.06 T and above. We obtained Γ_{mag} by measurements of dT/dH, which have the following advantages over the combination of M and C measurements. (1) Γ_{mag} can be obtained at very low fields (and also at zero-field), while it is very difficult with M and C because M becomes very small at low fields (impossible at zero-field because magnetization is zero). (2) Since it is a single measurement, possible error in Γ_{mag} is expected

to be smaller compared to the two separated measurements combined. We discuss the details of the measurement technique and the results on $YbRh_2Si_2$ around H_{cr}, including the un-explored field-range below H_{cr}. This work is done by the collaboration with H. S. Jeewan and P. Gegenwart and supported by DFG through research unit 960 (Quantum phase transitions).

TT 16.4 Tue 14:45 H19

Magnetic properties of $YbCo_2Si_2$ studied by neutron diffraction — •Nandang Mufti, Oliver Stockert, Koji Kaneko, Cornelius Krellner, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

While for most rare earth element R magnetic ordering in RT_2X_2 (T= transition metal and X = Si, Ge) has been thoroughly investigated, only very few results are available for Yb homologous. In this context $YbCo_2Si_2$ is very interesting because it is isoelectronic to quantum critical system $YbRh_2Si_2$. It presents a stable Yb^{3+} state which shows magnetic ordering at 1.7 K. We recently grew single crystals and started a extensive study of the magnetic properties of this compound. Magnetic susceptibility, specific heat, and electrical resistivity results evidenced a pronounced easy plane anisotropy and two magnetic transitions at $T_N \sim 1.7$ K and $T_L \sim 0.9$ K. Magnetization, susceptibility and magnetoresistance measurements indicate a complex B-T phase diagram with some anisotropy in the basal plane. Here, we will present the results of our investigation with single crystal and powder neutron diffractions in absence and under magnetic field up to 2.5 T. A commensurate magnetic structure with q = (0.25, 0.25, 1) and incommensurate magnetic structure with q= (0.25, 0.08, 1) are observed for the ground state and intermediate phase, respectively. The critical exponent β for T_N is obtained as $\beta = 0.369 \pm 0.03$ which is close to the expected value of 3D Heisenberg system. We shall propose a magnetic structure for both ordered phases.

TT 16.5 Tue 15:00 H19

Tuning the Eu valence in $EuPd_3B_x$ by B substitution and pressure - a joint experimental and theoretical study — •Miriam Schmitt[1], Roman Gumeniuk[1], Andreas Leithe-Jasper[1], Walter Schnelle[1], Marcus Schmidt[1], Angela Trapananti[2], Giuliana Aquilanti[2], Ulrich Schwarz[1], and Helge Rosner[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]European Synchrotron Radiat Facil, Grenoble, France

Valence changes induced by doping as well as internal or external pressure often lead to quantum critical phenomena. For $EuPd_3B_x$, an isostructural phase transition upon B substitution, attended by a change of its magnetic properties, was predicted by band structure theory [1]. According to our calculational results, the phase transition in $EuPd_3B_x$ can be explained by a change of the Eu valence related to a change of the 4f occupation. Upon B insertion, the Eu^{3+} in $EuPd_3$ changes to Eu^{2+} in $EuPd_3B_x$ ($x \geq 0.2$). By applying pressure this effect can be reversed, driving a magnetic Eu^{2+} to a non magnetic Eu^{3+} state. To challenge the prediction of the transitions we carried out XRD and XAS measurements for different B contents as well as for a fixed B content under high pressure. To elucidate the origin of the magnetic change, the experimental results are complemented by density functional based ab-initio band structure calculations using the LDA+U approach (to include strong electron correlations of 4f electrons) and the coherent potential approximation (CPA, to describe substitutional disorder).

[1] C. Loison *et al.*, Phys. Rev. B 75, 205135 (2007).

TT 16.6 Tue 15:15 H19

Larmor Diffraction in the Ferromagnetic Superconductor UGe_2 — •Robert Ritz[1], Dmitry Sokolov[2], Thomas Keller[3], Andrew Huxley[2], and Christian Pfleiderer[1] — [1]Physik Department E21, TU München, D-85748 Garching, Germany — [2]School of Physics and Astronomy, and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh EH9 3JZ, UK — [3]MPI für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Larmor Diffaction (LD) is a neutron resonance spin-echo technique which allows the study of the lattice constant as well the distribution of lattice constants. It was traditionally thought that neutron spin-echo measurements cannot be used in materials such as superconductors or ferromagnets, because they strongly depolarize a polarized neutron beam. In UGe_2 we are able to demonstrate that this technique may be applied in ferromagnetic superconductors with a magnetic Ising anisotropy. UGe_2 exhibits two ferromagnetic phases which are separated by a transiton at temperature T_x. With increasing hydrostatic pressure superconductivity emerges at the pressure for which T_x is suppressed. Using LD we studied the temperature dependence of the lattice constant as well as the distribution of lattice constants for all three axis of UGe_2 down to 0.5 K and at pressures up to 12 kbar.

TT 16.7 Tue 15:30 H19

Exploring the magnetocaloric effect in Cs_2CuCl_4 close to the field-induced quantum-critical point — •Georg Hofmann, Berd Wolf, Sebastian Belz, Natalija Krüger, Franz Ritter, Wolf Assmus, and Michael Lang — Physikalisches Institut, SFB/TR 49, Goethe-University Frankfurt am Main, 60438 Frankfurt am Main, Germany

The compound Cs_2CuCl_4 is a quasi-2D geometrically frustrated $S = 1/2$ antiferromagnet which orders antiferromagnetically below $T_N = 1.6$ K. By increasing an external field to $B_c \approx 8.5$ T [1], T_N is suppressed to zero which marks a field-induced quantum-critical point (QCP). The QCP, although inaccessible by experiment, manifests itself at finite temperature in an unusual sensitiveness of thermodynamic properties on the tuning parameter [2]. In fact, for a field-induced QCP, a diverging magnetocaloric effect (MCE) $\Gamma_B = -(\partial S/\partial B)_T/C$ is expected [2, 3]. Here we present measurements of the MCE in the vicinity of B_c for the title compound by using a step-like measuring technique which ensures quasi-adiabatic conditions. Our results reveal incipient divergencies of Γ_B upon approaching the QCP both as a function of field and temperature, consistent with the expectations [3].

[1] Radu et al., Phys. Rev. Lett. **95**, 127202 (2005).
[2] Zhu et al., Phys. Rev. Lett. **91**, 066404 (2003).
[3] Garst et al., Phys. Rev. B **72**, 205129 (2005).

TT 16.8 Tue 15:45 H19

Low temperature properties of single crystal Fe_2TiSn under high pressure and magnetic field — •Andreas Neubauer[1], Michael Schulz[1,2], Christian Pfleiderer[1], Peter Böni[1], Klaudia Hradil[2], and Günther Behr[3] — [1]Physik Department E21, Technische Universität München, 85748 Garching, Germany — [2]Technische Universität München, Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II),Lichtenbergstr. 1, 85748 Garching, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, PF270116, 01171 Dresden, Germany

Electronic structure calculations predict a paramagnetic ground state for the Heusler compound Fe_2TiSn. However, the experimental investigation of polycrystals showed weakly ferromagnetic behaviour ($T_C \sim 250$ K), where the magnetic properties are extremely sensitive to sample synthesis. We were able to grow, for the first time, single crystals of Fe_2TiSn by the optical float zoning using an UHV-compatible image furnace. The inverse AC susceptibility of the single crystals shows a paramagnetic Curie-Weiss-behaviour from room temperature down to around 5K, followed by a transition to a so far unidentified phase. Interestingly, the inverse susceptibility extrapolates through $T = 0$, a behaviour expected for ferromagnetic quantum criticality. We investigated the pressure dependence of the magnetization, the longitudinal magneto-resistance and the Hall effect. These data are supplemented by neutron depolarization measurements. Possible implications of our observations for the possible nature of quantum criticality in Fe_2TiSn will be discussed.

TT 16.9 Tue 16:00 H19

Vibrating Coil Magnetometry of quantum criticality in the Ising Ferromagnet $LiHoF_4$ — •Stefan Legl[1], Bastien Dalla Piazza[2], Karl Krämer[3], Henrik Ronnow[2], and Christian Pfleiderer[1] — [1]Physik Department E21, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany — [2]EPFL, CH-1015 Lausanne, Switzerland — [3]Department of Chemistry & Biochemistry, University of Bern, CH-3012 Bern, Switzerland

$LiHoF_4$ develops Ising ferromagnetism below a Curie temperature, $T_C = 1.54$ K. The easy-axis magnetization of $LiHoF_4$ has recently attracted great interest as a testing ground for theoretical studies of domain formation in Ising systems. This is contrasted by the properties of $LiHoF_4$ for magnetic field applied transverse to the Ising axis, where susceptibility measurements suggest the existence of a quantum critical point at a critical field $H_c = 4.90$ T. An outstanding issue in studies of $LiHoF_4$ are direct measurements of the magnetization parallel to an applied magnetic field, $M_\parallel$, as the principle order parameter of the ferromagnetic state. We have used a newly developed vibrating coil magnetometer (VCM) as combined with a top loading dilution re-

frigerator for measurements of the field and temperature dependence of $M_{\|}$ in $LiHoF_4$ down to mK temperatures. We present first results of our measurements and a critical discussion of the agreement and disagreement with previous work.

TT 17: SC: Iron-Based Superconductors - Theoretical Approaches

Time: Tuesday 14:00–16:15 Location: H20

TT 17.1 Tue 14:00 H20

Relation of structure, magnetism, doping and pressure in $AFe_{2-x}T_xAs_2$ (T=Co,Rh,Ru) — •Helge Rosner, Walter Schnelle, Deepa Kasinathan, Miriam Schmitt, Ulrich Schwarz, Michael Nicklas, Christoph Geibel, and Andreas Leithe-Jasper — MPI-CPfS Dresden, Germany

We present an overview of our recent investigations on the $SrFe_{2-x}T_xAs_2$ (T = Co, Ru, Rh) compounds. In our joint experimental and theoretical study, we report the influence of hydrostatic pressure and substitution at the Fe site on the magneto-structural and superconducting transitions. The magnetism is weakened upon the application of pressure as indicated by resistivity, X-ray data and density functional band structure calculations. Similar to substitution on the Sr site, substitutions on the Fe-site quench the magnetic transition and induce bulk superconductivity with T_c up to 20 K for ambient pressure and up to 27 K for underdoped $SrFe_{2-x}Co_xAs_2$ for pressures of 2.6GPa. In our analysis, we attempt to disentangle the interplay of charge doping and structural changes induced by the substitution and by external pressure.

TT 17.2 Tue 14:15 H20

Magnetism and pairing symmetries in a three-orbital model for pnictides — •Maria Daghofer[1], Andrew Nicholson[2,3], Adriana Moreo[2,3], and Elbio Dagotto[2,3] — [1]IFW Dresden, Dresden, Germany — [2]University of Tennessee, Knoxville, USA — [3]Oak Ridge National Laboratory, USA

While the shape of the Fermi surface (FS) obtained with the local density approximation (LDA) can be reproduced by a two-orbital model, three orbitals are needed to produce the degeneracy of the hole pockets. We discuss a three-orbital model including the xz, yz, and xy orbitals of the iron ions, which qualitatively reproduces the FS shape and orbital composition obtained by LDA calculations for undoped pnictides [1,2]. Since this model is not at half filling, orbital order becomes a possibility in addition to various magnetic phases. Using numerical techniques, we find an antiferromagnetic metal at realistic Coulomb interaction, while orbital order is only induced at at interaction strengths that are probably too strong to be realistic for pnictides. We also investigate possible pairing operators allowed by the lattice symmetry. We find that almost all of them lead to intra- as well as inter-band pairing, i.e., Cooper pairs that are formed by two electrons coming either from the same or from different bands. We also discuss consequences of inter-band pairing.

[1] A. Moreo, M. Daghofer, A. Nicholson, E. Dagotto, PRB **80**, 104507 (2009)

[2] M. Daghofer, A. Nicholson, A. Moreo, and E. Dagotto arXiv:0910.1573

TT 17.3 Tue 14:30 H20

Spin Density Waves in the Iron Pnictides - Itinerant Magnetic Excitations — •Johannes Knolle[1], Ilya Eremin[1,2], and Andrey Chubukov[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institut für Mathematische und Theoretische Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [3]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

We study the spin wave excitations of the parent iron-based superconductors employing the three band model which consists of one hole pocket centered around the Γ-point, and two elliptic electron pockets centered around $(\pi, 0)$ and $(0, \pi)$ points of the Brillouin zone (BZ), respectively. Without taking ellipticity into account, the spin wave excitations are degenerate at $(\pi, 0)$ and $(0, \pi)$ points representing the degeneracy of the underlying spin state. The ellipticity removes the degeneracy and selects the required $(\pi, 0)$ or $(0, \pi)$ state. Simultaneously, it also leaves only one gapless Goldstone mode. We analyze the dispersion of the spin waves along the symmetry points of the first BZ for various strengths of the ellipticity parameter and compare the results with available experimental data. We find that neutron scattering data on the damping of the spin waves and their dispersion can be well described within the itinerant description.

TT 17.4 Tue 14:45 H20

Itinerant spin excitations in the spin-density-wave state of the iron pnictides — •Philip Brydon and Carsten Timm — Technische Universität Dresden, Dresden, Germany

The proper understanding of the antiferromagnetism of the iron pnictide parent compounds is expected to provide important insights into the superconductivity of these materials. We consider a model where the spin density wave (SDW) arises from an excitonic instability of nested electron-like and hole-like Fermi pockets [1]. Using the random phase approximation, we obtain the transverse spin susceptibility within the SDW state, which allows us to determine the collective spin-wave dispersions and the single-particle continua [2]. Our results are compared to experimental findings, and the implications for electronic-only models of the SDW order are discussed.

[1] P. M. R. Brydon and C. Timm, Phys. Rev. B 79, 180504(R) (2009).

[2] P. M. R. Brydon and C. Timm, Phys. Rev. B 80, 174401 (2009).

15 min. break

TT 17.5 Tue 15:15 H20

The Curious Iron Pnictides: A Mottness Point of View — •Mukul Laad[1] and Luis Craco[2] — [1]Institut für Theoretische Physik, RWTH Aachen D-52056, Aachen, Germany — [2]MPI-CPfS, Nöthnitzer Strasse 40, 01187 Dresden, Germany

Based on perusal of various experiments, we propose that Fe pnictides are "bad metals" close to a Mott-Hubbard instability, as in the classic V_2O_3. First-principles LDA+DMFT calculations confirm this suspicion, giving excellent quantitative agreement with a host of one- and two-particle responses.

We have studied the instability of this "bad metal" to an unconventional SC, whose gap function has an admixture of extended-s and s_{xy} components. This, to our knowledge, is the first time that such an instability has been studied within LDA+DMFT.

Invited Talk TT 17.6 Tue 15:30 H20

Nature of Pairing in the FeAs Superconductors — •Siegfried Graser[1], Thomas A. Maier[2], Alexander F. Kemper[3], Peter J. Hirschfeld[3], and Douglas J. Scalapino[4] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]University of Florida, Gainesville, USA — [4]University of California, Santa Barbara, USA

A comparison of the new high-T_c superconductors of the iron pnictide and chalcogenide family to the cuprates reveals startling similarities between the two classes: both are layered materials with mainly 2D character, a conductivity that is dominated by d-electrons, and an antiferromagnetic or spin-density wave phase in proximity to the superconducting state. However, the pronounced multiband character of the iron pnictides, that becomes manifest in several disconnected Fermi surface sheets, distinguishes them from the cuprates and requires a multiorbital description of its electronic properties. This multiorbital character of the bands at the Fermi level together with the rich momentum structure of the Fermi surface allows for a wide variety of possible superconducting ground states. We have explored the symmetry of the superconducting state assuming a pairing mechanism based on the exchange of spin fluctuations using a 5-orbital tight-binding Hamiltonian fitted to the LDA band structure of LaOFeAs. We could show that not only the symmetry but also the anisotropy of the pairing state depends sensitively on the intra- and interorbital interaction parameters.

TT 17.7 Tue 16:00 H20

Superconductivity in the Fe-Pnictides - From first principle calculations to effective RG studies — •Christian Platt[1], Ronny Thomale[2], Andrei Bernevig[2], Carsten Honerkamp[3], and Werner Hanke[1] — [1]Universität Würzburg — [2]Princeton University — [3]RWTH Aachen

The functional Renormalization Group (fRG) is used to determine the superconducting (SC) mechansim in the ferropnictides, with the main emphasis on distiguishing universal and material-specific aspects. To this end we use a five-band d-orbital whose interactions, in contrast to earlier fRG studies, are not taken as scalar model parameters, but calculated "a priori" from constrained RPA calculations. We universally find a SC pairing instability, driven by inter-Fermi surface (FS) scattering and resulting in a sign-changing s+- wave order parameter. However, the gap anisotropy is shown to be dependent on material-specific orbital parameter deviations not only by the "non-interacting" (i.e. LDA) part of the d-orbital Hamiltonian, but also by self-energy corrections.

TT 18: TR: Quantum Coherence and Quantum Information Systems 1

Time: Tuesday 14:00–16:15 Location: H21

TT 18.1 Tue 14:00 H21

Optimized Pulse Sequences for the Suppression of Decoherence in Quantum Information — •Stefano Pasini and Götz S. Uhrig — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund

The dynamical decoupling (DD) aims at suppressing the decoherence by means of coherent control pulses. Even if devices exist where instantaneous pulses are an adequate approximation, experimentally a finite duration τ_p and a bounded amplitude are inevitable. They are the cause of additional errors which can be corrected by designing the pulse shape appropriately. The new pulse has the overall effect of an ideal, instantaneous pulse with the advantage of decoupling the spin (or qubit) from the bath up to the order $O(\tau_p^3)$ [1]. The limitation of the no-go theorem for π pulses [2] is avoided. Hence, the Uhrig sequence (UDD) [3], originally thought for ideal π pulses, works also for bounded control Hamiltonians [4]. Numerical simulations show that concatenated sequences of real pulses are effective against general decoherence.

[1] S. Pasini, P. Karbach, C. Raas and G.S. Uhrig, Phys. Rev. A **80**, 022328 (2009)

[2] S. Pasini, T. Fischer, P. Karbach and G.S. Uhrig, Phys. Rev. A **77**, 032315 (2008)

[3] G.S. Uhrig, Phys. Rev. Lett. **98**, 100504 (2007)

[4] G.S. Uhrig and S. Pasini, arXiv:0906.3605

TT 18.2 Tue 14:15 H21

Landau-Zener Transitions in a Dissipative Environment: Numerically Exact Results — •Peter Nalbach and Michael Thorwart — Freiburg Institute for Advanced Studies (FRIAS), Albert-Ludwigs-Universität Freiburg, Albertstraße 19, 79104 Freiburg, Germany

We study Landau-Zener transitions in a dissipative environment by means of the numerically exact quasiadiabatic propagator path-integral [1]. It allows to cover the full range of the involved parameters. We discover a nonmonotonic dependence of the transition probability on the sweep velocity which is explained in terms of a simple phenomenological model. This feature, not captured by perturbative approaches, results from a nontrivial competition between relaxation and the external sweep.

[1] P. Nalbach and M. Thorwart, Phys. Rev. Lett. 103, 220401 (2009)

TT 18.3 Tue 14:30 H21

Spin and entanglement dynamics in Double Quantum Dots due to hyperfine interaction: A homogenous coupling approach — •Bjoern Erbe and John Schliemann — Institute of Theoretical Physics, University of Regensburg

Quantum dot spin qubits are among the most promising and most intensively investigated building blocks of possible future solid state quantum computation systems [1]. One of the major limitations of the decoherence time of the confined electron spin is its interaction with surrounding nuclear spins by means of hyperfine interaction [2]. Apart from this adverse aspect, hyperfine interaction can act as a ressource of quantum information processing [3]. For the above reasons it is of key interest to understand the hyperfine induced spin dynamics.

We consider the hyperfine interaction in a double quantum dot in zero magnetic field. We give an exact solution of the model for homogenous hyperfine coupling constants and derive the dynamics therefrom. By a detailed investigation of the short time spin dynamics we calculate the decoherence time, which turns out to be in very good agreement with experimental data.

[1] D. Loss and D.P. DiVincenco, Phys. Rev. A 57, 120 (1998)

[2] J. Schliemann, A. Khaetskii, and D.Loss, J. Phys.: Condens Matter 15, R1809-R1833 (2003)

[3] see e.g.: J.M. Taylor, A. Imamoglu, and M.D. Lukin, Phys. Rev. Lett.91, 246802 (2003

TT 18.4 Tue 14:45 H21

Probing Phases of Interacting Polaritons in Circuit QED Setups — •Martin Leib and Michael Hartmann — TU München,Munich,Germany

Circuit QED systems pose a new paradym for reaching the strong coupling regime of photonic and atomic degrees of freedom and are thus ideal candidates for quantum simulation and computation. We are investigating one-dimensional arrays of transmission-line cavities, where each cavity is coupled to a transmon-qubit. This system can be used as a quantum many-body simulator, lowering the experimental requirements for prescission control with respect to the use as a quantum computing device. We exploit the intermediate qubit-harmonic oscillator regime of the transmon to simulate Bose-Hubbard physics. As a suitable experimental setup we consider a system where the first cavity is driven by a classical microwave source and the output voltage is monitored, with respect to signatures of a quantum phase transition, at the last cavity.

15 min. break

TT 18.5 Tue 15:15 H21

Exact matrix product solutions in the Heisenberg picture of an open quantum spin chain — Stephen Clark[1,2], Javier Prior[3,4,5], •Michael Hartmann[6], Dieter Jaksch[2,1], and Martin Plenio[3,5,7] — [1]Centre for Quantum Technologies, National University of Singapore, Singapore — [2]Clarendon Laboratory, University of Oxford, United Kingdom — [3]Institute for Mathematical Sciences, Imperial College London, United Kingdom — [4]Departamento de Física Aplicada, Universidad Politécnica de Cartagena, Spain — [5]QOLS, The Blackett Laboratory, Imperial College London, United Kingdom — [6]Technische Universität München, Physik Department, Garching, Germany — [7]Institut für Theoretische Physik, Universität Ulm, Germany

The classical simulation of the dynamics of open 1D quantum systems with matrix product algorithms can often be significantly improved by performing time evolution in the Heisenberg picture [1]. For a closed system that is quadratic in fermionic (or bosonic) fields, the time-evolution of a creation operator can be represented exactly with matrices of dimension two for arbitrary long times. Here we show that this exact solution can be significantly generalized to include the case of an open quadratic fermi chain subjected to master equation evolution with Lindblad operators that are linear in the fermionic operators [2].

[1] M.J. Hartmann et al., Phys. Rev. Lett. **102** 057202 (2009)

[2] S.R. Clark et al., arXiv:0907.5582

TT 18.6 Tue 15:30 H21

Two-resonator circuit QED: Dissipative Theory — •Georg M. Reuther[1], David Zueco[1], Frank Deppe[2], Elisabeth Hoffmann[2], Edwin P. Menzel[2], Thomas Weissl[2], Matteo Mariantoni[2], Sigmund Kohler[3], Achim Marx[2], Enrique Solano[4], Rudolf Gross[2], and Peter Hänggi[1] — [1]Institut für Physik, Uni Augsburg, D-86135 Augsburg — [2]Walther-Meißner-Institut, Bayer. Akademie der Wissenschaften, D-85748 Garching — [3]Instituto de Ciencia de

Materiales de Madrid, CSIC, E-29049 Madrid — [4]Departamento de Quimica Fisica, Univ. del Pais Vasco, E-48080 Bilbao

Managing the interaction between two quantum objects is a fundamental issue for quantum information processing. A promising approach is a two-resonator circuit quantum electrodynamics setup referred to as quantum switch [1]. Here, a superconducting qubit provides switchable coupling between the resonators. This requires operation in the dispersive regime, where the qubit transition frequency is far detuned from those of the resonators. In our contribution we present a dissipative theory for the quantum switch [2]. We derive an effective Hamiltonian beyond rotating-wave approximation and study the dissipative dynamics within a quantum master equation approach. We derive analytically how the qubit affects the dynamics and the coherence of the switch even if its state remains constant, and we estimate the strength of this influence. Our results are corroborated by numerical simulations. We acknowledge support from SFB631 and NIM.

[1] M. Mariantoni *et al.*, Phys. Rev. B **78**, 104508 (2008)
[2] G. M. Reuther *et al.*, arXiv:0911.2657

TT 18.7 Tue 15:45 H21

Ferromagnetic spin quantum bits — •Audrey Cottet[1,2] and Takis Kontos[1,2] — [1]Ecole Normale Supérieure, Laboratoire Pierre Aigrain, 24 rue Lhomond, F-75231 Paris Cedex 05, France — [2]CNRS UMR 8551, Laboratoire associé aux Universités Pierre et Marie Curie et Denis Diderot, France

We propose theoretically a scheme for implementing a spin quantum bit in a quantum dot circuit with ferromagnetic leads. This setup does not rely on any specific band structure and therefore can be realized with many different types of nanoconductors. In this talk, we will discuss its implementation with carbon nanotubes. We can reach the strong coupling limit between the electron spin and a superconducting photon cavity, with experimentally realistic parameters compatible with a slow enough decoherence of the spin quantum state. This allows us to envision the use of circuit cavity quantum electrodynamics methods for single spin manipulation and readout.

TT 18.8 Tue 16:00 H21

Spectroscopy of a Periodically Driven Qubit Coupled to a Non-Gaussian Bath — •Cheng Guo, Florian Marquardt, and Jan von Delft — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany

The dynamics and decoherence of solid-state qubits are often determined by a few non-Gaussian fluctuators. Paradigmatic models often used to represent the qubit-environment system like the spin-boson model cannot be applied here because they describe Gaussian-distributed fluctuations. The simplest model for non-Gaussian quantum noise is the so-called "quantum telegraph noise" model. It involves a qubit subject to the charge fluctuations of a single electron level that is tunnel-coupled to a reservoir. We use the adaptive time-dependent density-matrix renormalization group method (tDMRG) to study the dynamics of this model with arbitrary time-dependence. In particular, we present tDMRG-results on spectroscopy of the qubit under periodic driving.

TT 19: CE: Metal-Insulator Transition 2

Time: Wednesday 9:30–13:00 Location: H18

TT 19.1 Wed 9:30 H18

Charge, orbital and magnetic ordering in $La_{0.4}Sr_{1.6}MnO_4$ — •Holger Ulbrich[1], Daniel Senff[1], Olaf J. Schumann[1], Yvan Sidis[2], Paul Steffens[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, Saclay — [3]Institut Laue Langevin, Grenoble

The coupled ordering of charge orbital and spin (COS) degrees of freedom in the manganites constitutes a key element to understand the mechanism of CMR. 214 manganites are well-suited to study the COS state. The COS state of the half-doped layered material $La_{0.5}Sr_{1.5}MnO_4$ can be described by the Goodenough model [1-3]. The over-doped $La_{0.4}Sr_{1.6}MnO_4$ consists of 60% Mn^{4+} ions and 40% Mn^{3+} ions. Consequently there is no optimal checkerboard charge ordering possible. We suggest to put these excess of Mn^{4+} ions into stripes cutting the zig-zag chains. Investigations by neutron scattering emphasize this idea as incommensurable superstructure reflections of charges and orbitals could be found. The reflections of the magnetic ordering of Mn^{3+} are incommensurable as well, while the magnetic ordering of Mn^{4+} yields scattering at commensurable positions. These experiments are not in agreement with results by Larochelle *et al.* [4]. Stripe-like arrangement of Mn^{4+} ions are similar to the stripe phases in nickelates and cuprates. The order, however, is quite complex involving incommensurate ordering of orbitals, charges and Mn^{3+}-magnetic moments.

[1] D. Senff, *et al.*, Phys. Rev. Lett. 96, 257201 (2006).
[2] D. Senff, et al., Phys. Rev. B 77, 184413 (2008).
[3] J.B. Goodenough, Phys. Rev. 100, 564 (1955).
[4] S. Larochelle *et al.*, Phys. Rev. B 71, 024435 (2005).

TT 19.2 Wed 9:45 H18

Comparison of EELS and RIXS measurements for the single layer manganite $La_{1-x}Sr_{1+x}MnO_4$ — •Roberto Kraus[1], Jochen Geck[1], Matthias Schrade[1], Martin Knupfer[1], Bernd Büchner[1], and Pieter Glatzel[2] — [1]IFW Dresden, Germany — [2]ESRF Grenoble, France

The manganites show a variety of magnetic and electronic phases which are connected to charge, spin and orbital degrees of freedom. One example is the single layered perovskite $La_{1-x}Sr_{1+x}MnO_4$. Upon hole doping new in-gap excitations appear and up to now it is unclear if they are of charge-transfer or Mott-Hubbard type. To characterize the excitations in the system, we performed electron energy-loss spectroscopy (EELS) and resonant inelastic X-ray scattering (RIXS) of the Mn K-edge. The observed in-gap excitation shows a small positive dispersion and a clear positive shift as a function of temperature in the half-doped sample.

TT 19.3 Wed 10:00 H18

Orbital order in $La_{0.5}Sr_{1.5}MnO_4$: a failure of the local Jahn-Teller physics — •Hua Wu[1], C. F. Chang[1], Z. Hu[1], O. Schumann[1], J. C. Cezar[2], T. Burnus[1], N. Hollmann[1], N. B. Brookes[2], A. Tanaka[3], M. Braden[1], D. I. Khomskii[1], and L. H. Tjeng[4] — [1]II. Phys. Inst, Uni Köln — [2]ESRF, Grenoble, France — [3]Hiroshima Univ. Japan — [4]MPI Dresden

Orbital order (OO) occurs quite often in orbitally degenerate correlated transition-metal compounds. It has been generally accepted that there is one-to-one correspondence between a specific orbital order and a local Jahn-Teller distortion. Here we demonstrate that this is not always true, by demonstrating a failure of the local Jahn-Teller physics in the single-layered perovskite $La_{0.5}Sr_{1.5}MnO_4$ which is one of prototype OO materials. We studied both the site- and bond-centered charge orderings, crystal field levels, orbital states and their dependence on the varying local lattice distortions, through detailed ab initio electronic structure calculations. We conclude that this material has the site-centered charge ordering, and that the local Jahn-Teller physics fails and the type of occupied orbitals ($3x^2$–r^2/$3y^2$–r^2 ones) contradicts the local compression of $Mn^{3+}O_6$ octahedra which could require x^2–z^2/y^2–z^2 occupation. We explain this by the contribution of the long-range crystal-field in this anisotropic layered material and by the maximization of kinetic energy. Our theoretical results are confirmed by x-ray absorption linear dichroism.

TT 19.4 Wed 10:15 H18

Structural transformations due to electronic correlations in paramagnetic $KCuF_3$ and $LaMnO_3$ — •Ivan Leonov[1], Dmitry Korotin[2], Nadia Binggeli[3], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]ICTP and INFM-CNR Democritos National Simulation Center, Trieste, Italy

We present a computational scheme for *ab initio* total-energy calculations of materials with strongly interacting electrons using a plane-wave basis set [1]. It combines *ab initio* band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. The present approach allows us to investigate complex

materials with strongly interacting electrons and is able to treat atomic displacements, and hence structural transformations, caused by electronic correlations. Results obtained for paramagnetic $KCuF_3$ and $LaMnO_3$, namely an equilibrium Jahn-Teller distortion and antiferro-orbital order agree well with experiment. The structural optimization performed for paramagnetic $KCuF_3$ yields the correct lattice constant, equilibrium Jahn-Teller distortion and tetragonal compression of the unit cell. The present approach is able to determine correlation-induced structural transformations, equilibrium atomic positions and lattice structure in both strongly and weakly correlated solids in their *paramagnetic* phases as well as in phases with long-range magnetic order.

[1] I. Leonov, N. Binggeli, Dm. Korotin, V. I. Anisimov, N. Stojić, and D. Vollhardt, Phys. Rev. Lett. **101**, 096405 (2008).

TT 19.5 Wed 10:30 H18

Origin of Jahn-Teller distortion and orbital-order in $LaMnO_3$ — •Eva Pavarini[1] and Erik Koch[2] — [1]IFF und IAS, Forschungszentrum Jülich — [2]GRS, Jülich

The origin of the cooperative Jahn-Teller distortion and orbital-order in $LaMnO_3$ is central to the physics of the manganites. The question is complicated by the simultaneous presence of tetragonal and $GdFeO_3$-type distortions and the strong Hund's rule coupling between e_g and t_{2g} electrons. To clarify the situation we calculate the transition temperature for the Kugel-Khomskii superexchange mechanism by using the local density approximation+dynamical mean-field method, and disentangle the effects of super-exchange from those of lattice distortions. We find that super-exchange alone would yield $T_{\rm KK} \sim 650$ K. The tetragonal and $GdFeO_3$-type distortions, however, reduce $T_{\rm KK}$ to $\sim$550 K. Thus electron-phonon coupling is essential to explain the persistence of local Jahn-Teller distortions to $\gtrsim 1150$ K and to reproduce the occupied orbital deduced from neutron scattering.

TT 19.6 Wed 10:45 H18

First principles study of the electronic structure and phonon properties on double-layer manganites — •Omar De la Peña-Seaman, Rolf Heid, and Klaus-Peter Bohnen — Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Germany

We have studied the electronic and lattice dynamical properties of the tetragonal double-layer manganite system $La_{2-2x}Sr_{1+2x}Mn_2O_7$ ($x = 0.4$) within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation for modeling the alloy. The system has been investigated for non-magnetic and ferromagnetic phases. The performance of LDA and GGA exchange-correlation functionals on the properties under study was analyzed. We have used the experimental lattice constants, optimizing the internal structural parameters for each magnetic phase (non-magnetic and ferromagnetic). The electronic band structure as well as individual contributions to the density of states are discussed. The calculated phonon dispersion in [ξ00] and [ξξ0] high-symmetry directions for different magnetic phases are compared between them and with experimental data available in the literature. In addition, an analysis of the most representative phonon modes is performed, and the electron-phonon couplings discussed in detail.

TT 19.7 Wed 11:00 H18

THz and infrared spectroscopy in $FeCr_2S_4$ — •Joachim Deisenhofer[1], Yurii Goncharov[2], Franz Mayr[1], Dat Quach[3], Joanna Groza[3], Vladimir Tsurkan[1,4], and Alois Loidl[1] — [1]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia — [3]Department of Chemical Engineering and Materials Science, University of California, Davis, CA 95616, USA — [4]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chişinău, Republic of Moldova

We investigate the Jahn-Teller transition at $T_{JT} = 9$K in the CMR system $FeCr_2S_4$ by THz and IR spectroscopy. Below T_{JT} we observe the appearance of new phonon modes in the far-infrared region and new excitations in the THz regime. We attribute the latter to a splitting of the Fe^{2+} ground state due to the transition from a dynamic to a static Jahn-Teller distortion.

Invited Talk TT 19.8 Wed 11:15 H18

Spectroscopy on Strongly Correlated Electron Materials — •Liu Hao Tjeng — Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

One of the most intriguing aspects of transition metal materials is the wide variety of their physical properties. Although conceptually clean and beautiful, theoretical simplifications in terms of, for instance, a single band Hubbard model turn out to be inadequate. It now becomes clear that the interplay between the relevant charge, orbital and spin degrees of freedom of the metal ions involved determines the intricate balance between band formation and electron-correlation effects.

In this talk we would like to illustrate how synchrotron-based electron spectroscopies can contribute to the identification of the key parameters in the electronic structure of transition metal oxides, in particular those showing metal-insulator transitions as a function of temperature or doping. We use a combination of soft-x-ray absorption spectroscopy and photoemission, as well as the newly developed hard-x-ray photoelectron spectroscopy (HAXPES), to address issues related to the inter-site spin-spin and orbital-orbital correlations. Furthermore, we will address how accurate these phenomena can be theoretically described using the LDA+DMFT method and its most recent extensions.

In collaboration with Z. Hu, M. Haverkort, T. Koethe, C.F. Chang, H. Wu, T. Burnus, Y. Chin, N. Hollmann, H. Fujiwara, C. Schußler-Langeheine, H. Roth, M. Benomar, M. Reuther, C. Zobel, T. Lorenz, D. Khomskii, A. Tanaka, E. Pavarini, W. Reichelt, S. Barilo, J. Cezar, N. Brookes, H.H. Hsieh, H.J. Lin, C.T. Chen. Supported by SFB 608.

15 min. break

TT 19.9 Wed 12:00 H18

Absence of an electric potential gradient across the overlayer of $LaAlO_3/SrTiO_3$ heterostructures inferred from XPS — •Götz Berner[1], Michael Sing[1], Stefan Thiel[2], Jochen Mannhart[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Experimentelle Physik VI, Universität Augsburg

The origin of the interface electron gas (2DEG) in $LaAlO_3/SrTiO_3$ oxide heterostructures (LAO/STO) is a heavily discussed topic. Apart from possible influences of oxygen defects recent experimental and theoretical work suggests an electronic reconstruction as the driving mechanism for the 2DEG. In the most simple picture half an electron is transferred from the surface to the interface to neutralize the electric potential piling up across the polar LAO overlayers. Microscopically, density-functional (DFT) calculations find a potential gradient which shifts the LAO electronic states until the valence-band maximum crosses the chemical potential and electrons are transferred from the surface to the STO conduction-band minimum at the interface.

By x-ray photoelectron spectroscopy (XPS) this potential gradient should be observable as a significant broadening of the Al 1*s* core level. Moreover, probing the topmost LAO layer there should appear finite spectral weight at the chemical potential. However, in our XPS studies on several samples with different overlayer thicknesses none of these signatures is observed. In addition, we determined the band offsets of LAO and STO at the interface and arrived at values which suggest a flat band situation in contrast to the DFT calculations.

TT 19.10 Wed 12:15 H18

Possible localization of electrons at $LaAlO_3$-$SrTiO_3$ interfaces at finite temperatures — •Yang-Chung Liao[1], Nicolas Reyren[2], Stefano Gariglio[2], Christoph Richter[1], Rainer Jany[1], Stefan Thiel[1], Martin Breitschaft[1], German Hammerl[1], Thilo Kopp[1], Jean-Marc Triscone[2], and Jochen Mannhart[1] — [1]Experimental Physics VI, Center for Electronic Correlation and Magnetism, University of Augsburg, Augsburg, Germany — [2]DPMC, University of Geneva, Geneva, Switzerland

Intriguingly, the $LaAlO_3$-$SrTiO_3$ ($AlO_2/LaO/TiO_2/SrO$) interface possesses conducting electrons if the $LaAlO_3$ thickness exceeds 3 unit cells. By applying depleting gate fields in field-effect devices at finite temperatures, we observe the conducting interfaces to localize electrons. Below a critical carrier density, the interfaces display nonlinear current-voltage characteristics showing gap-like features. At higher carrier densities, the interface electron system is ohmic with a weak-localization type behavior. Based on current-voltage characteristics and magneto-transport properties, we trace the phase diagram of the $LaAlO_3$-$SrTiO_3$ interface electron system.

TT 19.11 Wed 12:30 H18

Microscopic origin of the electronic reconstruction at the $LaAlO_3/SrTiO_3$ interface — •Andrea Rubano[1], Domenico Paparo[2], Antigone Marino[2], Paolo Perna[2], Umberto Scotti di

Uccio[2], Fabio Miletto Granozio[2], Christoph Richter[3], Stefan Paetel[3], Jochen Mannhart[3], Lorenzo Marrucci[2], and Manfred Fiebig[1] — [1]HISKP, Universitaet Bonn, Bonn, Germany — [2]CNR-INFM Coherentia and Dip. di Scienze Fisiche, Università di Napoli Federico II, Italy — [3]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

$LaAlO_3/SrTiO_3$ interfaces are one of the most challenging topics in the field of perovskite oxides. Recently it was observed that a conductive two-dimensional electron gas (2DEG) emerges at the interface of these wide-gap insulators. The 2DEG formation occurs once $n \geq 4$ $LaAlO_3$ monolayers are deposited on top of the $SrTiO_3$. Although some macroscopic models have been proposed, our understanding on the microscopic scale is still at its infancy. Second harmonic (SHG) spectroscopy is an interface-only sensitive technique and, thus, an ideal tool to study these materials. Applying SHG, we demonstrate that a structural reorganization of the interfacial Ti-orbitals already occurs at $n = 3$, yet without any onset of conductivity, because the injected carriers are localized at the interface. The electronic reorganization at $n = 3$ leads to an abrupt increase of the SHG yield due to the enhancement of the polar asymmetry of the Ti $3d$ orbitals, and a crystal field splitting of the $d(xy)$ orbitals is observed.

TT 19.12 Wed 12:45 H18

Electronic reconstruction in thin $LaAlO_3$ films on $SrTiO_3$(001) via a $SrTiO_3$-capping layer — •Katrin Otte[1], Rossitza Pentcheva[1], and Warren E. Pickett[2] — [1]Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich — [2]Department of Physics, UC Davis

Novel electronic phenomena can be realized at the interface between polar (e.g. $LaAlO_3$) and nonpolar (e.g. $SrTiO_3$) band insulators. An intriguing example is the thickness dependent insulator-to-metal transition in thin $LaAlO_3$ films on $SrTiO_3$(001)[1]. Density functional theory calculations show that a strong lattice polarization allows several layers of $LaAlO_3$ on $SrTiO_3$(001) to remain insulating before an insulator-to-metal transition takes place at around 4 monolayers (MLs)[2]. We demonstrate here that an additional capping $SrTiO_3$ can trigger the electronic reconstruction already at two MLs of $LaAlO_3$. A surface O $2p$ state, similar to the surface states in $SrTiO_3$, is identified as the origin of this additional band shift.

Altogether, the $SrTiO_3$-capping layer represents an alternative pathway to tune the electronic reconstruction of the system leading to the formation of an electron-hole bilayer.

[1] S. Thiel et al., Science **313**, 1942 (2006).
[2] R. Pentcheva and W.E. Pickett, Phys. Rev. Lett. **102**, 107602 (2009).

TT 20: SC: Fabrication and Characterization of Iron-Based and Other Superconductors

Time: Wednesday 9:30–13:00 Location: H19

TT 20.1 Wed 9:30 H19

Preparation and transport properties of FeSe thin films — •Martin Jourdan, Sebastian ten Haaf, and Janek Maletz — Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany

Thin films of the presumably unconventional superconductor FeSe were prepared by molecular beam epitaxy (MBE). X-ray diffraction reveals epitaxial growth. The temperature dependent resistance of the samples depends crucially on the stoichiometry with variations in the order of 1% determining the observation or absence of superconductivity. The best samples show a critical temperature of 7K with a resistive transition width of 1K. Angular dependent measurements of the upper critical field reveal a pronounced anisotropy which is increasing with sample purity. Measurements of the Hall-effect in the normal conducting regime are related with sample stoichiometry as determined by energy dispersive x-ray spectroscopy (EDX) on thick films (thickness 600nm).

TT 20.2 Wed 9:45 H19

Metal-semiconductor transition and phase separation in superconducting $Fe_{1+y}Te_{1-x}Se_x$ single crystals — •Sahana Roessler[1], Dona Cherian[2], Sasidharan Harikrishnan[2], Handadi L Bhat[2], Suja Elizabeth[1], Frank Steglich[1], Steffen Wirth[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Science, C V Raman Avenue, Bangalore - 560012, India

We have investigated the influence of excess Fe on the electrical transport and magnetism of $Fe_{1+y}Te_{1-x}Se_x$ (y = 0.26, 0.15, 0.12 and x =0.32, 0.34, 0.36, respectively) single crystals. All three samples exhibit superconducting transitions with critical temperatures T_c (onset) $\sim$ 15 K in the resistivity measurements. It has been inferred from the width of the superconducting transition and the magnitude of the lower critical field H_{c1}, that excess Fe occupying interstitial sites in the chalcogen planes suppresses superconductivity. Further, the temperature dependence of resistivity in the normal state changes from metallic to semiconducting behavior with increasing Fe. From the dc-magnetization, linear and non-linear response of the ac-susceptibility, we show that the superconducting state for these compositions is inhomogeneous. A possible origin of this phase separation is due to a magnetic coupling between Fe in the chalcogen planes with those in the Fe-square lattice.

TT 20.3 Wed 10:00 H19

Single crystal growth and physical characterization of iron-pnictides $Ca(Fe_{1-x}Co_x)_2As_2$ — •Luminita Harnagea, Surjeet Singh, Gerd Friemel, Norman Leps, Friedrich Roth, Mahmoud Abdel-Hafez, Ulrike Stockert, Sabine Wurmehl, Günter Behr, Christian Hess, Rüdiger Klingeler, Martin Knupfer, and Bernd Büchner — Leibniz Institute for Solid State Materials Research (IFW) Dresden, Germany

Single crystals of iron-pnictides $Ca(Fe_{1-x}Co_x)_2As_2$ ($0 \leq x \leq 0.2$) were grown from Sn-flux using the conventional high temperature solution growth technique. All the grown crystals were found to be phase-pure crystallizing in a tetragonal $ThCr_2Si_2$-type structure. In particular, no trace of Sn incorporation in the structure was detected. Upon Co doping, the c-crystallographic axis of the tetragonal unit cell decreases, while a-axis shows a less significant variation. Crystals were plate-like exhibiting lateral dimensions up to 15 mm and 0.5 mm thick. The details of crystal characterization, including the chemical composition, growth habits and morphology of the grown crystals are presented. Effects of Co-doping on the structural/magnetic transition of $CaFe_2As_2$ are discussed from optical spectroscopy and temperature dependent resistivity and susceptibility studies.

TT 20.4 Wed 10:15 H19

Phase diagram of $Ca(Fe_{1-x}Co_x)_2As_2$ — •Ulrike Stockert, Mahmoud Abdel-Hafez, Luminita Harnagea, Surjeet Singh, Norman Leps, Liran Wang, Gerd Friemel, Sabine Wurmehl, Günter Behr, Christian Hess, Rüdiger Klingeler, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany

We report on magnetic and thermodynamic measurements on $Ca(Fe_{1-x}Co_x)_2As_2$ ($0 \leq x \leq 0.2$) single crystals grown from Sn-flux. Upon Co substitution, the first-order structural/magnetic phase transition of $CaFe_2As_2$ is split and shifted to lower temperatures. Simultaneously, superconductivity evolves at low T. The superconducting volume fraction depends sensitively on the Co content and reaches 100 % only above the optimum doping level of $x \sim 0.065$, as the magnetic and structural transitions are completely suppressed. We discuss the phase diagram of $Ca(Fe_{1-x}Co_x)_2As_2$ in consideration of recent investigations of $CaFe_2As_2$ under pressure, which revealed a sensitive pressure dependence of the structural/magnetic phase transitions and a T_c as high as 10 K at 3.5 kbar.

TT 20.5 Wed 10:30 H19

Single-crystal growth and characterization of ferro-pnictides $A(Fe,Co,Ni)_2As_2$ (A = Ba, Sr) and $(A_{1-x}K_x)Fe_2As_2$(A = Ba, Eu) — •S. Aswartham, S. Singh, G. Behr, N. Leps, G. Friemel, U. Stockert, S. Wurmehl, R. Klingeler, C. Hess, and B. Büchner — IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany

We employed a modified Bridgman and self-flux methods to grow single crystals of A(Fe, Co, Ni)$_2$As$_2$ (A = Ba, Sr) and $(A_{1-x}K_x)Fe_2As_2$(A

= Ba, Eu) series, respectively. Using these techniques large single-crystals with dimensions up to 25 x 10 mm^2 and thickness up to 1 mm were grown. Susceptibility and resistivity of these crystals were studied. Narrow superconducting transition widths ($\approx$ 0.5 K) and large residual resistivity ratios ($\approx$ 7) indicate the high-quality of our single crystals. Here we present details of our crystal growth methods, structural characterizations and physical properties.

TT 20.6 Wed 10:45 H19

Crystal growth and physical characterization of $Ba(Fe_{1-x}Co_x)_2As_2$ — •C. Nacke[1], G. Behr[1], S. Singh[1], N. Leps[1], G. Friemel[1], U. Stockert[1], H.H. Klauss[2], S. Wurmehl[1], C. Hess[1], R. Klingeler[1], and B. Büchner[1] — [1]Leibnitz Institute for Solid State and Material Research (IFW) Dresden, Germany — [2]TU Dresden, Institute for Solid State Physics, Germany

The vertical Bridgman technique was used to grow mm-size crystals of the $BaFe_2As_2$ compound and its Co-doped superconducting variants. With this technique the crystals were grown directly from a stoichiometric melt with the composition $Ba(Fe_{1-x}Co_x)_2As_2$. The resulting crystals were platelet-like and have lateral sizes up to 10 x 10 mm^2 and a thickness up to 1 mm. Analysis by X-ray diffraction and EDX confirm the correct Ba-122-phase. Measurements of magnetic susceptibility and electrical resistivity reveal superconducting properties of the Co-doped crystals. The suceptibility plots for the 10% Co-doping samples (x=0.1) show a sharp transition to superconductivity at T_c=23 K. This data are in good agreement with those from the resistivity. In particular, the zero-field μSR data show a pure Gaussian relaxation and confirm very high sample purity.

TT 20.7 Wed 11:00 H19

How Can We Raise T_c in $RO_{1-x}F_xFeAs$ Superconductors? — •Anke Köhler[1,2], Günter Behr[1], Marko Herrmann[1], and Wolfgang Hässler[1] — [1]IFW Dresden, PF 270116, 01171 Dresden — [2]Goethe-Universität Frankfurt am Main, Max-von-Laue-Str. 1, 60438 Frankfurt

By the discovery of $RO_{1-x}F_xFeAs$ (R = lanthanide) superconductors in the beginning of 2008, it was shown for the first time that a non-cuprate superconductor can reach a superconducting transition temperature T_c above 50 K. This offers new opportunities for the development of new high temperature superconductors. However, the superconductors with the highest T_c show the most difficulties in formation of the right phase. Problems are the incorporation of fluorine and the homogeneity of the samples. A further challenge is the structural instability for rare earth elements with small ion radius ($64 \leq Z \leq 71$). In our studies, several opportunities to overcome these difficulties are evaluated:

1. variation of the grain size of the initial powder
2. use of slightly non-stoichiometric initial composition
3. high-pressure synthesis

As a result, we raise the T_c of the material with a nominal composition $GdO_{1-x}F_xFeAs$ from 20 up to 40 K. In a $SmO_{0.9}F_{0.1}FeAs$-compound could be observed superconductivity above 50 K after a small As-reduction at the surface of the sample. Measurements of the final composition and structure will animate the discussion about the requirements for realization of the superconducting state.

15 min. break

TT 20.8 Wed 11:30 H19

Magnetic phase diagram of iron pnictide thin films — •Silvia Haindl, Martin Kidszun, Fritz Kurth, Kazumasa Iida, Alexander Kauffmann, Nadezda Kozlova, Jens Freudenberger, Jens Hänisch, Konstantin Nenkov, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, Institute for Metallic Materials, PO - Box 270116, D-01171 Dresden

The new iron pnictide superconductors with transition temperatures up to 55 K and high upper critical fields are found to be candidates for multiband superconductivity as it has been suggested by theory and experiment. A serious investigation, however, is restricted to single crystals and epitaxial thin films. Latter offer a defined current path (two-dimensionality) and a higher voltage resolution in transport measurements. Epitaxial $LaFeAsO_{1-x}F_x$ and Co-doped $BaFe_2As_2$ thin films have been successfully grown by pulsed laser deposition (PLD). We have performed transport measurements in static fields up to 14 T and pulsed fields up to 42 T for different crystallographic directions. The upper critical field and its temperature dependent anisotropy are discussed in terms of a two gap superconductivity scenario. In addition, the vortex matter has been studied using a vibrating sample magnetometer (VSM).

TT 20.9 Wed 11:45 H19

Anisotropy and vortex matter of LaFeAs(O,F) — •Martin Kidszun, Silvia Haindl, Jens Hänisch, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, Institute for Metallic Materials, PO - Box 270116, D-01171 Dresden, Germany

The successful growth of epitaxial LaFeAs(O,F) thin films opens the way to study intrinsic properties of this novel superconductors. Exploring the magnetic phase diagram up to 42 T we were able to investigate the temperature dependence and anisotropy of the upper critical field as well as the irreversibility field in this iron oxypinictide. The anisotropy of the irreversibility field was determined using a combination of resistive measurements in high magnetic fields and critical current densitie measurements. A substantial report about the anisotropy and the vortex matter will be given in this conribution.

TT 20.10 Wed 12:00 H19

Dynamic studies on the influence of strain on superconducting properties using piezoelectric substrates — •Sascha Trommler, Ruben Hühne, Patrick Pahlke, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

It is known that the application of strain has a significant influence on the functional properties of superconducting materials. Typically, thin films are prepared on substrates with a different lattice misfit inducing a biaxial tensile or compressive strain to study this effect. Unfortunately, this approach is often restricted to very thin films. Furthermore, it is difficult to correlate strain and superconductivity directly, as the preparation conditions and the resulting microstructure may severely affect the superconducting properties. An alternative approach is the preparation of superconducting films on single crystalline piezoelectric substrates enabling a dynamical variation of the induced strain by applying an electric field on the substrate. This approach is used to study the strain dependence of superconducting properties in different materials. Therefore, thin epitaxial YBCO, $La_{1-x}Sr_xCuO_4$ and $BaFe_{2-x}Co_xAs_2$ films were prepared on piezoelectric (001) $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ substrates. Depending on the lattice parameter of these materials, additional buffer layers are required to achieve an epitaxial growth of the superconductor on these substrates. Finally, results on the influence of strain on superconducting properties like the transition temperature will be presented for these materials using dynamic investigations.

TT 20.11 Wed 12:15 H19

Preparation and Characterization of $Ho_xLu_{1-x}Ni_2B_2C$ Thin Films — •Tim Niemeier, Karolin Tscharntke, Ruben Hühne, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, PF 270116, D-01171 Dresden

On the basis of the epitaxial growth of rare earth nickel borocarbide films [1], mixed phase borocarbide thin films $Ho_xLu_{1-x}Ni_2B_2C$ were successfully prepared for the first time. Pulsed Laser deposition with two stoichiometric $LuNi_2B_2C$ and $HoNi_2B_2C$ alloy targets and variable pulse counts on both targets were used to produce thin films with different chemical compositions. Using x-ray diffraction, a homogeneous phase was detected in the films. Texture measurements revealed that for most of the compositions, a high in-plane order could be preserved in the films for slighty adapted deposition parameters. The superconductive transition temperatures in dependence of the composition are close to those known from mixed phase polycrystalline samples [2]. Finally, an outlook to the behaviour of the upper critical field in the composition series will be given. Additional details on the deposition and the epitaxial growth will be discussed on an additional poster.

[1] T. Niemeier *et al.*, J. Phys.: Conf. Ser. 150 (2009) 052185

[2] J. Freudenberger *et al.*: J. Magnetism and Magnetic Materials 187 (1998) Nr. 3, S. 309-317

TT 20.12 Wed 12:30 H19

Effect of Gallium Doping on Superconductivity in Germanium — •R. Skrotzki[1], T. Herrmannsdörfer[1], V. Heera[2], O. Ignatchik[1], M. Uhlarz[1], A. Mücklich[2], M. Posselt[2], H. Reuther[2], B. Schmidt[2], K.-H. Heinig[2], W. Skorupa[2], M. Voelskow[2], C. Wündisch[2], J. Fiedler[2], M. Helm[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf (FZD) — [2]Institut für Ionenstrahlphysik und Ma-

terialforschung, FZD

We report recent discoveries of superconductivity in Ga-doped germanium fabricated by ion implantation and subsequent flash-lamp or oven annealing. Tuning the preparation parameters allows for varying both charge-carrier and Ga concentration in the resulting roughly 100 nm thin nano- or single-crystalline layers. Transport measurements on systematically prepared samples reveal that besides a needed charge-carrier concentration of more than 0.4 atom%, superconductivity occurs to be sensitive on the implanted Ga content which may also be attributed to a change in the phonon properties. Onset transition temperatures up to 1.4 K have been found for almost 10 atom% Ga. Further, we observe in-plane critical fields exceeding 1 T and being close to the Pauli-Clogston limit. An exceptionally low Cooper-pair density of around 10^{15} cm^{-3} turns out the extreme type-II character of superconductivity. Finally, our work adds to our previous report [1] and may help to understand superconductivity in doped elemental semiconductors in general.

[1] T. Herrmannsdoerfer et. al., Phys. Rev. Lett. 102, 1027003 (2009)

TT 20.13 Wed 12:45 H19

YBCO nanowires grown by the alumina template method — •Michael R Koblischka[1], Anjela Koblischka-Veneva[2], Vassil Skumryev[3], and Uwe Hartmann[1] — [1]Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Functional Materials, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [3]Institut Català de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

$YBa_2Cu_3O_x$ (YBCO) nanowires are grown by the anodized alumina template method, starting from pre-sintered YBCO powder. As templates, we have employed commercially available alumina templates with pore diameters of 30 nm and 100 nm, and an overall thickness of 50 μm. An oxygen annealing step is required to obtain superconducting nanowires. Superconductivity with a transition temperature of 88 K is confirmed by means of magnetic susceptibility measurements. The resulting nanowires are analyzed in detail employing electron microscopy and atomic force microscopy. The separation of the nanowires of the templates is not yet established, but individual nanowires of up to 10 μm length could be separated from the template. In several cases, the template pores are not completely filled by the superconducting material, which implies that the observed length is similar to what could be expected from regular grain growth. Resistance measurements using cut pieces of the filled templates were carried out as a function of temperature. These pieces were covered with Au films on top and bottom in order to provide the electric contacts. The measurements confirmed the magnetically determined critical temperatures.

TT 21: FS: Quantum Criticality in Strongly Correlated Metals

Time: Wednesday 9:30–13:00 Location: H20

Invited Talk TT 21.1 Wed 9:30 H20

Quantum Criticality, Kondo Breakdown, and Fermi Surfaces — •Qimiao Si — Dept of Physics & Astro, Rice U, Houston, TX, USA

Quantum criticality describes the collective fluctuations of matter undergoing a second order phase transition at zero temperature. Magnetic heavy fermion metals represent a prototype setting for quantum critical points (QCPs). Studies here have demonstrated quantum criticality as a mechanism for both non-Fermi liquid behavior and unconventional superconductivity. They have also illustrated the general notion of quantum criticality beyond the orthodox theory of order-parameter fluctuations. Here, I discuss these issues in the broader contexts, and address two types of antiferromagnetic QCPs, including a local quantum critical point [1] which contains the physics of a critical breakdown of the Kondo effect. Across such a QCP, there is a sudden collapse of a large Fermi surface to a small one. I also consider the proximate antiferromagnetic and paramagnetic phases, and these considerations lead to a global phase diagram [2]. Finally, I discuss the pertinent experiments, briefly address the case of ferromagnetic heavy fermions [3], and outline some issues for future studies.

[1] J.-X. Zhu, S. Kirchner, R. Bulla, & Q. Si, PRL 99, 227204 (2007) and to be published; Q. Si, S. Rabello, K. Ingersent & J. L. Smith, Nature 413, 804 (2001).

[2] Q. Si, arXiv:0912.0040; Physica B378, 23-27 (2006); S. J. Yamamoto and Q. Si, PRL 99, 016401 (2007).

[3] S. J. Yamamoto and Q. Si, arXiv:0812.0819.

Topical Talk TT 21.2 Wed 10:10 H20

Tuning magnetic quantum phase transitions — •Hilbert v. Löhneysen — Karlsruher Institut für Technologie, Physikalisches Institut und Institut für Festkörperphysik, D-76021 Karlsruhe

In the canonical quantum-critical heavy-fermion system (HFS) $CeCu_{6-x}Au_x$, a quantum critical point (QCP) can be obtained as a function of Au concentration at $x_c = 0.1$ or, for $x > x_c$, by hydrostatic pressure p or magnetic field B. The different behavior of B and x tuning of the QCP inferred from specific heat and resistivity, is corroborated by inelastic neutron scattering probing critical fluctuations [1], indicating that the (B, x, p) phase diagram for $T \to 0$ may exhibit several distinct phases. The Kondo temperature determined with UPS shows a sharp step at x_c, suggestive of a loss of complete Kondo screening [2]. Implications for QCP models for HFS will be discussed. - Uniaxial stress imposed on epitaxially grown $LaCoO_3$ films leads to the stabilization of a high-spin state, as opposed to bulk $LaCoO_3$ which is non-magnetic with S = 0 for $T \to 0$. Unexpectedly, ferromagnetism with T_C up to 80 K is observed in epitaxial films whose properties can be "strain-tuned" by choosing different substrates [3].

[1] O. Stockert et al., Phys. Rev. Lett. **99**, 237203 (2007)

[2] M. Klein et al., Phys. Rev. Lett. **101**, 266404 (2008)

[3] D. Fuchs et al., Phys. Rev. B **75**, 144402 (2007); B **77**, 014434 (2008)

Topical Talk TT 21.3 Wed 10:50 H20

Orbital-selective Mott transitions: Heavy Fermions and beyond — •Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Germany

Quantum phase transitions in metals are often accompanied by non-Fermi liquid behavior and the appearence of novel phases in the vicinity of the quantum critical point. Among the interesting theoretical concepts is that of an orbital-selective Mott transition, which - in heavy-fermion metals - is equivalent to a breakdown of the Kondo effect. I will discuss aspects of both the quantum critical regime and the possibly emerging paramagnetic non-Fermi liquid phase, dubbed fractionalized Fermi liquid. Electron-lattice coupling can turn the orbital-selective Mott transition into a quantum version of the Kondo volume collapse. In addition, I will discuss the realization of fractionalized Fermi liquids in single-band models of correlated electrons, with an eye towards cuprate superconductors.

10 min. break

Topical Talk TT 21.4 Wed 11:40 H20

Interaction of the magnetic instability and the Fermi surface reconstruction in $YbRh_2Si_2$ — •Sven Friedemann[1], Tanja Westerkamp[1], Manuel Brando[1], Steffen Wirth[1], Niels Oeschler[1], Philipp Gegenwart[1,2], Cornelius Krellner[1], Christoph Geibel[1], Frank Steglich[1], Silke Bühler-Paschen[3], Stefan Kirchner[4,5], and Qimiao Si[5] — [1]MPI CPfS, Dresden, Germany — [2]I. Physik. Institut, Georg-August-Universität, Göttingen, Germany — [3]Institut für Festkörperphysik, TU Wien, Austria — [4]MPI PKS, Dresden, Germany — [5]Physics and Astronomy Department, Rice University, Houston, USA

An antiferromagnetic (AF) quantum critical point (QCP) is conventionally described by the quantum generalization of finite-temperature phase transitions. By contrast, the newly proposed unconventional scenarios for heavy-fermion metals are based on the breakdown of the Kondo effect. $YbRh_2Si_2$ is a prototype of the latter class. Here, we report high-precision Hall effect data demonstrating the coincidence of the Fermi surface reconstruction and the AF QCP in the stoichiometric compound. In addition, we present results revealing the global phase diagram of $YbRh_2Si_2$ under positive and negative chemical pressure as realized by Co and Ir substitution on the Rh side. Surprisingly, this leads to a detachment of the AF QCP from the Fermi surface recon-

struction. In particular, negative pressure induces a separation of the two with an intermediate spin-liquid type ground state emerging in an extended field range. These results indicate a new quantum phase arising from the interaction of the Kondo breakdown and the AF QCP.

Topical Talk TT 21.5 Wed 12:20 H20

Novel electronic states near discontinous quantum phase transitions — •Philipp Gegenwart — I. Physikalisches Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

The collective low-energy excitations near quantum phase transitions (QPTs) lead to novel phenomena such as non-Fermi liquid (NFL) behavior, unconventional superconductivity or electronic nematicity. Here we focus on cubic ($Sr_{1-x}Ca_xRuO_3$) and layered ($Sr_3Ru_2O_7$) ruthenates. The former system, studied using thin films, displays a discontinuous ferromagnetic QPT with an extended NFL phase. In the latter system a novel phase displaying nematic-like transport anisotropies, which is bounded in magnetic field by two first-order metamagnetic transitions, is investigated by capacitive dilatometry on high-quality single crystals.

Work in collaboration with M. Schneider, C. Stingl, M. Schubert, K. Winzer, Y. Tokiwa, V. Mosneaga, F. Weickert, A.P. Mackenzie and M. Garst. Financial support by the DFG through SFB 602 and research unit 960 (Quantum phase transitions) is acknowledged.

TT 22: CE: Spin Systems and Itinerant Magnets

Time: Wednesday 9:30–13:15 Location: H21

TT 22.1 Wed 9:30 H21

Hydrodynamic Limit for the Spin Dynamics of the Heisenberg Chain — •Wolfram Brenig and Simon Grossjohann — Institute for Theoretical Physics, Technical University Braunschweig

We show that Quantum-Monte-Carlo calculations of the dynamic structure factor of the spin-1/2 antiferromagnetic Heisenberg chain at intermediate temperatures based on the stochastic series expansion method corroborate predictions for a diffusive behavior of the spin-dynamics at finite frequencies in the low-energy long wave-length limit. The temperature dependence of the scattering rate will be detailed and will be shown to be in good agreement with similar findings by bosonization and DMRG methods. Implications for NMR and spin-transport measurements will be discussed.

TT 22.2 Wed 9:45 H21

Non-abelian statistics in higher spin antiferromagnets — Burkhard Scharfenberger[1], Ronny Thomale[2], and •Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, KIT, 76128 Karlsruhe — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA

We conjecture, and provide some preliminary evidence, that spinons (and holons) in antiferromagnets with spin $S=2$ and higher generally obey non-abelian statistics (SU(2) level $k = 2S$ anyons for S integer). The line of argument is as follows. In one dimension, a paradigm for a general $S=1$ spin chain (the AKLT chain) can be obtained by projecting two dimer (or Majumdar-Ghosh) chains with $S=1/2$ together. Similarly, we can obtain an $S = 1$ spin liquid from projecting two $S = 1/2$ chiral spin liquids together [M.Greiter, J.Low Temp. Phys. 126, 1029 (2002)]. In both cases, a discrete symmetry is violated for the $S=1/2$ models, which is restored for $S=1$. We assume that the $S=1$ spin liquid provides a paradigm of the disorderd $S=1$ antiferromagnet. If this is correct, we may further assume that an $S = 2$ spin liquid generated by projecting two of these $S=1$ liquids together will in turn provide a paradigm of the disordered $S=2$ antiferromagnet. We provide evidence that the excitations of this $S=2$ spin liquid obey non-abelian statistics, and show that the degeneracy on a torus is $3 \times 3 = 9$, as expected for two species of Ising (SU(2) level $k=1$) anyons with opposite chiralities.

TT 22.3 Wed 10:00 H21

An FRG approach for quantum antiferromagnets — •Johannes Reuther and Peter Wölfle — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Germany

We consider spin-1/2 Heisenberg antiferromagnets on two dimensional lattices. In particular we study the melting of magnetic order as an effect of frustration. Examples for such models are the J_1-J_2-model or the Heisenberg model on a triangular or Kagome lattice. The last two lattices are examples for geometrically frustrated systems. We rewrite the spin operators in the Hamiltonians in terms of auxiliary fermions which enable us to perform diagrammatic approximations. For the auxiliary particle constraint an exact projection scheme proposed by Popov and Fedotov is available. In order to sum up diagrams in a controlled way we apply the Functional Renormalization Group (FRG) in conjunction with a cutoff procedure called Katanin truncation. Calculating the magnetic susceptibility and the spin-spin correlations we are able to distinguish between magnetically ordered and paramagnetic phases. We find phase diagrams in good agreement with numerical studies.

TT 22.4 Wed 10:15 H21

Spin dynamics in nearly critical magnets with quenched disorder — •Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Germany

Quanten phase transitions in quantum magnets, with coupled-dimer systems being prominent examples, have been extensively studied both experimentally and theoretically. In the absence of quenched disorder, the excitation spectrum near criticality is essentially understood. In contrast, relatively little is known about dynamical properties in the disordered case. Here we present numerical results for the fluctuation spectrum of coupled-dimer magnets with quenched disorder of random-mass type, obtained by a generalization of the bond-operator method. The results are directly applicable to doped dimer materials like (K,Tl)$CuCl_3$ and will also be discussed with an eye towards disordered stripe phases in cuprate superconductors.

TT 22.5 Wed 10:30 H21

Accurate spin susceptibilities for strongly correlated metals — •Lewin Boehnke[1], Olivier Parcollet[2], Michel Ferrero[3], and Frank Lechermann[1] — [1]1. ITP, Universität Hamburg, D-20355 Hamburg, Germany — [2]IPhT, CEA/DSM/IPhT-CNRS/URA 2306, CEA-Saclay, F-91191 Gif-sur-Yvette, France — [3]CPHT, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France

For many strongly correlated systems, the dynamical mean-field theory (DMFT) has proven its value as a numerically feasable and nevertheless physically sound approximation. In combination with the local density approximation (LDA), several material specific phenomena have been successfully studied. However, most of the former LDA+DMFT calculations in a manifest multi-orbital context were restricted to density-density interactions in the many-body hamiltonian and rather high temperatures. These restrictions rendered it difficult to accurately compute susceptibilities that are actually comparable with experimental data.

Due to the novel generation of continuous-time quantum-Monte-Carlo (CT-QMC) impurity solvers, these latter limitations have been lifted. Hence in this talk we want to present the computation of (frequency-dependent) spin susceptibilites for realistic correlated metals using the hybridization-expansion CT-QMC technique [1]. As a concrete example we will discuss the intriguing spin correlations in the strongly correlated Na_xCoO_2 system.

[1] P. Werner, A. Comanac, L. de' Medici, M. Troyer and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

TT 22.6 Wed 10:45 H21

Orbitally induced string formation in the spin-orbital polarons — •Krzysztof Wohlfeld[1], Andrzej M. Oleś[2,3], and Peter Horsch[3] — [1]IFW Dresden, Germany — [2]Jagellonian University, Poland — [3]Max-Planck-Institut für Festkörperforschung, Germany

We study the spectral function of a single hole doped into an *ab* plane of a Mott insulator $LaVO_3$ with antiferromagnetic (AF) spin order of $S = 1$ spins accompanied by alternating orbital (AO) order of active $\{yz, zx\}$ orbitals [1]. Starting from the respective t-J model, with spin-orbital superexchange and effective three-site hopping terms, we derive the polaron Hamiltonian and show that a hole couples simultaneously to the collective excitations of the AF/AO phase, magnons and or-

bitons. Next, we solve this polaron problem using the self-consistent Born approximation and find a stable quasiparticle solution — a spin-orbital polaron. We show that the spin-orbital polaron resembles the orbital polaron found in e_g systems, as e.g. in K_2CuF_4 or (to some extent) in $LaMnO_3$, and that the hole may be seen as confined in a string-like potential. However, the spins also play a crucial role in the formation of this polaron — we explain how the orbital degrees of freedom: (i) confine the spin dynamics acting on the hole as the classical Ising spins, and (ii) generate the string potential which is of the joined spin-orbital character. Finally, we discuss the impact of the results presented here on the understanding of the phase diagrams of the lightly doped cubic vanadates.

[1] K. Wohlfeld, A. M. Oleś, and P. Horsch, Phys. Rev. B **79**, 224433 (2009).

15 min. break

TT 22.7 Wed 11:15 H21

Dynamic topological spin clusters in the paramagnetic phase of MnSi. — •A. Hamann[1], D. Lamago[1,2], T. Wolf[1], H. v. Löhneysen[1], and D. Reznik[1] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA Saclay, France

At ambient pressure and below T_C spins in MnSi order in a helical ground state with the helix axis pinned by the crystal potential. At high pressure an exotic spin state forms referred to as partial order [1]. It is characterized by translational helical spin order but orientational disorder and the non-Fermi-liquid resistivity appears nearby in the phase diagram.

Our numerical calculations show that in the absence of the pinning potential isotropic near-neighbor chiral spin interactions of MnSi favor a glassy collection of topological spin clusters. These have the spectral signature of partial order. Their stability relative to the helical order increases with increasing temperature, and a competition with these clusters, not conventional fluctuations, melts the helical phase. Our detailed neutron scattering measurements fully confirm this prediction by identifying partial order at ambient pressure. We show that this partial order may explain most of the puzzling properties of MnSi including the two-component phase transition that was revealed by specific heat [2].

[1] C. Pfleiderer, D. Reznik et al., Nature **427**, 227 (2004)
[2] S. M. Stishov et al., Phys. Rev. B **76**, 052405 (2007)

TT 22.8 Wed 11:30 H21

Dynamics in the B-T phase diagram of MnSi measured with MIEZE — •Georg Brandl[1,2], Robert Georgii[1,2], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik Department E21, Technische Universität München, 85747 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, 85747 Garching, Germany

MIEZE (Modulation of IntEnsity by Zero Effort) has been proposed some time ago as a variant of the NRSE technique [1], having the advantage of preparing the beam modulation before the sample. This allows measurements under experimental conditions causing depolarization, such as magnetic samples or samples in an applied magnetic field without losing signal intensity, while keeping the high resolution of the spin echo technique. Yet, despite being potentially very attractive the MIEZE technique has so far not been used to tackle real scientific problems. We report the development of a MIEZE set up on the very cold neutron beam line MIRA at the FRM II. We have used the MIEZE technique at MIRA to study the skyrmion lattice in the B20 compound MnSi [2], a novel magnetic state composed of particle-like spin textures with non-trivial topology that forms in an applied magnetic field. We have measured the linewidth of the magnetic scattering at the position of the magnetic satellites throughout the B-T-diagram of MnSi. The results give us a clue on the stability of the various magnetic structures of MnSi.

[1] R. Gähler, R. Golub, T. Keller, Physica B, 180, 899 (1992)
[2] S. Mühlbauer et al., Science 323, 915 (2009)

TT 22.9 Wed 11:45 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: I. Crystal Growth, Magnetization and Specific Heat — •Andreas Bauer, Andreas Neubauer, Christian Franz, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

The helimagnetic transition in MnSi is suppressed under substitutional doping with Fe and Co on the Mn site. We report a comprehensive study of the magnetization and specific heat of single-crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$. With increasing concentration x the magnetic phase diagram remains essentially unchanged, exhibiting three phases (helical order, conical order and the Skyrmion lattice phase). In addition an extended cross-over regime exists between the paramagnetic and the helimagnetic state. When suppressing the magnetic modulations in an applied magnetic field, it is possible to infer the evolution of the underlying weakly ferromagnetic state as a function of x. In contrast to the pressure depencence of pure MnSi, which shows a first order quantum phase transition, we observe strong evidence for ferromagnetic quantum criticality.

TT 22.10 Wed 12:00 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: II. Small Angle Neutron Scattering — •Tim Adams[1], Sebastian Mühlbauer[1], Andreas Bauer[1], Andreas Neubauer[1], Christian Franz[1], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching, Germany

We report a comprehensive small angle neutron scattering study of the evolution of the magnetic phase diagram in $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$. With increasing concentration x the magnetic phase diagram remains essentially unchanged, exhibiting a well defined helimagnetic, conical and Skyrmion lattice phase up to $X \approx 0.5x_c$, where x_c is the critical concentration for which the helimagnetic transition temperature vanishes. Surprisingly, for concentrations $x \to x_c$ the magnetisation, susceptibility and specific heat are still akin the magnetic phase diagram of pure MnSi, but small angle neutron scattering suggests the emergence of complex spin textures. Similarities and differences with the pressure-temperature phase diagram of pure MnSi and the doped semiconductor $Fe_{1-x}Co_xSi$ will be discussed.

TT 22.11 Wed 12:15 H21

Quantum Phase Transitions in Single-Crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$: III. Magnetoresistance and Hall effect — •Christian Franz — Physik Department E21, Technische Universität München, München, Germany

Complex spin textures with non-trivial topology may generate anomalous contributions in the Hall conductivity, the so-called topological Hall effect, that provide direct evidence of non-vanishing winding numbers. We report a comprehensive study of the evolution of the spin structures and spin textures in $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ by means of the magnetoresistance and the Hall effect. Our study identifies the A-phase, located just below the helimagnetic transition, as a sykrmion lattice for a wide range of x. Combining the bulk properties and small angle neutron scattering with our Hall effect data additionally suggests the formation of non-trivial spin textures in parameter regimes outside the A phase when approaching quantum criticality under Fe- and Co-doping. Similarities and differences with pure MnSi and the doped semiconductor $Fe_{1-x}Co_xSi$ will be discussed.

TT 22.12 Wed 12:30 H21

Low-dimensional magnetic properties of anhydrous (black) dioptase. — •J. M. Law[1], C. Hoch[1], M.-H. Whangbo[2], and R. K. Kremer[1] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, U.S.A.

Hydrous dioptase, $CuSiO_3 \cdot H_2O$ is a low-dimensional quantum antiferromagnet. From a theoretical and experimental investigation it was proposed that hydrous dioptase is close to a quantum critical point.[1] Anhydrous dioptase, $CuSiO_3$ has a very similar magnetic lattice. We carried out a single-crystal structure determination and investigated the magnetic properties of anhydrous dioptase by carrying out specific heat and magnetic susceptibility measurements and performed a spin dimer analysis based on extended Hückel tight-binding calculations. We found that anhydrous dioptase conforms very well to a S=1/2 antiferromagnetic quantum chain model with uniform nearest-neighbor exchange interaction. Intra-chain interaction is by two orders of magnitude smaller than inter-chain superexchange and leads to long-range antiferromagnetic ordering at about 5 K.

[1] C. Gros *et al.*,*Europhys. Lett.* **2002**, *60*, 276.

TT 22.13 Wed 12:45 H21

Probing spin correlations in the highly frustrated magnets $CdCr_2O_4$ and $ZnCr_2O_4$ — •Christian Kant[1], Joachim Deisenhofer[1], Torsten Rudolf[1], Franz Mayr[1], Florian Schrettle[1], Vladimir Tsurkan[1,2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chisinau, Republic of Moldova

The spinel systems $CdCr_2O_4$ and $ZnCr_2O_4$ can be regarded as paradigms for highly frustrated systems where antiferromagnetic nearest-neighbor Heisenberg exchange leads to inherent frustration and considerable degeneracy of the magnetic ground state.

We performed optical, magnetic susceptibility, and specific heat measurements on single crystals of both compounds. From the magnetic susceptibility we estimate the nearest-neighbor and next-nearest neighbor exchange constants. The spin-spin correlation functions is derived from the magnetic susceptibility and the magnetic contribution to the specific heat. Comparing the frequency shift of the infrared optical phonons above T_N, we obtain the spin-phonon coupling constant in both systems.

TT 22.14 Wed 13:00 H21

High pressure studies in $Ca_3Ru_2O_7$ — •Oliver Welzel[1], Naoki Kikugawa[2], Andrew Mackenzie[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan — [3]Scottish Universities Physics Alliance, School of Physics & Astronomy, University of St Andrews, UK

The bilayer ruthenate $Ca_3Ru_2O_7$ undergoes first a magnetic transition ($T_N = 56$ K) and then a structural transition ($T_S = 48$ K) on cooling. Most of the Fermi surface is gapped out at low temperature, leading to a very low carrier density and small Fermi surface pockets. Pressure suppresses both T_N and T_S and, for $p > 3.5$ GPa, induces a third low temperature state, which has been known to be robust up to at least 7.5 GPa.

A detailed investigation of the unusual low temperature states of $Ca_3Ru_2O_7$ across the pressure-temperature-field phase diagram requires reliable access to hydrostatic pressures up to and beyond 10 GPa. We apply lithographic patterning and sputtering processes to anvil pressure cells in order to produce complex but robust lead patterns, which are integrated into the anvil surface. Patterns include multi-turn coils as well as eight-lead configurations for resistivity measurements.

Resistivity data in $Ca_3Ru_2O_7$ is presented, which indicates that the high pressure ordered state is fully suppressed at $p_c \simeq 9.5$ GPa. Beyond p_c, the in-plane resistivity follows a $T^{5/3}$ power-law down to below 1 K, suggesting ferromagnetic quantum criticality

TT 23: TR: Quantum Coherence and Quantum Information Systems 2

Time: Wednesday 14:00–17:00 Location: H18

TT 23.1 Wed 14:00 H18

Dynamics of strongly coupled Qubit-TLF systems — •Clemens Müller[1,2], Jared H. Cole[3,2], Jürgen Lisenfeld[4], Pavel Bushev[4], Alexander Shnirman[1,2], and Alexey V. Ustinov[4,2] — [1]Institut für Theorie der Kondensierten Materie, KIT, Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruhe, Germany — [3]Institut für Theoretische Festkörperphysik, KIT, Karlsruhe, Germany — [4]Physikalisches Institut, KIT, Karlsruhe, Germany

Spectroscopy of superconducting qubits often shows clear signatures of avoided crossings, indicating the presence of intrinsic two-level fluctuators (TLFs). Experiments are usually performed when the qubit is well detuned from resonance with these TLF since they are considered a source of decoherence. Alternatively one can tune the qubit in resonance with a TLF and observe the dynamics of the coupled multi-level system. We show results on rabi-spectroscopy in and near resonance with an individual TLF in the regime where both the coupling between qubit and TLF as well as the Rabi-frequency is strong. In addition we report on driving the system with high power, when the effect of higher levels in the qubit become important. This may pave the way towards understanding the microscopic nature of the TLFs.

TT 23.2 Wed 14:15 H18

Dissipative dynamics of driven quantum systems: a combined Floquet-Van-Vleck approach — •Johannes Hausinger, Carmen Vierheilig, and Milena Grifoni — Universität Regensburg, 93040 Regensburg, Germany

We investigate open quantum systems which are coupled to a classical, time-periodic field. Popular approximations to solve those time-dependent systems are the rotating wave approximation (RWA) and/or a perturbative expansion in the driving amplitude. In our work we combine Floquet theory with Van Vleck perturbation theory, which allows us to go beyond the RWA results and to arbitrary strong driving amplitudes, thus providing insight in so far not well explored parameter regimes. Environmental influences are accounted for by solving the Floquet-Bloch-Redfield master equation for the system's dynamics.

Our approach can be applied for example to examine the behavior of qubits in the strong driving regime leading to so-called dressed states and multi-photon Rabi oscillations [1]. We solve the corresponding spin-boson problem and give analytical results for the renormalized Rabi frequency, dephasing and relaxation times of the qubit going beyond the known RWA and high-frequency results [2].

Further, we apply the above formalism to a driven qubit-detector system; i.e., we couple the qubit to a linear/nonlinear oscillator, which represents for example the read-out by a dc-SQUID and investigate the resulting modifications of the dissipative qubit dynamics.

[1] C. M. Wilson et al., Phys. Lett. **98**, 257003 (2007)
[2] J. Hausinger, and M. Grifoni, arxiv:0910.0356 (2009)

TT 23.3 Wed 14:30 H18

Josephson quartic oscillator as a superconducting phase qubit — •Alexander Zorin[1] and Fabio Chiarello[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Istituto di Fotonica e Nanotecnologie, CNR, 00156 Rome, Italy

Due to interplay between the cosine Josephson potential and parabolic magnetic-energy potential the radio-frequency SQUID with the screening parameter value $\beta_L \equiv (2\pi/\Phi_0)LI_c \approx 1$ presents an oscillator circuit which energy well can dramatically change its shape. Ultimately, the magnetic flux bias of half flux quantum $\Phi_e = \Phi_0/2$ leads to the quartic polynomial shape of the well and, therefore, to significant anharmonicity of oscillations ($> 30\%$). We show that the two lowest eigenstates in this symmetric global minimum perfectly suit for designing the qubit which is inherently insensitive to the charge variable, always biased in the optimal point and allows efficient dispersive and bifurcation-based readouts. Moreover, in the case of a double-SQUID configuration (dc SQUID instead of a single junction) the transition frequency in this Josephson phase qubit can be easy tuned within an appreciable range allowing variable qubit-qubit and qubit-resonator couplings.

Invited Talk TT 23.4 Wed 14:45 H18

Superconducting Flux Qubits in Circuit QED and Detection of Weak Microwave Signals — •Achim Marx[1], Alex Baust[1], Elisabeth Hoffmann[1], Matteo Mariantoni[1], Edwin P. Menzel[1], Thomas Niemczyk[1], Manuel Schwarz[1], Thomas Weissl[1], Enrique Solano[2], Juan J. Garcia-Ripoll[3], Frank Deppe[1], Hans Hübl[1], and Rudolf Gross[1] — [1]Walther-Meissner-Institut and TU München, Germany — [2]Universidad del País Vasco and Ikerbasque Foundation, Bilbao, Spain — [3]Instituto de Fisica Fundamental, CSIC, Madrid, Spain

Superconducting qubits behave as artificial two-level atoms. Coupling them to on-chip microwave resonators has given rise to the field of circuit quantum electrodynamics, where fundamental quantum properties can be investigated. Here, we present spectroscopy data on single and two flux qubits coupled to a coplanar transmission line resonator. The strong coupling regime can be readily accessed both for inductive and galvanic coupling. The inherent tunability of the artificial atoms allows to control the symmetry properties of the coupled qubit-resonator system. Systems consisting of several resonators, which can be coupled by using superconducting qubits can be used to generate quantum microwave signals. To detect such weak microwave signals on a single photon level we have developed a signal recovery method based

on a cross-correlation technique. This method has been successfully applied to analyze thermal microwave states and propagating signals on a single photon level. We acknowledge support from SFB 631, NIM, UPV/EHU Grant GIU07/40 and European project EuroSQIP.

TT 23.5 Wed 15:15 H18

Spectral properties of single-qubit lasers — •Stephan André[1,2], Valentina Brosco[3], Alexander Shnirman[2,4], 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]Dipartimento di Fisica, Università "La Sapienza", P.le A. Moro 2, 00185 Roma, Italy — [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Recent experiments demonstrated lasing and cooling of the electromagnetic field in an electrical resonator coupled to a superconducting qubit [1]. In this work, we theoretically investigate the spectral properties of single-qubit lasers by numerically solving the full Liouville equation for the density matrix. We extend the usual quantum optics description to acccount for strong qubit-resonator coupling and to include the effects of low-frequency noise.

We present results for the linewidth and the lineshape of the emission spectrum. We find that the linewidth grows with the qubit-resonator coupling strength beyond the lasing transition, thus deteriorating the lasing state [2]. Our results also show that quantum correlations have a significant effect on the spectral properties and that low-frequency noise might explain the shape and width of the emission spectrum observed in the experiment.

[1] O. Astafiev *et al.*, Nature **449**, 588 (2007)
[2] S. André *et al.*, arXiv:0908.4227 (2009)

TT 23.6 Wed 15:30 H18

Coupling of a quantum oscillator to a superconducting flux qubit at its symmetry point — •Pascal Macha[1], Arkady Fedorov[2], Alexey K. Feofanov[3], Pol Forn-Diaz[2], Evgeni Il'ichev[1], Alexey. V. Ustinov[3], Kees Harmans[2], and J. E. Mooij[2] — [1]Institute of Photonic Technology, Jena, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — [3]Karlsruhe Institute of Technology, Germany

Resonant coupling of a quantum oscillator ($\hbar\omega > k_B T$) in the low–photon limit to a flux qubit at its symmetry point provides optimal conditions for the realization of cavity-QED experiments, i.e. long coherence times and the largest qubit–oscillator coupling. We report an experiment demonstrating this regime using the recently developed tunable gap flux qubit [1]. The control over the energy barrier height enables us to tune the gap of the flux qubit in and out of resonance with a superconducting LC resonator. We performed spectroscopic measurements of the qubit–oscillator system and demonstrate vacuum Rabi oscillations for various representative cases. We find that the decay time of these oscillations for the qubit operated at its symmetry point is not affected by 1/f flux noise and is only limited by the quality factor of the resonator. This work contributes to the development of advanced quantum information processing schemes with superconducting qubits.

[1] F. G. Paauw, A. Fedorov, C. J. Harmans, and J. E. Mooij, PRL **102**, 090501 (2009)

15 min. break

TT 23.7 Wed 16:00 H18

Selection rules for multiphoton excitations in a qubit-resonator system — Thomas Niemczyk[1], •Frank Deppe[1,2], Hans Huebl[1], Edwin Menzel[1], Fredrik Hocke[1], Elisabeth Hoffmann[1,2], Manuel Schwarz[1], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik Department E23, Technische Universität München, 85748 Garching, Germany

The theoretical analysis of a qubit-resonator system reveals selection rules at certain symmetry points of the qubit. In the case of a superconducting flux qubit, this symmetry of the double-well potential can be broken in a controlled way by changing the external magnetic field. Only then, odd and even multiphoton processes can coexist at the same flux bias. We illustrate this phenomenon with spectroscopy measurements of a superconducting flux qubit strongly coupled to an onchip coplanar waveguide resonator. Our studies extend up to three-photon driving and clearly show the transition from strict selection rules to a regime of coexistent multiphoton excitations.

Financial support via SFB631 and the Excellence Initative via NIM is gratefully acknowledged.

TT 23.8 Wed 16:15 H18

Strong coupling of two flux qubits to a colanar waveguide resonator — •Thomas Niemczyk[1], Hans Huebl[1], Frank Deppe[1,2], Edwin Menzel[1], Manuel Schwarz[1], Elisabeth Hoffmann[1,2], Fredrik Hocke[1], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik Department E23, Technische Universität München, 85748 Garching, Germany

The field of circuit QED opens new possibilities in both quantum information processing and studies of fundamental quantum mechanics "on a chip". Central building blocks are qubit circuits, which interact with on-chip superconducting microwave resonators. Of particular importance is the strong-coupling regime, where the coupling strength exceeds all relevant decay rates in the system. Here, we present spectroscopic measurements on two superconducting flux qubits strongly coupled to a coplanar waveguide resonator.

Finacial support via SFB631 and the Excellence Initative via NIM is gratefully acknowledged.

TT 23.9 Wed 16:30 H18

Dual-path measurements of propagating microwave signals at the quantum level for circuit QED — •Edwin P. Menzel[1], Matteo Mariantoni[1], Frank Deppe[1], Miguel Angel Araque Caballero[1], Alexander Baust[1], Elisabeth Hoffmann[1], Thomas Niemczyk[1], Achim Marx[1], Rudolf Gross[1], Enrique Solano[2], Kunihiro Inomata[3], Tsuyoshi Yamamoto[3,4], and Yasunobu Nakamura[3,4] — [1]Walther-Meissner-Institut and TU München, Garching, Germany — [2]Universidad del Pais Vasco and Ikerbasque Foundation, Bilbao, Spain — [3]RIKEN, Wako, Japan — [4]NEC Corporation, Tsukuba, Japan

Few-photon propagating microwave signals can be characterized by means of a beam splitter and two amplification chains. We show that such a setup is robust against random noise added by the amplifiers. Even if this noise is much larger than the signal itself, the first two signal moments and, hence, Gaussian states can be analyzed via correlation measurements. We discuss possible applications of the dual-path method for detecting squeezed states generated by a superconducting Josephson parametric amplifier and in circuit QED setups.

We acknowledge support from SFB631, NIM, UPV/EHU Grant GIU07/40 and European project EuroSQIP.

TT 23.10 Wed 16:45 H18

Josephson current and quantum cavity modes — Jakob Hammer[1] and •Marco Aprili[2] — [1]Universität Regensburg, Germany — [2]Laboratoire de Physique des Solides, France

Extended Josephson junctions support resonant quantum cavity modes in the weak link. We succeeded to excite selected modes in a controlled manner and to detect this excitations as modifications of the Fraunhofer interference pattern of the junction. Furthermore very small numbers of thermally excited photons are reflected in the shape of the switching current histogram. In addition we observed an increase of the Josephson critical current when the microwave frequency is slightly detuned from the cavity mode resonance. This effect is consistant with cavity induced phase cooling.

TT 24: SC: Properties, Electronic Structure, Mechanisms

Time: Wednesday 14:00–18:45 Location: H19

TT 24.1 Wed 14:00 H19

Tight-binding parameterization of the O-doped high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ — •Kateryna Foyevtsova[1], Hai Ping[2], Hem Kandpal[1], Harald Jeschke[1], Roser Valenti[1], and Peter Hirschfeld[2] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]University of Florida, Gainesville, Florida 32611, USA

Recent scanning tunneling microscopy studies of several hole-doped high-T_c cuprate superconductors reveal a positive correlation between the position of a dopant atom and the size of local superconducting gap. These findings can be explained in the framework of spin exchange mediated pairing theories of superconductivity in cuprates, provided that in the parent compound certain modifications of local electronic structure occur due to a dopant, which has been so far neither proved nor disproved.

We present a Density Functional Theory study on oxygen-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ aimed at gaining insight into the dopant-induced variations of electronic structure of this high-T_c superconductor. In our study, we develop a method to characterize the $Bi_2Sr_2CaCu_2O_{8+\delta}$ bandstructure in terms of a single-band tight-binding (TB) Hamiltonian. We present three alternative TB models and critically discuss the achievements and drawbacks of the proposed approach. The discussion is supplemented by comparison of the spin susceptibilities and the pairing strengths calculated in the random-phase approximation from the derived TB models.

TT 24.2 Wed 14:15 H19

Superconducting Coherence Peak in the Electronic Excitations of a Single-Layer Bi2201 Cuprate Superconductor — •Jia Wei[1,2], Martin Aeschlimann[1], and Donglai Feng[2] — [1]Department of Physics, University of Kaiserslautern, Fachbereich Physik, Erwin Sch€oodinger Str. 46, 67663 Kaiserslautern, Germany — [2]1Department of Physics, Surface Physics Laboratory (National Key Laboratory) and Advanced Materials Laboratory, Fudan University, Shanghai 200433, P. R. China

Angle resolved photoemission spectroscopy study is reported on a high quality optimally doped Bi(La)2201 high-Tc superconductor. In the antinodal region with a maximal d-wave gap, the symbolic superconducting coherence peak, forming a so-called "peak-dip-hump" (PDH) structure, which has been widely observed in multi-CuO_2-layer cuprate superconductors, is unambiguously observed in a single-layer system. We have discovered the PDH in the antinodal region of the La-Bi2201. The 19 meV peak-dip separation seriously challenges models based on electron-phonon interactions. Meanwhile, this energy scale is much smaller than its counterparts in multi-layered compounds, but correlates with the energy scales of spin excitations in single layer cuprates. Our data provide a critical piece to the global picture of the bosonic mode and gap in cuprates, which would help to eventually resolve controversial issues and uncover the "glue" of high-T_c superconductivity.

TT 24.3 Wed 14:30 H19

Polarized XAS on single layer Bi-cuprates: Probing the ground state beyond the conventional $d_{x^2-y^2}$ picture — •Beate Müller, Ahmad Ariffin, Rüdiger Mitdank, Lenart Dudy, Peter Hlawenka, Alica Krapf, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt Universität Berlin, Newtonstr. 15, 12489 Berlin

CuL_3 and OK XAS studies on the single layer Bi-cuprate (Pb,Bi)2201 with different combinations of La and Pb substitutions and thus varied doping levels are presented. A polarization dependence within the CuO_2 plane was found which should not exist following the assumptions of a one-band model based on $d_{x^2-y^2}$ symmetric Zhang-Rice singlets. This dependence on the azimuthal angle modulates spectral features believed to be related to the Zhang-Rice singlet. Its characteristics over angle reveals signatures that move beyond the expected $d_{x^2-y^2}$ symmetry and point towards the inclusion of axial orbitals as proposed by Anderson et al. [J. Phys. Chem. Solids 56, 1573 (1995)] and Pavarini et al. [Phys. Rev. Lett. 87, 047003 (2001)].

TT 24.4 Wed 14:45 H19

High-Temperature optical behavior of Bi-based cuprates — •Georg Rohringer[1], Alessandro Toschi[1], Daniele Nicoletti[2], Paolo Calvani[2], Stefano Lupi[2], Massimo Capone[3], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology — [2]CNR-INFM Coeherentia and Department of Physics, University of Rome "La Sapienza" — [3]CRS SMC, CNR-INFM and Department of Physics, University of Rome "La Sapienza"

The optical conductivity $\sigma(\omega)$ and the optical spectral weight W provide important information about the physical properties of strongly correlated systems[1,2]. This is the case for cuprates, where DMFT calculations have shown the important role of the quasiparticle renormalization factor Z, which manifests itself in a strong temperature (T) dependence of W at low T. We analyze here new experimental results for the normal phase of two Bi-based cuprates up to 500K. The comparison between our DMFT calculations and the experimental data for W allows for a full understanding of the observed deviation ($\propto T^4$) from the low-temperature T^2 behavior in the framework of a Sommerfeld expansion with strongly renormalized coefficients[3].

[1] L. Baldassarre et al., Phys.Rev. B **77**, 113107 (2008)
[2] A. Toschi et al., Phys.Rev.Lett. **95**, 097002 (2005)
[3] D. Nicoletti, O. Limaj, P. Calvani, G. Rohringer, et al. in preparation.

TT 24.5 Wed 15:00 H19

Importance of local correlations for the order parameter of high-T_c superconductors — •Matthias Balzer and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Germany

Using an extension of the variational cluster approximation (VCA), the relevance of bath degrees of freedom in a cluster-embedding approach for the size of the d-wave superconducting order parameter is studied within the hole- and electron-doped two-dimensional Hubbard model at zero temperature. We discuss results obtained for a reference system consisting of a plaquette of four correlated and four bath sites in addition and compare with results obtained via VCA for the plain plaquette without bath sites on the one hand and with results from previous cellular (plaquette) dynamical mean-field calculations on the other. It is shown that local, i.e. temporal, correlations are essential: Including a single bath degree of freedom considerably decreases the order parameter and provides a substantial gain of binding energy. Bath sites are also seen to partially compensate for the artificial breaking of translational symmetry introduced by the real-space quantum cluster approach.

15 min. break

Invited Talk TT 24.6 Wed 15:30 H19

Fermi Surface Evolution in an Electron-Doped Cuprate Superconductor Revealed by High-Field Magnetotransport — •Mark Kartsovnik — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

Establishing the Fermi surface topology and its dependence on carrier concentration is fundamentally important for understanding the role of electronic correlations and resulting ordering instabilities in superconducting paring in high-T_c cuprates. I will present recent experiments on magnetic quantum oscillations in the electron-doped cuprate $Nd_{2-x}Ce_xCuO_4$ providing direct evidence for a well-defined continuous Fermi surface and its evolution with doping level. Most interestingly, the Fermi surface is found to be reconstructed, most likely due to a magnetic ordering which occurs at a critical doping level significantly exceeding the optimal doping. Besides quantum oscillations, we have found semiclassical angle-dependent magnetoresistance oscillations (AMRO) which are directly related to the geometry of the underlying Fermi surface. The analysis of the AMRO in combination with the Shubnikov-de Haas data shows that a superlattice potential survives over the entire superconducting doping range. This suggests an intimate relation between magnetic ordering and superconductivity.

The work was done in cooperation with T. Helm, W. Biberacher, M. Bartkowiak, I. Sheikin, M. Lambacher, A. Erb, N. Bittner, J. Wosnitza, and R. Gross and supported by the DFG via Research Unit 538 and EuroMagNET II.

TT 24.7 Wed 16:00 H19

Angle-dependent interlayer magnetoresistance in the normal state of the electron-doped cuprate $Nd_{1-x}Ce_xCuO_4$ — •Toni Helm[1], Mark Kartsovnik[1], Pavel Grigoriev[2], Michael Lambacher[1], Andreas Erb[1], Ilya Sheikin[3], and Rudolf Gross[1] — [1]Walther-Meissner-Institit, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]L.D. Landau Institute for Theoretical Physics, Russian Ac. Sci., Chernogolovka, Russia — [3]Grenoble High Magnetic Field Laboratory, Grenoble, France

We report on systematic studies of the normal-state *c*-axis magnetoresistance of high quality single crystals of $Nd_{2-x}Ce_xCuO_4$ as a function of magnetic field orientation, performed for a broad range of Ce concentrations. In underdoped compounds, the major effect of magnetic field comes from coupling to spins in a magnetically ordered system. Notably, the spin-dependent magnetotransport prevails even for superconducting compositions, up to the optimal doping level. In the overdoped regime, the conventional orbital coupling of charge carriers to a magnetic field becomes dominant. Most interestingly, overdoped samples exhibit features characteristic of the so-called angle-dependent magnetoresistance oscillations (AMRO). We analyze the data using the semiclassical kinetic model and discuss the results in terms of the geometry of the Fermi surface responsible for the AMRO.

The work was supported by the DFG via Research Unit 538 and EuroMagNET II under the EU contract.

TT 24.8 Wed 16:15 H19

Superconducting fluctuation regime in $HgBa_2CuO_{4+\delta}$ revealed by microwave measurements — •Neven Barišić[1,3], Mihael S. Grbić[2], Antonije Dulčić[2], Yuan Li[3], Xudong Zhao[3], Guichuan Yu[3], Martin Dressel[1], Martin Greven[3,4], and Miroslav Požek[2] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany — [2]Department of Physics, Faculty of Science, University of Zagreb, P.O. Box 331, HR-10002 Zagreb, Croatia — [3]Department of Physics, Stanford University, Stanford, California 94305, USA — [4]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

Superconducting (SC) fluctuations belong to fundamental properties of high-T_c superconductors. Although studied by various experimental techniques the highest temperature at which the superconducting fluctuations can be observed, is not yet unambiguously determined. Thus, an alternative experimental verification of the SC fluctuation regime is desirable. We are proposing a novel approach to microwave conductivity measurements to elucidate the phase diagram of high- T_c. Measurement are performed on a model high-T_c material: $HgBa_2CuO_{4+\delta}$. From a set of the single c-axis data for a sample close to optimal doping we can clearly discern the opening of the pseudogap at T*=185 (15) K, the appearance of the superconducting fluctuations at a much lower temperature T'=105 (2) K, and the full transition to the superconducting state at the critical temperature T_c=94.3 K. Thus, with the presently acquired high sensitivity we establish that the superconducting fluctuations extend only to about 10 K above T_c.

TT 24.9 Wed 16:30 H19

The magnetic resonance mode in high-temperature superconductors — •Klaus W. Becker[1] and Steffen Sykora[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Department of Physics and Astronomy, Rutgers University, USA .

The origin of the magnetic resonance mode in cuprates, measured by inelastic neutron scattering, is still subject of controversy. In this talk, we investigate the resonance mode on the basis of the t-J model using a microscopic renormalization approach which is called projector based renormalization method (PRM). Thereby, the strong correlations are strictly obeyed. The approach was applied to the cuprates before in order to explain ARPES experiments in the pseudogap and in the superconducting region. The method also allows to evaluate the inelastic neutron scattering in the superconducting state of the cuprates. The theoretical results turn out to be in perfect agreement with the experimental findings.

TT 24.10 Wed 16:45 H19

Microscopic approach to high-temperature superconductors: Superconducting phase — •Steffen Sykora[1,2] and Klaus W. Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Department of Physics and Astronomy, Rutgers University, USA

An understanding of the superconducting pairing mechanism of the high-temperature superconductors leading to an unprecedented high transition temperature T_c is still lacking. Starting from the *t*-*J* model, in this talk we present a microscopic approach to investigate physical properties of the superconducting phase in the framework of a novel renormalization scheme called PRM. This approach is based on a stepwise elimination of high-energy transitions using unitary transformations. We find a renormalized 'free' Hamiltonian for correlated electrons for the superconducting phase. Our microscopic approach allows us to explain the experimental findings in the underdoped as well as in the optimal hole doping regime. Our results turn out to be in good agreement with experiment: The superconducting order parameter shows *d*-wave symmetry with a coherence length of a few lattice constants. In good agreement with experiments, we find no superconducting solutions for very small hole doping. Furthermore, we calculate the ARPES spectral function along the Fermi surface. The spectra display peak-like structures which are caused alone by coherent excitations in a small range around the Fermi energy.

15 min. break

TT 24.11 Wed 17:15 H19

Plasmons and interband transitions of $Sr_{14-x}Ca_xCu_{24}O_{41}$ investigated by electron energy-loss spectroscopy — •Friedrich Roth, Martin Knupfer, Christian Hess, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Electron energy-loss spectroscopy has been used to investigate the loss-function between 0 and 70 eV of singel-crystalline $Sr_{14-x}Ca_xCu_{24}O_{41}$, composed of two-leg Cu_2O_3 ladders and edge-sharing CuO_2 chains, with various compositions. We found significant exitations in the low-energy range which are different for momentum transfer q parallel to the **a**- and **c**-axes. Comparison with reflectivity data from literature [1] shows a good agreement with our data. Also the disperions of a charge-carrier plasmon like in $Bi_2Sr_2CaCu_2O_8$ [2] was obeserved for $Sr_3Ca_{11}Cu_{24}O_{41}$.

[1] Osafune, T. et al., Phys. Rev. Lett. **78** 1980 (1997)
[2] Nücker, N. et al., Phys. Rev. B **39** 12379 (1989)

TT 24.12 Wed 17:30 H19

Optical conductivity of $LuNi_2B_2C$ in the terahertz range — •T. Fischer[1], A. V. Pronin[1], J. Wosnitza[1], T. Niemeier[2], and B. Holzapfel[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, 01171 Dresden, Germany

Using a backward-wave-oscillator-based setup in a Mach-Zehnder interferometer arrangement, we have measured the temperature- and frequency-dependent transmission and phase-shift spectra of $LuNi_2B_2C$ films on MgO substrates in the range 200 GHz - 1.4 THz. From the measured spectra, we have directly calculated the complex optical conductivity. We observe a clear signature of the superconducting energy gap in the spectra. In the talk, a comparison of the experimentally obtained spectra with theoretical predictions for a multi-band superconductor will be given.

TT 24.13 Wed 17:45 H19

Low temperature disorder of the stripe phase in layered nickelates — Christoph Trabant[1], Marcel Buchholz[1], Chun-Fu Chang[1], Ralf Feyerherm[2], Enrico Schierle[2], Esther Dudzik[2], Alexander Komarek[1], Agung Nugroho[3], Mohammed Benomar[1], Liu Hao Tjeng[1,4], Markus Braden[1], and •Christian Schüssler-Langeheine[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Helmholtz-Zentrum Berlin — [3]Institut Teknologi Bandung — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

In hole-doped layered nickelates and cuprates a collective order of charge and spin degrees of freedom is found, the so-called stripe phase. The holes arrange in lines, which act as domain walls for the antiferromagnetic order on the hole-poor sites. This order is formed upon cooling with a gradual increase of the correlation length. Remarkably the correlation length goes through a maximum and decreases again upon further cooling: The stripe order breaks apart at low temperatures. Generally not observed in neutron experiments, this effect has been predicted by theory as a consequence of competition between Coulomb repulsion and lattice potential. Also the effect of static disorder has been discussed. We present a systematic study of low-temperature disorder in doped nickelates using resonant diffraction in the conventional and soft x-ray range. We find that this effect depends mainly on the

total doping level and affects spin order and charge order in a similar way. The influence of static disorder is found to be small. Funded by the DFG through SFB 608 and by the BMBF project 05KS7PK1.

TT 24.14 Wed 18:00 H19

Origin of the nondispersive wavevector component at $\vec{q} = (3/4, 0)$ in the electronic structure of cuprate superconductors — •Jürgen Röhler — Universität zu Köln, 50937 Köln

A direct spectroscopic fingerprint of phase-incoherent precursor superconductivity in cuprates was recently obtained by spectroscopic imaging spectroscopy uncovering up to $T = 1.5\ T_c$ dispersive Bogoliubov quasiparticle excitations ($\pm E < 35$ meV) which coexist with true nondispersive and locally symmetry breaking excitations at the pseudogap energy scale ($\pm E \simeq 120$ meV) [1]. While the low-energy excitations are homogenously distributed in r-space, the high-energy excitations appear as static domains (width $4a$) scattered in random orientation on the xy-plane, but along no preferred Cu-O direction. This "glassy" component of the electronic structure is in conflict with "stripes" flowing preferrentially in one Cu-O direction. The $4a$ wide O-Cu-O-Cu-O-Cu-O-Cu-O domains exhibit an internal $3a$ structure by dominant charge contrast maxima at the central O site and the two outmost Cu sites. We analyze the corresponding wavevector components at $\vec{q} = (3/4, 0); (0, 3/4)$ as a signature of bond centered quartets of Zhang-Rice hole singlets forming pseudomoleculss with a characteristic length of $3a$ [2]. The internally antiferromagnetic $3a$ pseudomolecules may act as bosonic pairing centers exchanging resonantly paired quasiparticles with the dispersive low-energy sector of the superconducting condensate.

[1] J. Lee et al., Science **325** (2009), 1099.
[2] J. Röhler, Physica C**460-62** (2007), 374.

TT 24.15 Wed 18:15 H19

Ferromagnetism and d-wave superconductivity in the 2D Hubbard model — Carsten Honerkamp[1], •Christoph Husemann[2], Jutta Ortloff[3], and Manfred Salmhofer[2] — [1]Institut für Theoretische Physik C, RWTH Aachen, Germany — [2]Institut für Theoretische Physik, Universität Heidelberg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

By using the functional renormalization group we compute detailed momentum dependencies of the scale-dependent interaction vertex of the 2D (t,t')-Hubbard model. Compared to previous studies we improve accuracy by separating dominant parts from a remainder term. The former explicitly describe, for example, the interaction of Cooper pairs or spin operators. Applying the method to the repulsive Hubbard model we find d-wave superconductivity or ferromagnetism for larger next-to-nearest neighbor hopping amplitude |t'| at Van Hove Filling. Both ordering tendencies strongly compete with each other.

TT 24.16 Wed 18:30 H19

Conserving T-matrix theory of superconductivity — •Klaus Morawetz[1,2], Pavel Lipavský[3,4], Bretislav Šopík[4], and Michael Männel[5] — [1]University of Applied Science Münster, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Center for Condensed Matter Physics, Universidade de Brasília, 70904-910, Brasília-DF, Brazil — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [5]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Any many-body approximation corrected for unphysical repeated collisions in a given condensation channel is shown to provide the same set of equations as they appear by using anomalous propagators. The ad-hoc assumption in the latter theory about non-conservation of particle numbers can be released. In this way the widespread used anomalous propagator approach is given another physical interpretation. A generalized Soven equation follows which improves any approximation in the same way as the coherent potential approximation (CPA) improves the averaged T-matrix for impurity scattering. A selfconsistent T-matrix theory of many-Fermion systems is proposed. In the normal state the theory agrees with the Galitskii-Feynmann approximation, in the superconducting state it has the form of the renormalized Kadanoff-Martin approximation. The two-particle propagator satisfies the Baym-Kadanoff symmetry condition which guarantees that the theory conserves the number of particles, momentum and energy.

TT 25: FS: Iron-Based Superconductors

Time: Wednesday 14:00–18:00 Location: H20

Invited Talk TT 25.1 Wed 14:00 H20

Fermiology of Fe-Pnictide Superconductors Revealed by Quantum Oscillations — •James Analytis — Stanford Linear Accelerator Center

The iron-pnictide superconductors are a new class of materials with unique superconducting and magnetic properties. Many theoretical frameworks describing these materials rely heavily on the nature of the size and topology of the Fermi surface. The classic method of determining the Fermi surface is by looking at oscillations in the magnetization as a function of field. These oscillations, known as the de Haas-van Alphen effect, are extremely powerful in determining the full three-dimensional topology of the FS, in addition to the quasiparticle renormalization to the effective mass. In the present study we measure the Fermi surface of the superconducting P-doped BaFe2As2 using this technique and describe the consequences for theories of pnictide superconductivity.

Topical Talk TT 25.2 Wed 14:30 H20

Magnetic degeneracy and hidden metallicity of the spin density wave state in Fe-based superconductors — •Ilya Eremin — MPI fuer Physik komplexer Systeme, 01187 Dresden, Germany

In my talk, I will analyze spin density wave (SDW) order in iron-based superconductors and electronic structure in the SDW phase. We consider an itinerant model for $Fe-$pnictides with two hole bands centered at $(0, 0)$ and two electron bands centered at $(0, \pi)$ and $(\pi, 0)$ in the unfolded BZ. A SDW order in such a model is generally a combination of two components with momenta $(0, \pi)$ and $(\pi, 0)$, both yield (π, π) order in the folded zone. Neutron experiments, however, indicate that only one component is present. We show that $(0, \pi)$ or $(\pi, 0)$ order is selected if we assume that only one hole band is involved in the SDW mixing with electron bands. A SDW order in such 3-band model is highly degenerate for a perfect nesting and hole-electron interaction only, but we show that ellipticity of electron pockets and interactions between electron bands break the degeneracy and favor the desired $(0, \pi)$ or $(\pi, 0)$ order. We further show that stripe-ordered system remains a metal for arbitrary coupling. We analyze electronic structure for parameters relevant to the pnictides and argue that the resulting electronic structure is in good agreement with ARPES experiments. We discuss the differences between our model and $J_1 - J_2$ model of localized spins.

Topical Talk TT 25.3 Wed 15:00 H20

Muon spin relaxation and Moessbauer studies of iron pnictide superconductors — •Hans-Henning Klauss[1], H. Maeter[1], T. Dellmann[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], Y. Pashkevich[3], C. Hess[4], R. Klingeler[4], B. Büchner[4], A. Leithe-Jasper[5], H. Rosner[5], C. Geibel[5], W. Schnelle[5], M. Braden[6], and J. Litterst[7] — [1]Technische Universität Dresden, Germany — [2]PSI Villigen, Switzerland — [3]Donetsk Phystech NASU, Ukraine — [4]IFW Dresden, Germany — [5]MPI-CPfS, Dresden, Germany — [6]Universität Köln, Germany — [7]Technische Universität Braunschweig, Germany

We have determined the electronic phase diagrams and order parameters of $ReO_{1-x}F_xFeAs$ and $(Sr,Eu)Fe_{2-x}Co_xAs_2$ superconductors. The results prove an important role of the structural distortion for the SDW magnetism [1-3] and reveal two gap multiband superconductivity. We examined the interplay of iron and rare earth magnetic order in $ReO_{1-x}F_xFeAs$. The undoped compounds show different magnetic coupling strength of the rare earth ion to the antiferromagnetic iron layers ranging from independent order to strong polarization of the rare earth moments by the ordered iron [4]. Finally, we present recent studies on $(Ca,Sr,Ba,Eu)Fe_2As_2$ [5] and $(Fe_2As_2)(Sr_4T_2O_6)$based pnictide superconductors.

[1] H. Luetkens, et al., Phys. Rev. Lett.,101, 2008
[2] H.-H. Klauss, et al., Phys. Rev. Lett., 101, 2008
[3] H. Luetkens, et al., Nature Materials, 8, 2009
[4] H. Maeter et al., Phys. Rev. B., 80, 2009
[5] R. Khasanov et al., Phys. Rev. Lett., 102, 2009

15 min. break

Topical Talk TT 25.4 Wed 15:45 H20

Interplay among lattice, orbital and spin degrees of freedom in iron pnictides — •Roser Valenti — Institute of Theoretical Physics, Goethe University, Frankfurt am Main, Germany

By means of ab initio molecular dynamics calculations as well as dynamical mean field theory considerations, we investigate the role of lattice, orbital and spin degrees of freedom in iron pnictides. We analyze the nature of magnetism as well as the origin of structural and magnetic phase transitions under pressure in the 1111 and 122 families and discuss their implications on the superconductor behavior of these materials.

Topical Talk TT 25.5 Wed 16:15 H20

Lattice dynamics and magnetism in layered iron based superconductors — •Thomas Brückel[1,2], Yixi Su[2], Yinguo Xiao[1], and Ranjan Mittal[2] — [1]Forschungszentrum Jülich, Institut für Festkörperforschung IFF, 52425 Jülich, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science JCNS, Outstation at FRM II, 85747 Garching, Germany

The discovery of superconductivity in layered iron based compounds at critical temperatures of up to some 56 K has attracted much attention by the solid state physics community. Scattering methods, in particular neutron scattering and resonant x-ray scattering, prove crucial to access microscopic information about these new classes of compounds. We have employed inelastic neutron scattering to study the phonon density of states as well as full phonon dispersion relations [1]. The proximity to magnetism suggests that magnetic order and spin fluctuations play an important role in these compounds [2]. We will review our experimental findings on ordering phenomena and spin- and lattice excitations and discuss their possible relevance for superconductivity.

[1] R. Mittal et al., Phys. Rev. B 78 (2008), 104514; R. Mittal et al., Phys. Rev. B 78 (2008), 224518 (R); R. Mittal et al., PRL 102 (2009), 217001; R. Mittal et al., Phys. Rev. B 79 (2009), 144516; R. Mittal et al., Phys. Rev. B 79 (2009), 214514

[2] Y. Su et al., Phys. Rev. B 79 (2009), 064504; Y. Xiao et al., Phys. Rev. B79, 060504 (R)

15 min. break

TT 25.6 Wed 17:00 H20

ARPES studies on FeAs-based superconductors and their parent compounds — •Jörg Fink[1,2], S. Thirupathaiah[1], R. Ovsyannikov[1], H.A. Dürr[1], S. de Jong[3], Y. Huang[3], R. Huisman[3], M.S. Golden[3], A. Gloskovskii[4], Y.Z. Zhang[5], H.O. Jeschke[5], R. Valenti[5], H.S. Jeevan[6], P. Gegenwart[6], and A. Erb[7] — [1]HZ Berlin — [2]IFW Dresden — [3]U Amsterdam — [4]U Mainz — [5]U Frankfurt — [6]U Göttingen — [7]WMI Garching

We report high-resolution ARPES studies of the electronic structure of $BaFe_{2-x}Co_xAs_2$, $Ba_{1-x}K_xFe_2As_2$, FeTe(Se), and $EuFe_2As_2$. The results are compared with DFT band structure calculations. From photon energy dependent measurements, information on the band dispersion perpendicular to the Fe layers could be derived. with increasing Co doping in $BaFe_{2-x}Co_xAs_2$, the dimensionality increases and, due to the filling of the hole pockets, the nesting condition decreases. In the AFM phase of $EuFe_2As_2$ back-folded bands strongly hybridize with the non-folded bands leading to the opening of gaps around both high-symmetry points. This transforms the large Fermi surface of the PM phase into droplet Fermi surfaces in the AFM low-T phase.

TT 25.7 Wed 17:15 H20

Energy and temperature dependence of spin fluctuations in electron-doped iron arsenide superconductors — •Dmytro Inosov[1], Jitae Park[1], Philippe Bourges[2], Dunlu Sun[1], Yvan Sidis[2], Astrid Schneidewind[3,4], Klaudia Hradil[4,5], Daniel Haug[1], Chengtian Lin[1], Bernhard Keimer[1], and Vladimir Hinkov[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]LLB, CEA-CNRS, CEA Saclay, France — [3]Inst. für Festkörperphysik, TU Dresden, Germany — [4]FRM-II, TU München, Garching, Germany — [5]Institut für Physikalische Chemie, Univ. Göttingen, Germany

Using inelastic neutron scattering we have studied the spin excitations in optimally doped $BaFe_{1.85}Co_{0.15}As_2$ ($T_c = 25$ K) over a wide range of temperatures and energies. We present the results in absolute units and find that the normal state spectrum carries a weight comparable to underdoped cuprates. In contrast to cuprates, however, the spectrum agrees well with predictions of the theory of nearly antiferromagnetic metals, without complications arising from a pseudogap or competing incommensurate spin-modulated phases. We also show that the temperature evolution of the resonance energy follows the superconducting energy gap, as expected from conventional Fermi-liquid approaches. Our observations point to a surprisingly simple theoretical description of the spin dynamics in the iron arsenides and provide a solid foundation for models of magnetically mediated superconductivity.

TT 25.8 Wed 17:30 H20

Doping evolution of the electronic density of states and the gap symmetry in Co-doped 122 iron pnictides — •Frédéric Hardy[1], Thomas Wolf[1], Peter Schweiss[1], Peter Adelmann[1], Robert A. Fisher[2], Rolf Heid[1], Robert Eder[1], Hilbert v. Löhneysen[1], and Christoph Meingast[1] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA

Iron pnictides represent a new class of multiband superconductors which offer new possibilities for studying the interplay between magnetism and superconductivity. In these materials, solid experimental evidence for any particular pairing state remains elusive because several probes point to different conclusions. Some of these apparent contradictions may arise from the influence of the magnetic instability, which is expected to strongly alter the gap topology, from impurity effects, or from experimental difficulties like sample inhomogeneities. Here, we present a critical analysis of our own specific-heat and thermal expansion-data, realized on high-quality flux-grown Co-doped 122 single crystals, for doping levels that cover the entire phase diagram.

TT 25.9 Wed 17:45 H20

Mössbauer high pressure and magnetic field studies of the superconductor FeSe — Vadim Ksenofontov[1], Gerhard Wortmann[2], Ivan Trojan[3], Taras Palasyuk[3], Sergey Medvedev[3], Michail Eremets[3], Tyrel M. McQueen[4], Richard J. Cava[4], and •Claudia Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]Department of Physics,University of Paderborn, Paderborn, Germany — [3]Max-Planck-Institute for Chemistry, Mainz, Germany — [4]Department of Chemistry, Princeton University, Princeton, USA

Superconducting FeSe has been investigated by Mössbauer spectroscopy applying high pressure and strong external magnetic fields. It was found that pressure-induced structural phase transition between tetragonal and hexagonal modifications is accompanied by increased distortion of local surrounding of Fe atoms. Appearance of the hexagonal phase above 7.2 GPa is accompanied by degradation of superconducting properties of FeSe. Low-temperature measurements demonstrated that the ground states in both orthorhombic and hexagonal phases of FeSe are nonmagnetic. Mössbauer measurements in the external magnetic field below transition to the superconducting state revealed zero electron spin density on Fe atoms. Interpretation of Mössbauer spectra of FeSe in the Shubnikov phase is discussed.

TT 26: CE: Heavy Fermions

Time: Wednesday 14:00–18:45 Location: H21

TT 26.1 Wed 14:00 H21

Evolution of the Electron Spin Resonance (ESR) in the $CeFeAs_{1-x}P_xO$ doping series — •Tobias Förster, Anton Jesche, Cornelius Krellner, Jörg Sichelschmidt, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden

The $CeFeAs_{1-x}P_xO$ compounds are structural homologues of the RTPnO (R: rare earth, T: transition metal, Pn: P or As) high temperature superconductors. The doping series owns a rich magnetic phase diagram driven by chemical pressure: CeFeAsO shows spin density wave (SDW) type order of Fe at $T_{SDW} \approx 140$ K and antiferromagnetic order (AFM) of Ce^{3+} at $T_N = 4$ K. By substituting P for As the SDW order disappears and the Ce magnetism initially becomes ferromagnetic (FM). Finally CeFePO is a heavy fermion metal with a large Sommerfeld coefficient and no magnetic order[1,2].
In our contribution we present the results of an ESR study on high quality poly- and single crystalline samples from the $CeFeAs_{1-x}P_xO$ doping series, covering the hole doping range. We find no signal, neither from Fe nor from Ce, in the samples with SDW and Ce-AFM. The ESR, which originates from the Ce^{3+} ions, appears when the SDW order of Fe vanishes and the Ce magnetism becomes FM. This is in agreement with our earlier work on CeRuPO and CeOsPO[3]. We will discuss the temperature and doping dependence of the ESR parameters.

[1] Y. Luo et al., arXiv **0907** 2961v1 (2009)
[2] E. Brüning et al., Phys. Rev. Lett. **101**, 117206 (2008)
[3] C. Krellner et al., Phys. Rev. Lett. **100**, 066401 (2008)

TT 26.2 Wed 14:15 H21

Complex interplay of Ce 4f and Fe 3d magnetism in CeFe(As,P)O as seen from ^{31}P and ^{75}As NMR. — •Rajib Sarkar, Michael Baenitz, Anton Jesche, Frank Steglich, and Cristoph Geibel — Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The rare earth (R) transition metal (T) pnictides RTPnO(Pn:P or As) earn special attention because of the high T_C superconductivity in $CeFeAsO_{1-x}F_x$, whereas the magnetism of the undoped system stays unexplored. CeFePO is a heavy fermion metal with a high γ value (700 mJ/mol K^2) in the vicinity of a ferromagnetic (FM) instability [1]. Here magnetism is solely governed by Ce-4f state whereas in CeFeAsO Fe 3d states themself order AFM at about T≅150 K. Therefore investigation on CeFe(As,P)O allows to study the crossover between Kondo and RKKY physics to 3d magnetic order. Yongkang Luo et. al. recently published a rather complex phase diagram with two critical points obtained from bulk properties. NMR provides a microscopic tool for studying the interplay between Ce 4f and Fe 3d magnetism. We report on ^{31}P (I=1/2) and ^{75}As (I=3/2) NMR studies on $CeFeAs_{1-x}P_xO$ with x=0, 0.05, 0.3, and 0.9.

[1] Brüning et . al., PRL 101, 117206 (2008).
[2] Luo et . al., arXiv:0907.2961v1.

TT 26.3 Wed 14:30 H21

Ferromagnetic 4f Correlations in the Oxypnictides $CeFe_{1-x}Ru_xPO$: A ^{31}P NMR Study — •Eva Maria Brüning, Cornelius Krellner, Michael Baenitz, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

CeTPO (T = Ru, Os, Fe), homologues of the new oxypnictide superconductors, show dissimilar types of ground states. CeRuPO is a rare example of a ferromagnetically ordered Kondo-lattice system ($T_C = 15$ K), whereas CeOsPO shows antiferromagnetic order and weak Kondo interaction ($T_N = 3.5$ K) [1]. CeFePO is a paramagnetic heavy fermion system in the vicinity of ferromagnetic order [2]. Therefore it became very interesting to investigate the solid solution series $CeFe_{1-x}Ru_xPO$ ($x = 0.1, 0.2$) to trace the crossover from a ferromagnetically correlated heavy fermion system ($x = 0$) to a ferromagnetically ordered metal ($x = 1$) through a possible quantum critical point. We applied the microscopic NMR method on polycrystals and performed a temperature and field dependent ^{31}P NMR study. The investigations of the Knight shift $^{31}K(T)$ and spin-lattice-relaxation rate $^{31}(1/T_1)$ of the new systems $CeFe_{1-x}Ru_xPO$ ($x = 0$, $x = 0.1$, $x = 0.2$) are presented.

[1] C. Krellner, N. S. Kini, E. M. Brüning, K. Koch, H. Rosner, M. Nicklas, M. Baenitz, C. Geibel *Phys. Rev. B*, **76**; 104418 (2007)
[2] E. M. Brüning, C. Krellner, M. Baenitz, A. Jesche, C. Geibel, F. Steglich, *Phys. Rev. Lett*, **101**; 117206 (2008)

TT 26.4 Wed 14:45 H21

Electronic structure and thermodynamic properties of $Ce_{3+x}Rh_4Sn_{13-x}$. — •Monika Gamza[1,2], Walter Schnelle[1], Roman Gumeniuk[1], Michael Nicklas[1], Ulrich Burkhardt[1], Andrzej Slebarski[3], Lev Akselrud[4], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]Institute of Materials Science, University of Silesia, Katowice, Poland — [3]Institute of Physics, University of Silesia, Katowice, Poland — [4]Ivan Franko National University of Lviv, Ukraine

Recently we reported on the electronic structure and the magnetic properties of the strongly correlated compound $Ce_3Rh_4Sn_{13}$ [1]. The combined theoretical and experimental study indicated an unusual sensitivity of the magnetic ground state on the local composition. This prompted us to inspect the homogeneity range of Ce and Sn in this system.

Here, we present the results of magnetization, resistivity and specific heat measurements on the series of compounds $Ce_{3+x}Rh_4Sn_{13+x}$ ($0 \leq x \leq 0.6$) for temperatures down to 350 mK and in applied magnetic fields up to 7 T. The experimental study is accompanied by first principles electronic structure calculations. The changes in electronic structure and ground state properties for the series of $Ce_{3+x}Rh_4Sn_{13+x}$ are analysed with respect to the substitution of Sn by Ce. Furthermore, the crystal structure of the parent compound $Ce_3Rh_4Sn_{13}$ has been reinvestigated in detail. Superstructure has been found.

[1] Gamza M *et al.*, J. Phys.: Condens. Matter **20** 395208 (2008)

TT 26.5 Wed 15:00 H21

Investigation of the metamagnetic transition in $Ce_{1-x}La_xTiGe$ polycrystals — •Micha Deppe, Nubia Caroca-Canales, Franziska Weickert, Stefan Lausberg, Manuel Brando, Christoph Geibel, and Frank Steglich — Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

CeTiGe is a new heavy Fermion system with a Kondo energy scale of the order of 50 K. Our investigations of the specific heat, magnetic susceptibility and resistivity of polycrystals evidenced a paramagnetic heavy Fermi liquid with a Sommerfeld coefficient $\gamma_0 \approx 300$ mJ/molK^2 at low temperatures. The temperature dependence of the susceptibility and of the specific heat reveal a maximum at 24 K and 16 K, respectively, indicating that the full $J = 5/2$ state of Ce^{3+} is involved in the formation of the heavy Fermion ground state [1].
DC magnetization measurements at 1.8 K up to 14 T on pure CeTiGe showed a step like increase of the magnetization $\Delta M \approx 0.7\ \mu_B$/Ce at $B_{MM} \sim 13.5$ T, which evidences a pronounced metamagnetic transition (MM). Here we shall focus on the development of the MM phase boundary in $Ce_{1-x}La_xTiGe$ upon increasing La content using $\rho(B)$ and $M(B)$ measurements. The observation of a hysteresis in $\rho(B)$ and $M(B)$ at B_{MM} for $Ce_{1-x}La_xTiGe$, which vanishes at $x = 0.6$, is a strong hint for a first order phase transition, in contrast to the crossover behavior reported for $CeRu_2Si_2$[2]. Thus the metamagnetic transition in CeTiGe represents a unique case among Kondo lattice systems.

[1] M. Deppe et al. J. of Phys.: Condensed Matter 21, (2009) 206001.
[2] P. Haen et al. J. of Low Temp. Phys. 67 (1987).

15 min. break

TT 26.6 Wed 15:30 H21

Field-induced coupled superconductivity and spin density wave order in the heavy fermion compound $CeCoIn_5$ — •Johannes Spehling[1], Hans-Henning Klauss[1], Robert Heffner[2], Eric Bauer[2], Jeff Sonier[3], and Nicholas Curro[4] — [1]Institut für Festkörperphysik, TU Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico , U.S.A. — [3]Department of Physics, Simon Fraser University, Burnaby, Canada — [4]Department of Physics, UC Davis, California, U.S.A

In strong magnetic fields the Heavy Fermion superconductor $CeCoIn_5$

shows a first order transition from the normal state into the SC phase [1]. Several modulated SC phases are suggested at high magnetic fields in $CeCoIn_5$, e.g., the spin singlet FFLO [2] and mixed singlet/triplet phases (Q-phase) [3]. We have carried out transverse field muSR measurements between 2 T and 5 T (H parallel c-axis) on single crystalline $CeCoIn_5$ in a temperature range between 25 mK and 7 K. In addition to the standard modulation perpendicular to the applied field due to the vortex lattice, a longitudinal modulation is expected. For the modulated high field phases in a local probe experiment an additional line or a static line broadening should occur. Our data clearly evidence the fielddriven change from second to first order transition at an applied field of 4.8 T. Temperature and field dependence of the muon spin relaxation rate support the formation of a mode-coupled SC and AFM ordered phase in $CeCoIn_5$ for fields directed parallel to the c-axis.

[1] A. Bianchi et al., PRL 91, 187004 (2003).
[2] P. Fulde and R.A. Ferrell, Phys. Rev. 135, A550 (1964).
[3] A. Aperis et al., arXiv:0902.0553.

TT 26.7 Wed 15:45 H21

Planar cross-type junctions on microcrystals of $CeCoIn_5$ thin films — •Oleksandr Foyevtsov and Michael Huth — Johann Wolfgang Goethe University, Frankfurt am Main, Germany

We present results on the preparation and electrical measurements of superconductor-insulator-superconductor cross-type junctions with variable barrier strength on microcrystal isolated from $CeCoin_5$ thin films.

The films have been grown by molecular beam epitaxy. The morphology of the films grown by this method demonstrates a strong tendency to form microcrystals, which makes it difficult to obtain reliable tunneling contacts. Nevertheless, it is still possible to prepare such junctions with an artificial barrier on individual microcrystals.

Films were pre-patterned by optical lithography for contact pad preparation. Then, ion/electron beam induced deposition (FIBID/FEBID) techniques were used for the preparation of both, the barriers and the counter electrodes on selected microcrystals. As artificial barriers we used carbonaceous deposits prepared with FEBID. The counter electrodes prepared using FIBID from $W(CO)_6$ precursor, which was also previously characterized on cross-type planar junctions with aluminum counter electrode.

TT 26.8 Wed 16:00 H21

Scanning Tunneling Spectroscopy studies of heavy fermion metals — •Stefan Ernst[1], Steffen Wirth[1], Cornelius Krellner[1], Christoph Geibel[1], Frank Steglich[1], Zachary Fisk[2], John L. Sarrao[3], and Joe D. Thompson[3] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Department of Physics and Astronomy, University of California at Irvine, USA — [3]Los Alamos National Laboratory, Los Alamos, USA

We report Scanning Tunneling Microscopy/Spectroscopy (STM/S) experiments on single crystals of the heavy fermion intermetallic compounds $CeCoIn_5$, $CeIrIn_5$, and $YbRh_2Si_2$. The tunneling experiments were conducted at temperatures down to 300 mK under ultra–high vacuum conditions. Methods have been established to facilitate *in-situ* sample cleaving.

$CeCoIn_5$ and $CeIrIn_5$ exhibit unconventional superconductivity (SC) at ambient pressure. A gap compatible with d-wave symmetry of the order parameter was observed in the conductance spectra of $CeCoIn_5$. The presence of a gap–like feature in a temperature range above T_c may indicate the existence of a precursor state to SC. Based on atomically resolved topography data, the possible influence of a modified surface structure on STS is discussed.

For the case of $YbRh_2Si_2$, we speculate that the tunneling spectra reveal signatures of a Kondo resonance related to the Yb ions.

TT 26.9 Wed 16:15 H21

Electron Spin Resonance of $YbRh_2Si_2$ under pressure — •J. Sichelschmidt[1], H.-A. Krug von Nidda[2], D. Zakharov[2], I. Fazlishanov[3], J. Wykhoff[1], T. Gruner[1], C. Krellner[1], C. Klingner[1], C. Geibel[1], F. Steglich[1], and A. Loidl[2] — [1]MPI Chem. Physik fester Stoffe, 01187 Dresden — [2]EP V, EKM, Univ. Augsburg, 86135 Augsburg — [3]E. K. Zavoisky Phys. Techn. Inst., 420029 Kasan, Russia

We investigated the electron spin resonance (ESR) in the heavy-fermion metal $YbRh_2Si_2$ by applying hydrostatic pressure up to 3 GPa. We found that pressure increases the temperature dependence of the g factor and broadens the ESR line. These effects are similar to those observed in $Yb(Rh_{1-x}Co_x)_2Si_2$ where Co substitution for Rh induces chemical pressure. However, the effect of chemical and external pressure on the ESR is not identical indicating the relevance of Co induced disorder on the spin dynamics. We compare our pressure ESR results with the behavior of the Gd ESR in $CeAl_3$ [1]. This reveals a similar behavior pointing on one hand to a local character Yb^{3+}-ESR, on the other hand on the properties of a heavy quasiparticle spin resonance upon changing the hybridization strength between $4f$ and conduction electrons [2]. Both findings are consistent with the properties of a collective $4f$-conduction electron spin mode which is supported by the Kondo effect [3].

[1] B. Elschner, A. Loidl, Handb.Phys.Chem.Rare Earths **24**, 221(1997)
[2] P. Wölfle, E. Abrahams, arXiv **0909** 3552v1 (2009)
[3] B.I. Kochelaev et al., Eur. Phys. J. B **72** (2009)

TT 26.10 Wed 16:30 H21

Evidence for unconventional d-wave superconducting state in $CeCu_2Si_2$ — •Hugo A. Vieyra[1], David Parker[2], Hirale S. Jeevan[3], Christoph Geibel[1], Frank Steglich[1], and Niels Oeschler[1] — [1]Max Planck Institute for Chemical Physics of Solids. Dresden 01187, Germany — [2]US Naval Research Laboratory. Washington, DC 20375, USA — [3]I. Physik. Institut, Georg-August-Universität Göttingen, Göttingen 37077, Germany

The heavy-fermion $CeCu_2Si_2$ represents a prime system to study unconventional superconductivity in the vicinity of a magnetic instability. Within the homogeneity range of pure $CeCu_2Si_2$ different ground states can be obtained. S-type crystals exhibit a superconducting transition at T_c=0.6 K, whereas A/S-type show in addition antiferromagnetic order at T_N=0.8 K. In recent years, the synthesis techniques have been optimized in order to obtain large high-quality single crystals with well defined ground state properties. This allows the systematic study of the superconducting order parameter and its variation at the border with magnetic order. In this work, we present angular dependent resistivity measurements on high-quality S- and A/S-type single-crystalline $CeCu_2Si_2$ samples. The experimental results for the angular dependence of the upper critical field B_{c2} as well as theoretical calculations taking into account effects like the strong Pauli paramagnetism, hint towards an unconventional d-wave symmetry of the order parameter in $CeCu_2Si_2$.

TT 26.11 Wed 16:45 H21

Study of the temperature dependence of the magnetic excitations in $CeCu_2Ge_2$ — •Astrid Schneidewind[1], Oliver Stockert[2], Karin Schmalzl[3], Enrico Faulhaber[1], Micha Deppe[2], and Michael Loewenhaupt[4] — [1]Joint Research Group Helmholtz-Zentrum Berlin - Technische Universität Dresden, Garching, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France — [4]Institut für Festkörperphysik, Technische Universität Dresden, Dresden, Germany

Long-range antiferromagnetic order establishes in the heavy fermion compound $CeCu_2Ge_2$ below T_N = 4.15 K with an amplitude modulated structure and an ordering wave vector $\mathbf{Q}_{AF}$ = (0.28 0.28 0.543) [1]. Due to the Kondo effect the ordered moment is slightly reduced to $m \approx 1.0\mu_B$ at low temperatures [1].
We performed inelastic neutron scattering on a $CeCu_2Ge_2$ single crystal to study the low energy magnetic excitations in the ordered state. At lowest temperatures, dispersive spin waves have clearly been observed. At the magnetic zone centre the spin waves are gapped with $\Delta E \approx 0.55$ meV. The excitation spectrum changes with increasing temperatures and the gap closes giving rise to quasielastic scattering just below T_N. The distinct behaviour of the magnetic excitation spectra can be related to the different magnetically ordered phases in $CeCu_2Ge_2$.

[1] A. Krimmel et al., Phys. Rev. B 55 (1997) 6416.

15 min. break

TT 26.12 Wed 17:15 H21

Drude response of slow and fast electrons in the heavy-fermion compound UNi_2Al_3 — •Marc Scheffler[1], Julia P. Ostertag[1], Katrin Steinberg[1], Martin Dressel[1], and Martin Jourdan[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

The unusual metallic behavior of heavy-fermion compounds at low

temperatures is caused by mobile charge carriers with a large effective mass. This mass enhancement (compared to normal electrons) goes hand in hand with a reduction of the transport scattering time, which can directly be studied with optical spectroscopy: the characteristic Drude roll-off moves to very low frequencies. Here we combine microwave and THz spectroscopy to study thin films of the heavy-fermion compound UNi_2Al_3 in a broad frequency range.

At frequencies of a few GHz, a full Drude response indicates the dynamics of the heavy electrons in UNi_2Al_3. Surprisingly, at considerably higher frequencies (around 300 GHz) we observe a similar structure that is very reminiscent of Drude behavior. We interpret these two features as the Drude response of - at low frequencies - correlated, slow electrons and - at higher frequencies - uncorrelated, fast electrons. The temperature dependence and anisotropy of these two Drude roll-offs correspond to each other. These results also shed new light on previous studies of the related compound UPd_2Al_3.

TT 26.13 Wed 17:30 H21

Enhanced thermoelectricity and strong correlations in $FeSb_2$ — •Niels Oeschler[1], Peijie Sun[1], Simon Johnsen[2], Bo B. Iversen[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Chemistry, University of Aarhus, Aarhus, Denmark

$FeSb_2$ was recently identified as a narrow-gap semiconductor with indications of strong electron-electron correlations. Around 10 K the thermopower S assumes huge absolute values of more than 40 mV/K. It has been shown that the thermopower of $FeSb_2$ is of diffusive nature and strongly enhanced due to the appearance of strong correlations. By substituting Te on the Sb site, an atom with one extra electron relative to Sb, an evolution from a semiconducting ground state into a metallic one is observed for small Te content. The thermopower of $FeSb_{1.98}Te_{0.02}$ is linear in T as expected for metals, however, with enhanced slope compared to the free-electron predictions. Deduced from specific heat and Hall effect measurements the effective charge-carrier mass m^* is determined to be as large as 15 times the free electron mass, consistent with the enhanced thermopower.

TT 26.14 Wed 17:45 H21

Theory of spin exciton in the Ce-based unconventional superconductors — •Alireza Akbari[1], Ilya Eremin[1], Peter Thalmeier[2], and Peter Fulde[1] — [1]Max Planck Institute for the Physcis of Complex Systems, D-01187 Dresden, Germany — [2]Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

The feedback spin resonance was observed in inelastic neutron scattering (INS) experiments for numerous unconventional superconductors. In particular a different kind of feedback has been found in the Ce-based ferropnictides. We analyze the influence of unconventional superconductivity on crystalline electric field (CEF) excitations of rare-earth ions. Our theoretical model shows that the resonant magnetic excitations of the conduction electrons below T_c is a result of the formation of the bound state in the 4f-electron susceptibility at energies well below the CEF excitation energy. The transition between CEF split Ce-4f states has anomalous shift and line-width which is explained as an effect of coupling to resonant 3d spin excitations below T_c giving evidence for a $S^{\pm}$ state.

[1] S. Chi et al Phys. Rev. Lett. 101, 217002 (2008).

[2] G. Yu, et al, arXiv:0803.3250 (unpublished).

[3] A. Akbari, I. Eremin, P. Thalmeier, and P. Fulde, Phys. Rev. B, 80, 100504R (2009).

TT 26.15 Wed 18:00 H21

Phonons and the coherence scale of models of heavy fermions — •Marcin Raczkowski[1], Peng Zhang[1,2], Fakher F. Assaad[1], Thomas Pruschke[3], and Mark Jarrell[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics and Astronomy, Louisiana State University, Baton Rouge LA 70803, USA — [3]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

We consider models of heavy fermions in the strong coupling or local moment limit and include phonon degrees of freedom on the conduction electrons [1]. Due to the large mass or low coherence temperature of the heavy fermion state, it is shown that such a regime is dominated by vertex corrections which leads to the complete failure of the Migdal theorem. Even at weak electron-phonon couplings, binding of the conduction electrons competes with the Kondo effect and substantially reduces the coherence temperature, ultimately leading to the Kondo breakdown. Those results are obtained using a combination of the slave boson method and Migdal-Eliashberg approximation as well as the dynamical mean-field theory approximation. [1] arXiv:0910.2954v1

TT 26.16 Wed 18:15 H21

Charge Fluctuations and the Valence Transition in Yb under Pressure — Erik R. Ylvisaker[1], •Jan Kuneš[2], Andrew K. McMahan[3], and Warren E. Pickett[1] — [1]Department of Physics, University of California, Davis, California, USA — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany — [3]Lawrence Livermore National Laboratory, Livermore, California, USA

Materials, whose atomic state cannot be approximated by a single Slater determinant, are said to have fluctuating or intermediate valence. Using dynamical mean-field theory we investigate the physics of elemental Yb, which exhibits a valence transition under pressure accompanied by a crossover from the fluctuating to the intermediate valence behavior. By comparison to other rare-earth materials (Ce, Nd, Pr) we show that fluctuating and intermediate valence regimes can be distinguished by the charge susceptibility. A large charge susceptibility can explain the softness of Yb in the valence transition region.

TT 26.17 Wed 18:30 H21

Phase diagram of heavy fermions and valence fluctuators — •Veljko Zlatic — Institut für Festkörperforschung, Forschungszentrum Jülich, 52428 Jülich, Germany

The phase diagram of heavy fermions is obtained by the scaling solution of the periodic Anderson model with the crystal feld split states. The results explain the phase boundaries revealed by pressure and doping experiments on intermetallic compounds with Ce, Yb and Eu ions. A detailed comparison with the pressure experiments on $CeRu_2Ge_2$, Yb_2Pd_2Sn and doping experiments on $EuCu_2(Si_xGe_{1-x})_2$ is provided as an illustration.

TT 27: CE: Poster Session

Time: Wednesday 14:00–18:00 Location: Poster D1

TT 27.1 Wed 14:00 Poster D1

Soft-Mode Behaviour of Phonons in the CDW Systems $NbSe_2$ and $TiSe_2$ — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank A. Weber[2], Stephan Rosenkranz[2], John-Paul A. Castellan[2], and Ray Osborn[2] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, P.O.Box 3640, D-76021 Karlsruhe — [2]Neutron & X-ray Scattering Group, Materials Science Division, Argonne National Laboratory, 9700 S Cass Ave, Argonne, IL, 60439

We investigated the soft-mode behaviour of phonons in the CDW systems $NbSe_2$ and $TiSe_2$ both theoretically in DFT-based ab-initio phonon calculations and experimentally by means of X-ray scattering. For $NbSe_2$, our calculations predict the development of a phonon instability on reduction of the thermal broadening of the electronic states, in good agreement with the experimental findings. For $TiSe_2$, our theoretical description correctly indicates a softening of the phonon dispersions in the experimentally observed critical regions of the Brillouin zone. However, the effect predicted here by our DFT-description appears to be too weak to explain the experimentally observed CDW instability.

TT 27.2 Wed 14:00 Poster D1

Dilatometric Investigations at the Charge-Ordering Transition in $(TMTTF)_2X$ — •Daniel Hofmann[1], Mariano de Souza[1], Christian Balz[1], P. Foury-Leylekian[2],

A. Moradpour[2], J.-P. Pouget[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue Str. 1, SFB/TR49 D-60438 Frankfurt (M), Germany — [2]Laboratoire de Physique des Solides, Université Paris Sud, CNRS UMR 8502, Orsay, France

We report results of high-resolution measurements of the c^*-axis expansivity (α_{c^*}) at the charge-ordering (CO) transition for the quasi-1D $(TMTTF)_2X$ compounds with X = Br and SbF_6 and make a comparison with previous results for the X = PF_6 and AsF_6 salts [1]. For X = SbF_6, due to the screening of the long-range Coulomb forces, a sharp λ-type anomaly is observed at T_{CO}, which contrasts with the step-like mean-field anomaly at T_{CO} for PF_6 and AsF_6, where CO occurs in the Mott-Hubbard charge-localized regime. For the latter two salts, a negative contribution to α_{c^*} is observed above T_{CO}. This effect is assigned to the anions' rigid-unit modes, which become inactive for $T < T_{CO}$. Measurements for the X = Br salt, where such rigid-unit modes are absent, reveal no traces of such negative contribution to α_{c^*}, confirming the model based on the anions' rigid-unit modes for the X = PF_6 and AsF_6 salts [1].

[1] M. de Souza *et al.*, Phys. Rev. Lett. **101**, 216403 (2008).

TT 27.3 Wed 14:00 Poster D1

Energy gap in charge-density-wave systems — •Reinhard Rossner[1], Hans-Martin Eiter[1], Michela Lavagnini[2], Leonardo Tassini[1], Bernhard Muschler[1], Jiun-Haw Chu[3], Nancy Ru[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, D-85748 Garching, Germany — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, Stanford, California 94305, USA

The rare-earth tri-tellurides show a phase transition to a charge-density-wave ground state, some of them at temperatures well above 300 K. As a consequence an energy gap Δ opens up. We observed this gap in $DyTe_3$ and $LaTe_3$ by measuring the electronic Raman effect as a function of polarization in the temperature range from 6 K to 311 K. The gap becomes more pronounced with decreasing temperature. The magnitudes of Δ are in agreement with those obtained by other experimental techniques such as angle-resolved photoemission spectroscopy. The polarization dependence allows us to study the anisotropy of the gap.

TT 27.4 Wed 14:00 Poster D1

X-ray absorption of hole-doped and electron-doped $Pr_{1-x}Ca_xMnO_3$: Doping-dependent transfer of spectral weight — •Stephan Uebe[1,2], Andrea Assmann[1,2], Michael Merz[1], Prabir Pal[3], Manas Dalai[3], Biju Sekhar[3], Hilbert von Löhneysen[1,2], Peter Nagel[1], and Stefan Schuppler[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, Germany — [3]Institute of Physics, Bhubaneswar, India

Transition metal oxides like the manganites have intriguing physical properties, many of which are based on unusual interrelations between spin, charge, and orbital degrees of freedom. To better understand the phenomena of charge/orbital ordering (CO/OO) and to possibly isolate the fundamental properties which serve as a driving force for CO/OO we have investigated $Pr_{1-x}Ca_xMnO_3$ with temperature-dependent near-edge x-ray absorption spectroscopy. With respect to CO/OO, $Pr_{1-x}Ca_xMnO_3$ becomes especially interesting since it is a narrow band system with almost identical radii of Pr^{3+} and Ca^{2+}. Changes in the tolerance factor can, therefore, directly be attributed to the t_{2g} and e_g orbital occupation. The present data clearly show that the spectral weight and, thus, the number of unoccupied states near the Fermi energy directly tracks the Ca doping level x. A small but distinct redistribution with temperature between the t_{2g} and e_g states at E_F is observed. Implications of the spectroscopic data will be discussed.

TT 27.5 Wed 14:00 Poster D1

EELS-study of $La_{1-x}Sr_{1+x}MnO_4$ — •Matthias Schrade, Roberto Kraus, Pascal Reutler, Jochen Geck, Martin Knupfer, and Bernd Büchner — Institute for Solid State Research, IFW Dresden

The layered manganite $La_{1-x}Sr_{1+x}MnO_4$ displays a strong interplay of charge-, spin-, and orbital degrees of freedom, which results in complex electronic properties.

We performed a detailed electron energy loss spectroscopy (EELS) study in order to clarify the charge dynamics in these materials as a function of doping and temperature.

A new feature at 1.8 eV rapidly gains spectral weight with increasing x. This low energy excitation shows little dispersion, but for x > 0.25 an additional excitation appears around 1 eV for high q-values.

At low T, the magnetic superstructure for half doping could be observed, coinciding with a 0.3 eV-shift of the 1.8 eV-excitation. An interpretation of the physical origin of the different excitations will be proposed.

TT 27.6 Wed 14:00 Poster D1

Orbitons and bi-orbitons in $GdVO_3$ and YVO_3 observed by RIXS — •Luis Mäder[1], Komalavalli Thirunavukkuarasu[1], Eva Benckiser[2,1], Giacomo Ghiringhelli[3], Marco Moretti[3], Graeme R. Blake[4], Nandang Mufti[4], Agung A. Nugroho[5,4], Thomas T. M. Palstra[4], Maurits Haverkort[2], Thorsten Schmitt[6], 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]PSI, Villigen

In an orbitally ordered state, one expects that exchange interactions between orbitals on neighbouring sites give rise to a novel kind of elementary excitations, so called orbitons, which are analogous to spin waves in a magnetically ordered state.

Here, we report on the observation of orbital excitations in YVO_3 and $GdVO_3$ by means of high-resolution resonant inelastic x-ray scattering (RIXS) across the V $L_{3,2}$ (V $2p \rightarrow$ V $3d$) and O K (O $1s \rightarrow$ O $2p$) edges with the new SAXES beamline at the PSI, Villigen.

Due to the excellent resolution of 60 meV, we are able to resolve two different features in the low energy regime. We interpret them as one- and bi-orbiton excitations in good agreement with our optical data [1]. We compare our data with results on $YTiO_3$ and $LaTiO_3$ by Ulrich et al. [2], who attribute the spectral weight at low energies mainly to bi-orbiton excitations.

[1] E. Benckiser *et al.*, New J. Phys. **10**, 053027 (2008).
[2] C. Ulrich *et al.*, PRL **103**, 107205 (2009).

TT 27.7 Wed 14:00 Poster D1

HAXPES analysis of $LaAlO_3/SrTiO_3$ thin films grown under various oxygen partial pressures — •Florian Pfaff[1], Andreas Müller[1,3], Götz Berner[1], Wolfgang Drube[2], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik IV, University of Würzburg — [2]HASYLAB DESY, Hamburg — [3]Inorganic Materials Science, University of Twente

At the interfaces of epitaxially grown oxide heterostructures novel phases with unexpected properties may be generated. E.g., for $LaAlO_3/SrTiO_3$ (LAO/STO) a quasi-2DEG is found, if more than four monolayers (ML) of LAO are grown on STO. As possible explanations intrinsic, i.e. electronic reconstruction, but also extrinsic effects like oxygen vacancies are discussed. To analyze the influences of oxygen vacancies, we performed hard x-ray photoelectron spectroscopy (HAXPES) measurements on samples with two and five ML LAO grown under various oxygen partial pressures (10^{-5} mbar, 10^{-3} mbar, and 10^{-1} mbar) by pulsed laser deposition (IMS, U Twente). We used angle-dependent HAXPES on the Ti $2p$ core level to determine the Ti^{3+}/Ti^{4+} ratio, which clearly depends on the growth pressure. Unexpectedly, the five ML sample grown at 10^{-1} mbar - a pressure for which oxygen vacancies should be largely suppressed - shows no Ti^{3+} at all, which is in agreement with its insulating behavior observed in transport measurements, but casts electronic reconstruction as only possible origin for the 2DEG formation into doubt. However, other explanations for the insulating behavior could be involved, like an increased interface roughness or possible Sr-La intermixing.

TT 27.8 Wed 14:00 Poster D1

Preparation and characterization of $PdCoO_2$ thin films grown by Pulsed Laser Deposition — •Stefan Hirsch, Philipp Komissinskiy, and Lambert Alff — TU Darmstadt, Materialwissenschaft, Darmstadt, Deutschland

$PdCoO_2$ has a hexagonal delafossite crystal structure with the lattice constants of a = 2.83 Å and c = 17.74 Å, and a low resistivity of 4.7 $\mu\Omega$cm perpendicular to the c-axis at 260 K [1]. The aforementioned property is unusual for an oxide material and makes it interesting for thin film applications as an electrode in epitaxial all-oxide heterostructures.

The thin films were produced by pulsed laser deposition (PLD). Single crystals of $PdCoO_2$ were synthesised out of $PdCl_2$ and CoO in evacuated silica tubes. The crystals were grinded, pressed and sin-

tered to a cylindrical pellet to obtain a target for the PLD process. The growth mechanism of the thin films on single crystal substrates was monitored by reflection high energy electron diffraction (RHEED). The thin films were characterized by X-ray diffraction, atomic force microscopy, magnetisation and resistivity measurement from 4.2 to 300 K.

The authors thank DFG GK 1035.

[1] M.Tanaka et al., J. Physical Society of Japan 65, 3973 (1996)

TT 27.9 Wed 14:00 Poster D1

Superconductivity in the hybrid dichalcogenide 18R-$SnSe_2\{CoCp_2\}_x$ — •Michael Herzinger, Robert Miller, Sandra Altmannshofer, Ernst–Wilhelm Scheidt, and Wolfgang Scherer — Lehrstuhl für Chemische Physik und Materialwissenschaft, Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany

We report on electronical and thermodynamical properties of the superconducting hybrid materials 18R-$SnSe_2\{CoCp_2\}_x$ ($0 < x < 0.25$). These materials were synthesized by intercalation of the host layered dichalcogene $SnSe_2$ with the organometalic compound cobaltocene ($CoCp_2$).

These materials indicate a highly anisotropic superconducting behavior, which is observed in resistivity as well as susceptibility measurements parallel and perpendicular to the $SnSe_2$-layers. This is also reflected in the coherence length ratio, e.g. for 18R-$SnSe_2\{CoCp_2\}_{0.1}$, perpendicular to the layers of $\xi_\perp(0) = 7$ Å and parallel $\xi_{||}(0) = 717$ Å.

This study was done for different $CoCp_2$-concentration and demonstrates a quasi two-dimensional superconductor with designable physical properties depending on the degree of intercalation.

TT 27.10 Wed 14:00 Poster D1

Hard x-ray photoemission spectroscopy on $LaAlO_3/LaNiO_3$ multilayers — •Patrick Helmecke[1], Götz Berner[1], Michael Sing[1], Johannes Walde[1], Eva Benckiser[2], Georg Cristiani[2], Hanns-Ulrich Habermeier[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universiät Würzburg — [2]MPI-FKF Stuttgart

Recently, oxide heterostructures attract attention due to novel physical properties at their interfaces. A case in point is the 1/1 heterostructure LaO-NiO_2-LaO-AlO_2 (LAO/LNO/LAO). For that it has recently been predicted that by substrate-imposed strain one of the two conductions bands can be pushed up such that it is almost completely depleted. Inclusion of electron-electron interactions would shift this band further up, inducing a single Fermi surface (FS) sheet which resembles that of the high-T_c superconducting cuprates with prospects to carry high-temperature superconductivity as well [1].

While experimentally it is not yet possible to fabricate the 1/1 heterostructure with the required precision, we analyzed multilayers with layer thicknesses between 2uc and 4uc by means of hard-x-ray photoelectron spectroscopy to access the buried LNO layers. Interestingly, from Ni core-level spectra we have found evidence for a charge-transfer in the 2uc/2uc sample to Ni which might have an important impact on the FS topology and hence the idea to artificially design a cuprate-like FS.

[1] P. Hansmann, X. Yang, A. Toschi, G. Khaliullin, O. K. Andersen, and K. Held, Phys. Rev. Lett. 103, 016401 (2009).

TT 27.11 Wed 14:00 Poster D1

Single crystal growth of $CeNi_2Ge_2$ using floating zone technique — •Christoph Bergmann[1], H. S. Jeevan[1], Christoph Geibel[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

$CeNi_2Ge_2$ is a well-known paramagnetic moderate heavy fermion compound with the electronic specific heat $\gamma \approx 350$ mJ/K^{2}mol. It shows pronounced non-Fermi liquid behavior, which could be related to a nearby anti-ferromagnetic quantum critical point. Similar to its homologue compound $CeCu_2Si_2$, $CeNi_2Ge_2$ displays a strong sensitive of its low-temperature physical properties to tiny changes in the composition in its physical properties, possibly due to site interchange of Ni and Ge. Aiming to determine the fermi surface, we have grown single crystals of $CeNi_2Ge_2$ using a floating-zone technique. We prepare the feed rod of $CeNi_2Ge_2$ using induction melting or arc melting methods. With these methods we got good quality of single crystals and try to increase the residual resistivity ratio by varying the initial composition. Here we will discuss the relation between the single crystal growth conditions for our floating zone technique, the initial composition and the properties of the obtained single crystal especially their residual resistivity ratio. Additionally we have grown and investigated a crystal with 20% Pd doping to get an anti-ferromagnetic ground state.

Work supported by DFG through SFB 602 and research unit "Quantum phase transitions".

TT 27.12 Wed 14:00 Poster D1

Magnetic anisotropy of flux-grown of $CeAu_2Ge_2$ — •Veronika Fritsch[1], Gerda Fischer[1], Peter Pfundstein[2], Bernd Pilawa[1,3], and Hilbert v. Löhneysen[1,3] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Laboratorium für Elektronenmikroskopie, 76131 Karlsruhe, Germany — [3]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76131 Karlsruhe, Germany

$CeAu_2Ge_2$ crystallizes in the well-known tetragonal $ThCr_2Si_2$ structure. Although the high anisotropy of this crystal structure is often reflected in its magnetic properties, most previous investigations were performed on polycrystals. We succeeded in the growth of $CeAu_2Ge_2$ single crystals in Au-Ge flux as well as in Sn flux. X-ray powder diffraction measurements and EDXS measurements indicate that in the latter case Sn atoms from the flux are incorporated in the samples. We present measurements of the magnetization M demonstrating a strong dependence of the magnetic properties on the flux employed: $M(B)$ curves with the field B aligned along the easy axis in the temperature regime of magnetic order ($T_N = 14.4$ K) reveal with decreasing temperature an increasing number of metamagnetic-like transitions in the Au-Ge-flux grown sample, but only a single one (with increasing field) or two (with decreasing field) metamagnetic-like transitions in the Sn-flux grown sample. With the magnetic field aligned along the hard axis no indication of magnetic order is found in the $M(T)$ curves for small B, where the $M(T)$ curves for the easy axis show a sharp maximum.

TT 27.13 Wed 14:00 Poster D1

Sample preparation and magnetic properties of $CeTiGe_3$ — •Wolfram Kittler[1], Gerda Fischer[1], Veronika Fritsch[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76131 Karlsruhe, Germany

$CeTiGe_3$ crystallizes in the hexagonal $BaNiO_3$-structure (space group $hP10 - P6_3/mmc$), which is also known as hexagonal perovskite. We prepared polycrystals by conventional argon-arc melting with subsequent annealing and quenching in liquid nitrogen. The x-ray powder diffraction patterns showed no traces of impurity phases in our samples, however small deviations from the Curie-Weiss law might be attributed to some impurities still present in the sample. We present measurements of magnetization and electrical resistivity in the temperature range between 1.5 and 300 K in magnetic fields up to 5 T. The resistivity ratio at $T = 1.5$ K of $RRR = 26$, in comparison to the previously reported value of approximately 13 [1], confirms the rather good quality of our samples. The magnetization data show that $CeTiGe_3$ is one of the rare ferromagnetic dense Kondo-lattice compounds with a Curie temperature of $T_C = 14$ K and direction-average magnetic moment of 0.94 μ_B as inferred from the $M(B)$ curves at $B = 5$ T for $T = 5$ K.

[1] P. Manfrinetti et al., Solid State Commun. **135**, 444 (2005).

TT 27.14 Wed 14:00 Poster D1

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-Institut für Chemische Physik fester Stoffe, Dresden, Germany

We present a detailed electron spin resonance (ESR) study on a series of single crystals $Yb(Rh_{1-x}Co_x)_2Si_2$ with Cobalt concentrations x from 0 to 1. All compositions show well defined ESR spectra which can be ascribed to a bulk Yb^{3+} resonance. The pure system $YbRh_2Si_2$ is located in the vicinity of an antiferromagnetic quantum critical point. The magnetic ordering of this system ($T_N = 72$ mK) is stabilized by pressure as it is expected for Yb-Kondo lattice compounds. Doping with Cobalt corresponds to applying chemical pressure. Accordingly, the Néel-temperature is increased to $T_N = 1.7$ K in the pure system $YbCo_2Si_2$, confirming a decrease of the hybridization between conduction electrons and Yb^{3+} $4f$-spins. The anisotropies of the ESR

g-factor and the ESR linewidth ΔB for three different frequencies (L, X, Q-band) and in a temperature range from $T \approx 1.5\,\mathrm{K}$ to $\approx 10\,\mathrm{K}$ are presented and discussed here. A significant decrease of the anisotropy from $x = 0$ to 1 is observed.

TT 27.15 Wed 14:00 Poster D1

Low-temperature magnetization measurements on $\mathbf{Yb(Rh_{0.93}Co_{0.07})_2Si_2}$ — •Luis Pedrero, Manuel Brando, Cornelius Krellner, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

In the heavy-fermion compound $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ a detailed study of the thermodynamic and transport properties at low temperature has shown that the energy scale $T^*(H)$, associated with the Fermi surface reconstruction, vanishes inside the magnetic phase $T_N(H)$, where $T_N = 0.4$ K at zero field [1]. This discovery raises questions as (i) which energy scale is more relevant for quantum criticality in this system, (ii) where are located the strongest signatures of quantum fluctuations (at the critical field of T^* or of T_N) and (iii) which is their intrinsic nature.
To get more insights, we have performed several isofield $M(T)$ and isothermal $M(H)$ magnetization measurements on a high-quality single crystal of $Yb(Rh_{0.93}Co_{0.07})_2Si_2$, to obtain a magnetization grid $M(T, H)$ across the magnetic phase diagram. According to the definition of the Grüneisen ratio $\Gamma_H = -(dM/dT)_H/C_H$ and the Maxwell relation $(dM/dT)_H = (dS/dH)_T$ we could then map the entropy $S(H)$ in and outside the magnetic phase and - supported by specific heat measurements - analyse the divergence of $\Gamma_H(T)$ at both critical fields for T^* and T_N. A direct comparison with the theory will be presented.
[1] S. Friedemann *et al.*, Nat. Phys. **5** (2009) 465.

TT 27.16 Wed 14:00 Poster D1

Low-T magnetic phase diagram of $\mathbf{Yb(Rh_{0.73}Co_{0.27})_2Si_2}$ — •Stefan Lausberg[1], Christoph Klingner[2], Cornelius Krellner[1], Manuel Brando[1], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Physics Department E14, TU München, James-Franck Str., 85748 Garching, Germany

The heavy fermion system $YbRh_2Si_2$ is situated close to a quantum critical point. At $T_N = 70$ mK it shows a transition to an antiferromagnetic (AFM) phase. Under pressure T_N increases and a second AFM phase emerges at a temperature $T_L < T_N$. Both phases persist up to 8 GPa [2]. Isoelectronic substitution of Rh by Co leads to a similar effect as pressure, apart from the fact that at a Co concentration of 27 % both transition temperatures seem to merge [3].

In this contribution we present low-temperature ac-susceptibility $\chi'(T, H)$ and resistivity $\rho(T, H)$ measurements of high-quality single crystals of $Yb(Rh_{0.73}Co_{0.27})_2Si_2$. We observe just a single magnetic transition in zero field down to 20 mK, which is of the 2^{nd} order. Increasing the field T_N is suppressed at about $\mu_0 H_c \approx 0.53$ T where the phase boundary line drops very rapidly. This suggests that the phase line could become 1^{st} order although no hysteresis is seen at H_c. Furthermore we observe Fermi liquid behavior around the critical field and within the AFM phase.

[1] S. Mederle *et al.*, JMMM **226-230** (2001) 254-255
[2] G. Knebel *et al.*, JPSJ **75** (2006) 114709
[3] C. Klingner, Diploma Thesis (2009), Dresden.

TT 27.17 Wed 14:00 Poster D1

Far-infrared optical conductivity of $\mathbf{CeCu_2Si_2}$ — •Alexander Herzog[1], Jörg Sichelschmidt[1], Shin-ichi Kimura[2], Christoph Geibel[1], Hirale Jeevan[1], and Frank Steglich[1] — [1]MPI Chem. Physik fester Stoffe, 01187 Dresden — [2]UVSOR, Institute for Molecular Science, Okazaki 444-8585, Japan

We investigated the optical reflectivity of a S/A-type single crystal of the heavy-fermion metal $CeCu_2Si_2$ in the energy range 3 meV – 30 eV for temperatures between 8K – 300K. Our preliminary results for the charge dynamics indicate a behavior that is expected for a formation of a coherent heavy quasiparticle state [1]: Upon cooling we observe a narrowing of the Drude-like part of the optical conductivity corresponding to an enhancement of the quasiparticle effective mass and scattering time. Furthermore, towards cooling down to $T = 8$ K a redistribution of spectral weight occurs essentially from the energy region below 0.6 eV towards energies below 3 meV.

[1] L. Degiorgi, Rev. Mod. Phys. **71**, 687 (1999)

TT 27.18 Wed 14:00 Poster D1

In situ preparation of $\mathbf{CeIn_3}$ thin films by co-sputtering — •Alexander Zaitsev[1], Andre Beck[1], Rainer Fromknecht[1], Markus Wissinger[1], Rudolf Schneider[1], Jochen Geerk[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe

Thin films of the heavy fermion material $CeIn_3$ were prepared in situ on 10x30 mm^2 r-cut sapphire substrates by simultaneous dc sputtering of two stoichiometric $CeIn_3$ targets and dc sputtering of a pure In target in argon gas. The sputtering power of 40 W at each $CeIn_3$ target and 400 W at the In target allowed the deposition of $\sim$0.5 μm thick $CeIn_3$ films within 40 seconds on the substrate held at 500-550 °C. The resultant films were continuous, smooth and stoichiometric as measured by EDX, although sparse In outgrowths of $\sim$1 μm size were also observed. According to XRD analysis the films were predominatly (111) oriented, with minor amount of (100) and (110) oriented phases. The dependence of the electrical resistivty on temperature was typically that of bulk $CeIn_3$ with a clear maximum at around 50 K, followed by a linear decrease of resistivity towards lower temperatures. At 10 K a kink in ρ(T) indicated the antiferromagnetic ordering of $CeIn_3$. The residual resistivity ratio $\rho(50K)/\rho(1.4K) = 3$ was reasonably high for the textured thin film material.

TT 27.19 Wed 14:00 Poster D1

Anisotropy in the microwave conductivity of $\mathbf{UNi_2Al_3}$ — •Katrin Steinberg[1], Marc Scheffler[1], Martin Dressel[1], and Martin Jourdan[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

In the heavy-fermion compound UNi_2Al_3, the free charge carriers show an enhanced effective mass at low temperatures due to electronic correlations. This mass enhancement and a strongly enhanced scattering time can be observed in the microwave conductivity spectrum. The frequency dependent complex conductivity shows a Drude roll-off at a few GHz. From directionally dependent dc studies it is known that UNi_2Al_3 exhibits a pronounced transport anisotropy at low temperatures. To resolve whether the conductivity at microwave frequencies is anisotropic as well, we have prepared strip-shaped thin-film samples of UNi_2Al_3 and measured their conductivity in a broadband microwave Corbino spectrometer with the current parallel to the a-axis or to the c-axis of the hexagonal crystal structure. We present the frequency- and temperature-dependent microwave conductivity (45 MHz to 40 GHz and 1 K to 300 K, respectively) of UNi_2Al_3. The conductivity spectra exhibit clear Drude roll-offs in both crystallographic directions. They are anisotropic, in consistence with the dc transport. From the measured spectra we obtain the effective mass and scattering rate for both crystal axes and we study their temperature dependence.

TT 27.20 Wed 14:00 Poster D1

Equivalence of pressure and concentration tuning in $\mathbf{CeCu_{6-x}Au_x}$ — •O. Stockert[1], A. Hamann[2], V. Fritsch[2], A. Schneidewind[3], and H. v. Löhneysen[2] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Joint Research Group Helmholtz-Zentrum Berlin - Technische Universität Dresden, FRM-II, Garching, Germany

In the prototypical heavy-fermion system $CeCu_{6-x}Au_x$ two different quantum critical scenarios are discussed: the conventional spin-density-wave (SDW) scenario introduced by Hertz, Millis and Moriya and the local scenario by Schröder, Coleman, Si. While concentration and pressure tuning the quantum phase transition (QPT) are described by the local critical scenario, magnetic field tuning the QPT results in the conventional SDW scenario. In order to study how far the analogy between Au substitution and hydrostatic pressure holds, we performed elastic neutron scattering experiments on single crystalline $CeCu_{5.5}Au_{0.5}$ and investigated the magnetic structure under hydrostatic pressure. At a pressure of $p = 8$ kbar the Néel temperature and the propagation vector of the magnetic structure attain almost the values of $CeCu_{5.7}Au_{0.3}$. This concentration-pressure analogy away from the QPT is highly remarkable, since the ambient-pressure magnetic structures of $CeCu_{5.5}Au_{0.5}$ and $CeCu_{5.7}Au_{0.3}$ are quite different. The change of the magnetic structure of $CeCu_{5.5}Au_{0.5}$ under pressure appears to be of first order and to be determined by slight changes in the nesting properties of the Fermi surface. We will discuss our findings in comparison to the different QPTs in the system $CeCu_{6-x}Au_x$.

TT 27.21 Wed 14:00 Poster D1

Luttinger-Ward functional approach in the Eliashberg frame-

work : A systematic derivation of scaling for thermodynamics near a quantum critical point — •Adel Benlagra[1], Ki-Seok Kim[2], and Catherine Pépin[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]Institut de physique Théorique, CEA Saclay, France — [3]Pacific Center for Theoretical Physics, POSTECH, Pohang, South Korea

The poster by Duc-Anh Le et. al. originally scheduled for TT 27.21 has been withdrawn and was replaced by this poster.

We used the Luttinger-Ward (LW) functional in the Eliashberg framework to derive scaling expressions for the free energy from a microscopic model for two models of quantum criticality : the standard theoretical framework called the Hertz-Moriya-Millis theory and the Kondo breakdown model, one possible scenario for heavy-fermion quantum transitions, for which the effective theory is given by a U(1) gauge theory.

The LW functional approach allows to take into account the fluctuation corrections in a systematic way. The Eliashberg framework allows to use the proper level of approximation to get, self-consistently, the correct scaling for thermodynamics near the quantum critical point. We have shown that, at the one loop level, the fermionic excitations give a Fermi Liquid contribution whereas the singular part of the free energy for both models is due to the collective bosonic excitations. In particular, the Kondo breakdown QCP is characterized by two length scales : one is the correlation length for hybridization fluctuations, and the other is that for gauge fluctuations, analogous to the penetration depth in superconductors.

TT 27.22 Wed 14:00 Poster D1

Spin density wave quantum phase transition in the $LuFe_2Ge_2/YFe_2Ge_2$ system — •Zhuo Feng and Malte Grosche — Quantum Matter Group, Cavendish Laboratory, J J Thomson Avenue, Cambridge, CB3 0HE, U.K.

In intermetallic transition metal compounds, spin density wave order and studies of the associated quantum critical point are still comparatively rare. $LuFe_2Ge_2$ has been reported to exhibit spin density wave order below 9K, and its isoelectronic sister compound YFe_2Ge_2 is paramagnetic. Together, they form an attractive system for probing spin density wave quantum criticality. We have grown high quality crystals of YFe_2Ge_2 and $LuFe_2Ge_2$ using flux as well as radio frequency induction methods. YFe_2Ge_2 exhibits an unusually high Sommerfeld coefficient of the specific heat capacity C/T at 1 K in excess of 100 mJ/(molK^2) and still rising significantly with decreasing temperature, as well as an anomalous temperature dependence of the electrical resistivity, $\rho \sim T^{3/2}$. High-pressure measurements are under way in $LuFe_2Ge_2$, to investigate its magnetic phase diagram near the magnetic quantum phase transition, and to examine the associated quantum critical behaviour.

TT 27.23 Wed 14:00 Poster D1

Ferromagnetic quantum phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider[1], Vasile Moshnyaga[1], Philipp Gegenwart[1], Markus Wissinger[2], and Dirk Fuchs[2] — [1]I. Physikalisches Institut, Georg-August Universität Goettingen,Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Postfach 3640, 76021 Karlsruhe, Germany

We report results on $Sr_{1-x}Ca_xRuO_3$ thin films which have been grown epitaxially on $SrTiO_3$ substrates by metalorganic aerosol deposition. The films are characterized using X-ray diffraction, room-temperature STM, as well as atomic-resolution transmission electron microscopy. The physical properties are investigated by electrical resistivity and magnetization measurements. We observe a continuous suppression of itinerant electron magnetism with T_C=160K for $SrRuO_3$ with increasing Ca concentration x in $Sr_{1-x}Ca_xRuO_3$ towards $T_C \to 0$ for x_c=0.7. At x>0.7 indications for non-Fermi liquid behavior are found in the low-temperature resistivity. For selected thin films the measurements are extended to mK temperatures. We also report low-temperature electrical resistivity measurements on thin films grown at KIT Karlsruhe by pulsed-laser deposition on various different substrates. Work supported by DFG through SFB 602, TP A19.

TT 27.24 Wed 14:00 Poster D1

Low temperature magnetoresistance of different strongly correlated metals close to a quantum phase transition — •M. Schubert, K. Winzer, M. Schneider, H.S. Jeevan, and P. Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We report measurements of the electrical resistance at temperatures down to 15 mK in magnetic fields up to 7 Tesla on different intermetallic systems, which are located close to a quantum phase transition. Both heavy-fermion systems like $YbRh_2(Si_{1-x}Ge_x)_2$ and $CeAu_2In_4$ as well as transition metal oxides ($Sr_{1-x}Ca_xRuO_3$ thin films) are investigated. The results are compared with different theoretical scenarios. Our work is supported by the DFG through SFB 602 and research unit "Quantum phase transitions".

TT 27.25 Wed 14:00 Poster D1

Quantum Dissipation in Spin Systems: Spin-Boson Model and its Quantum Phase Transition — •André Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, Campus, 66123 Saarbrücken

Our interest is focused on quantum-dissipative effects in spin systems. These effects play a highly interesting role in several fields of physics, like the decoherence of qubits or charge transfer in donor-acceptor systems. Mainly, the spin-boson model, which describes a two-level system coupled to a bosonic bath with a spectral density $J(\omega) \propto \omega^s$ will be discussed. We developed a new Monte Carlo algorithm to explore the quantum phase transition between the localized and delocalized phase of this model in the sub-Ohmic regime ($0 < s < 1$). The applied method, which is based on the path integral approach to Quantum Monte Carlo computations, works in continuous time and uses cluster updates of worldline-segments to investigate the quantum critical point effectively.

In addition, we are considering extensions within this framework like an alternative approach, where the bosonic environment is simulated explicitly or more general setups with multiple interacting spins.

[1] A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. 102, 030601 (2009)

TT 27.26 Wed 14:00 Poster D1

Shubnikov-de Haas oscillations in $Ca_3Ru_2O_7$ under pressure — •Lina Klintberg[1], Swee Goh[1], Naoki Kikugawa[2,3], Andrew Mackenzie[2], Michael Sutherland[1], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, United Kingdom — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews, Fife KY16 9SS, United Kingdom — [3]National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan

The bilayer ruthenate $Ca_3Ru_2O_7$ undergoes a series of phase transitions on cooling, which lead to a low carrier density state at low temperature. Hydrostatic pressure is applied on this material in order to track the Fermi surface whilst tuning and ultimately suppressing the high temperature phase transitions. Quantum oscillations in the Hall component of $Ca_3Ru_2O_7$ are investigated as a function pressure using a piston-cylinder cell. As the pressure is increased, the oscillation frequency decreases systematically, suggesting that the Fermi pockets shrink. Owing to the size of the frequencies and to the non-linear background, the evolution of the effective masses cannot be determined accurately enough to extract a trend other than that they remain of the order of $0.6m_e$. Further work at higher pressures is under way, using anvil cells, to track the evolution of the Fermi surface through the pressures where the magnetic and structural transitions eventually are suppressed.

TT 27.27 Wed 14:00 Poster D1

Quantum phase transition in a two-subband quantum wire — •Tobias Meng[1], Mehul Dixit[2], Markus Garst[1], Julia Meyer[3,2], and Achim Rosch[1] — [1]Universität zu Köln — [2]Ohio State University — [3]Universite Joseph Fourier Grenoble

We consider a quantum wire with two subbands close to the Lifshitz transition, at which the second band starts to get filled as a function of an external gate voltage. This quantum phase transition is, generically, characterized by pronounced correlations as the electrons in the second subband are strongly interacting: the diverging density of states close to the band bottom leads to unitary two-particle scattering in the low-energy limit. This effectively generates nodes in the many-body wavefunction of electrons with different spin polarization, and, as a result, the electrons in the second band behave effectively as spinless fermions. We argue that, as a consequence, the interaction between the subbands is dominated by non-local contributions similar to the case of spin-polarized electrons [1,2]. We present an analysis of the leading instabilities at small densities of particles in the second band.

[1] J.S. Meyer, K.A. Matveev, and A.I. Larkin, Phys. Rev. Lett.

98, 126404 (2007)
[2] M. Sitte et al., Phys. Rev. Lett. 102, 176404 (2009)

TT 27.28 Wed 14:00 Poster D1

The ferromagnetic phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films studied by noise spectroscopy — •Adham Amyan[1], Pintu Das[1], Jens Brandenburg[2], Jens Müller[1], Melanie Schneider[3], Vasily Moshnyaga[3], and Philipp Gegenwart[3] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt am Main, Germany. — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany. — [3]Physikalisches Institut, Georg-August Universität Göttingen, Göttingen, Germany.

Fluctuation (noise) spectroscopy is a powerful tool to investigate the intrinsic dynamics of charge carriers coupled to lattice vibrations and defects, or magnetic and electronic excitations. In principle, one can access the autocorrelation function describing the kinetics of the fluctuating carriers. We employ an *ac*-technique to study the excess $1/f$-type noise at different temperatures and magnetic fields for samples $Sr_{1-x}Ca_xRuO_3$ with various Ca concentrations x. In particular, in our low-frequency studies we are interested in the energy distribution of fluctuators causing the excess noise in the vicinity of the ferromagnetic transition in the energy range of 1 meV-1 eV. To this end, we use a phenomenological random fluctuation model and compare the noise data to complementary measurements of the Hall effect. Also, we are investigating the differences of the low-temperature dynamical properties as a function of Ca doping, in particular close to the ferromagnetic quantum phase transition, where $T_C \to 0$ for $x_c = 0.7$.

Work supported by the DFG through the Emmy Noether-program and SFB 602.

TT 27.29 Wed 14:00 Poster D1

Multiple phase transitions in YbPd — •Stefanie Grünheit, Jeevan S. Hirale, Yoshifumi Tokiwa, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

Cubic YbPd is an interesting strongly-correlated electron system, as previous ^{170}Yb-Mössbauer measurements have suggested two different Yb charge states at low temperatures; one magnetic and the other one nonmagnetic in equal proportions [1]. We have synthesized large YbPd polycrystals and investigate their physical properties by electrical resistivity, magnetic susceptibility, specific heat and thermal expansion at temperatures down to 20 mK. Four phase transitions at 0.6 K, 1.9 K, 105 K and 125 K are found. While the two higher ones are presumably related to a structural distortion, which may result in two inequivalent Yb-sites, the two lower ones are of clear antiferromagnetic origin. At lowest temperatures, the Sommerfeld coefficient amounts to 200 mJ/(mol K^2) and a reduced entropy of about one quarter of $R \log 2$ at 1.9 K is found. These results are discussed in terms of a coexistence of mixed-valent and magnetic Yb-sites. To investigate the microscopic origin of the various transitions, synchroton and neutron scattering experiments are under way.

Work supported by DFG through research unit 960 (Quantum phase transitions).

[1] P. Bonville et al., Phys. Rev. Lett. 57 (1986) 2733.

TT 27.30 Wed 14:00 Poster D1

Metal-insulator transitions in layered ruthenates — Johanna Brand[1], •Anna Silex[1], Olaf J. Schumann[1], Michael Gottschlich[1], Steven Price[1], Navid Qureshi[1], Paul Steffens[1,2], Daniel Löwen[1], Yvan Sidis[3], Arsène Goukassov[3], Beatrice Gillon[3], Satoru Nakatsuji[4], Jason Farrell[5], Naoki Kikugawa[5], Andrew Mackenzie[5], Karin Schmalzl[2], and Markus Braden[1] — [1]II. Physik, Uni Köln — [2]ILL, Grenoble — [3]LLB, Saclay — [4]ISSP, Tokio, Japan — [5]Univ. of St. Andrews, Scotland

Ca- and Sr-Ruthenates are far more interesting than the structural similarity with the cuprates initially suggested. By doping the single or double layer materials, many interesting phenomena are observed. Substituting Ti into Sr_2RuO_4 stabilizes a spin-density wave (SDW) phase that still is metallic, in which the static ordering corresponds to the dominating magnetic instability in pure Sr_2RuO_4. On the other hand, the doping of Ti into the double layer material $Sr_3Ru_2O_7$ seems to induce a SDW type magnetic order with larger impact on the electronic properties. The SDW phase in Ti-doped $Sr_3Ru_2O_7$ does not seem to be related with the magnetic instabilities of the parent phase. In both Sr-ruthenates the impact of the Ti-doping on the crystal structure is small and changes slightly across the magnetic transition. However, we find a strong influence of the Ti-substitution in Ti-doped $Ca_3Ru_2O_7$ which significantly stabilizes a weakly non-metallic phase. This can be seen in the transition temperature and in the resistivity jump. A pronounced flattening of the lattice is discussed as a general feature accompanying the metal-insulator transition in layered ruthenates.

TT 27.31 Wed 14:00 Poster D1

Doping dependent behaviour of potassium intercalated pentacene films: watching out for correlation effects — •Andreas Ruff[1], Joep Loos[1], Michael Sing[1], Jens Pflaum[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Experimentelle Physik 6, Universität Würzburg

Recently, evidence for a band-filling controlled Mott metal-insulator transition (MIT) was reported for strongly potassium (K) doped pentacene (PEN) films on silicon substrates by conductivity measurements [1]. We have investigated the system K_xPEN on silicon with different orientations by means of photoelectron spectroscopy to follow the evolution of the spectral function with doping. The high quality of our PEN films is demonstrated by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED) measurements. In the ultraviolet photoemission spectra (UPS) one can observe the gradual filling of the former lowest unoccupied molecular orbital (LUMO) with K evaporation time. Additionally, conductivity measurements have been carried out to observe the MIT. To clarify the growth mode of the films images of the surface were taken with an atomic force microscope (AFM). Despite the drastic change in conductivity, no spectroscopical evidence neither for the metallic regime nor for the Mott transition has been observed as yet.

[1] M.F. Craciun et al, PRB 79, 125116 (2009)

TT 27.32 Wed 14:00 Poster D1

The metal-to-insulator transition in organic charge-transfer salts studied by noise spectroscopy — •Robert Rommel[1], Pintu Das[1], Adham Amyan[1], Jens Müller[1], Jens Brandenburg[2], and Dieter Schweitzer[3] — [1]Goethe-Universität Frankfurt, SFB/TR49, Frankfurt am Main — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden — [3]3. Physikalisches Institut, Universität Stuttgart

The organic $(ET)_2X$ compounds are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. In particular, the interplay of onsite and intersite Coulomb interaction on the one hand and the coupling to the lattice degrees of freedom on the other hand are interesting to investigate with respect to the different kinds of metal-to-insulator transition (MIT) in this class of materials. We employ a new technique, fluctuation (noise) spectroscopy, for the quasi-2D $(ET)_2X$ salts to study the low frequency dynamics of the correlated electrons. Our experimental setup allows for measuring the resistance fluctuations in the frequency range from 1 mHz to above 100 Hz for systems showing an MIT in a wide temperature range covering variations of the samples' resistance noise of many orders of magnitude (e.g. 10^{-8}–$10^6\ \Omega^2$/Hz). We employ a simple random fluctuation model to study the distribution of activation energies of the specific fluctuations causing the excess, 1/f-type noise. We compare different kinds of MIT regarding the mechanisms for slow electron dynamics.

TT 27.33 Wed 14:00 Poster D1

Pressure-induced phase transition in $ZnCr_2Se_4$ spinel — •Kaneez Rabia[1], Leonetta Baldassarre[1], Vladimir Tsurkan[2,3], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, Germany — [2]Experimentalphysik V, Universität Augsburg, Germany — [3]Insitute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Republic of Moldova

Among the various transition metal chalcogenide spinels, the chromium spinels with the formula ACr_2X_4, with A=Zn,Cd or Hg, and X=O,S or Se, were most extensively investigated because of their unusual optical, electrical, and magnetic properties. The Cr^{3+} ions with the electron configuration $3d^3$ occupy the B sites with an octahedral environment. Under the action of the octahedral crystal field the Cr 3d levels split into a lower t_{2g} triplet, each orbital being singly occupied, and an excited eg doublet; the resulting bulk material is a Mott insulator with S=3/2. These compounds show a wide variety of magnetic properties ranging from those of a strongly frustrated antiferromagnet to a Heisenberg ferromagnet.

In the present study we studied the optical response of $ZnCr_2Se_4$ in refection mode as a function or pressure. Our results suggest the occurrence of a sluggish structural phase transition and the tendency

of charge delocalization starting from 12 GPa. We will also discuss the pressure dependence of the high-energy electronic excitations, which are assigned to onsite crystalfield transitions.

TT 27.34 Wed 14:00 Poster D1

Magnetic and electronic properties in Chromates $R\mathbf{CrO_3}$ and the Vanadate $\mathbf{K_2V_8O_{16}}$ (Hollandite) — •A. C. Komarek[1,2], M. Isobe[3], T. Möller[1], M. Hoelzel[4,5], A. Senyshyn[4,5], D. Trots[6], M. T. Fernandez-Diaz[7], T. Hansen[7], M. Azuma[8], Y. Ueda[3], J. Hemberger[1], T. Unruh[5], J. R. Stewart[7,9], M. Grüninger[1], D. I. Khomskii[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]TU München, Physics Departement E21, D-85748 Garching, Germany — [3]Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan — [4]Technische Universität Darmstadt, Material und Geowissenschaften, Petersenstrasse 23, D-64287 Darmstadt, Germany — [5]TU München, FRM-II, Lichtenbergstr. 1, D-85747 Garching, Germany — [6]Hasylab/DESY, Notkestr. 85, D-22607 Hamburg, Germany — [7]Institut Laue-Langevin, 38042 Grenoble, France — [8]Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan — [9]ISIS facility, Rutherford Appleton Laboratories, STFC, Chilton, Didcot OX11 0DE, UK

$CaCrO_3$ is a $3d^2$ transition metal oxide with perovskite structure. Regarding the magnetism in such correlated electron systems, ferromagnetism usually comes along with metallic and antiferromagnetism (AFM) with insulating properties. Due to our neutron and optical measurements $CaCrO_3$ seems to be a rare example of a fully 3-dim. AFM transition metal oxide. $K_2V_8O_{16}$ is a mixed-valent vanadium oxide which exhibits a MI-transition at 160 K. Below T_{MI} we found a strong dimerization resembling on the monoclinic M2-phase in VO_2.

TT 27.35 Wed 14:00 Poster D1

Temperature dependent optical conductivity of $\mathbf{RVO_3}$ (R=Y, Gd), $\mathbf{LaSrFeO_4}$ and $\mathbf{RCoO_3}$ (R=La, Eu) studied by ellipsometry — •Julia Küppersbusch[1], Kostiantyn Shportko[1], Agung Nugroho[2], Thomas Palstra[2], Navid Qureshi[1], Marco Reuther[1], Thomas Lorenz[1], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

Spin and orbital degrees of freedom play a decisive role in strongly correlated transition-metal oxides. Spin and orbital correlations for instance have a strong impact on the optical transitions from the lower to the upper Hubbard band. Our aim is a systematical study to understand the importance of spin/orbital correlations and also excitonic effects on the temperature dependence of the optical spectra. We use ellipsometry from 0.75 to 5.5 eV and show results on RVO_3, $LaSrFeO_4$, and $RCoO_3$.
The $3d^5$ configuration of $LaSrFeO_4$ does not show orbital degrees of freedom, the spins order at 350 K, thus the behavior at lower temperatures offers a reference for the influence of the lattice. The T dependence of the optical data of $3d^2$ RVO_3 can be well described on the basis of spin/orbital correlations. The $3d^6$ compounds $RCoO_3$ allow to study the effect of a spin-state transition on the optical data.

TT 27.36 Wed 14:00 Poster D1

LDA+DMFT study of $\mathbf{LaCoO_3}$ — •Evgeny Gorelov and Eva Pavarini — IFF and IAS, Forschungszentrum Jülich, 52425 Jülich

$LaCoO_3$ has attracted a lot of attention because of its spin-state transitions, the nature of which has been debated since decades. In this work we study $LaCoO_3$ by means of the LDA+DMFT (local-density approximation + dynamical mean-field theory) method. Using the downfolding procedure based on the N-th Order Muffin-Tin Orbital approach, we calculate ab-initio $3d$ Wannier functions and construct the corresponding 5-band Hubbard model. We solve this model within dynamical mean-field approximation. We use the weak-coupling CT-quantum Monte Carlo method as impurity solver; this allows us to take into account the full rotationally-invariant Coulomb interaction, including the pair-hopping and spin-flip terms. We also retain the full self-energy matrix in orbital space. We analyze the competition between crystal-field splitting and Hund's rule coupling.

TT 27.37 Wed 14:00 Poster D1

Variational Monte Carlo study of the one-dimensional $t-t'$ Hubbard model — •Luca F. Tocchio[1], Claudius Gros[1], and Federico Becca[2] — [1]Institute for Theoretical Physics, Goethe-University Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main, Germany — [2]CNR-INFM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Beirut 2, I-34151 Trieste, Italy

We present a Variational Monte Carlo study of the one-dimensional Hubbard model with nearest and next-nearest neighbour hopping. After settling the metal-insulator transition, we describe the spin properties of the model, studying their behaviour across the metal-insulator transition and inside the insulating phase. The spin properties are then shown to be related to the single-particle spectrum in the optimized variational wave function. Moreover, we find that the metal-insulator transition can be already characterized at a mean-field level, since the underlying Fermi surface renormalizes to perfect nesting at the transition.

TT 27.38 Wed 14:00 Poster D1

Spectral properties of the three-dimensional Hubbard Model — •Sebastian Fuchs[1], Emanuel Gull[2], Matthias Troyer[3], Mark Jarrell[4], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Physics, Columbia University, W 120th Street New York, NY 10027, USA — [3]Institut für Theoretische Physik, ETH Zürich, Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland — [4]Louisiana State Universtity, Baton Rouge, LA 70803, USA

We calculate momentum resolved single-particle spectra of the three-dimensional Hubbard Model. We perform Quantum Monte Carlo (QMC) simulations inside and outside the antiferromagnetically symmetry broken phase in the vicinity of the metal-insulator transition. The full lattice model is approximated by the Dynamical Cluster Approximation (DCA) and the resulting cluster model is solved using a QMC algorithm in continuous imaginary time. The absence of a time discretization error and Monte Carlo measurements in Matsubara frequencies enable us to analytically continue the self-energies directly by a Maximum Entropy calculation. Thus, momentum resolved single-particle spectra can be determined using Dyson's equation.

TT 27.39 Wed 14:00 Poster D1

The role of the double counting correction in the LDA+DMFT method - a systematic study. — •Michael Karolak, Tim Wehling, German Ulm, and Alexander Lichtenstein — I. Institut für theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

An intrinsic issue of the LDA+DMFT approach is the so called double-counting of interaction terms. How to choose the double-counting potential in a manner that is both physically sound and consistent is unknown. We have conducted an extensive study of the charge transfer system NiO in the LDA+DMFT framework using quantum Monte Carlo and exact diagonalization as impurity solvers. By explicitely treating the double-counting correction as an adjustable parameter we systematically investigated the effects of different choices for the double-counting on the spectral function. Different methods for fixing the double counting can drive the result from Mott insulating to almost metallic.

TT 27.40 Wed 14:00 Poster D1

Non-linear integral equations for transfer matrices of Chalker Coddington network models — •Win Nuding and Michael Brockmann — Bergische Universitä Wuppertal, Germany

We analyse the eigenvalues of the transfer matrices of an integrable Chalker Coddington model on the basis of the work by Gade and by Essler, Frahm and Saleur. We derive from the Bethe ansatz equations a finite system of non-linear integral equations. Whereas in the Bethe ansatz the system size L is equal to the number of unknown Bethe ansatz roots, L enters the non-linear integral equations just as an external control parameter. We present solutions of the non-linear integral equations. From these the eigenvalues of the transfer matrices are obtained.

TT 27.41 Wed 14:00 Poster D1

Calculating Thermodynamic Properties using Stochastic Sampling within the DMRG framework — •Stefan Kremer[1,2] and Peter Schmitteckert[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Laboratoire CRISMAT, UMR 6508 CNRS-ENSICAEN, and IRMA, Caen, France — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

In order to calculate thermodynamic properties a method within the

framework of the Density Matrix Renormalisation Group (DMRG) is proposed. This method combines the Imaginary Time Evolution with the ideas of Stochastic State Sampling proposed by J. Jaklič and P. Prelovšek. In their approach obtaining thermodynamic states within Exact Diagonalisation is accomplished by the means of stochastic sampling of the Hilbert space. Thermodynamic expectation values of conserved quantities at a specific temperature can then be evaluated since they correspond to the quantum mechanical expectation values with respect to such states. Performing an evolution of the states in imaginary time will therefore represent a cooling of the system. In the proposed method the Hilbert space is sampled stochastically where the low energy region is sampled with a higher weight for the purpose of evaluating the thermodynamic expectation values at low temperature. Results for the specific heat of spinless fermionic rings are compared to predictions from Exact Diagonalisation.

TT 27.42 Wed 14:00 Poster D1

Screening of U in a three-band Hubbard model — •Clemens Adolphs and Erik Koch — German Research School for Simulation Sciences, FZ-Jülich and RWTH Aachen University, 52425 Jülich

We study the screening of the Hubbard interaction. As a concrete example, we consider a three-band Hubbard model with a central, half filled band, one filled band below, and an empty band above. We use the Lanczos algorithm to solve this model for small chains and calculate the spectral function. We then investigate a one-band Hubbard model where the renormalized interaction energy, U, for the one-band Hubbard model is calculated from the charging energy of the central orbital in the atomic limit of the original model. Comparing the spectral functions of the two models, we determine in which cases a one-band description using such a static renormalized U is feasible.

TT 27.43 Wed 14:00 Poster D1

Variational matrix product states for nano chains — •Andrej Schwabe and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany

We discuss a variational matrix product states (VMPS)[1,2] code, where the coefficients of the test wave function Ψ are assumed as product of site dependent matrices $\mathbf{A}^i$. The advantageous matrix product operator (MPO) representations is used, which allows to construct a generic algorithm, almost independent of the Hamiltonian H. In order to optimize the code and to account for physical properties of H, the wave function transformation as well as $U(1)$ symmetries have been implemented. Furthermore, the corrected one-site algorithm, recently proposed by White [3], is incorporated in our VMPS code at several approximation stages. We perform a benchmark test to study the impact of both the corrected one-site algorithm and the implementation of the $U(1)$ symmetries on CPU time and accuracy of the results.
The technique is applied to ferromagnetic nano chains in one dimension, described by inhomogeneous Hubbard-type models with site dependent Hubbard-U. The magnetic phase diagram and its dependence on the chain length are investigated. We discuss the emergence of the magnetic exchange coupling (e.g. RKKY) within and between the nano particles. Size and distance dependencies are studied as well as the competition with the Kondo effect.

[1] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005)
[2] F. Verstraete et al., Advances in Physics **57**, 143 (2008)
[3] S. R. White, Phys. Rev. B **72**, 180403 (2005)

TT 27.44 Wed 14:00 Poster D1

On the existence of the excitonic insulator phase in the extended Falicov-Kimball model: a vectorial slave-boson approach — •Bernd Zenker[1], Dieter Ihle[2], Franz Xaver Bronold[1], and Holger Fehske[1] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany — [2]Institut für Theoretische Physik, Universität Leipzig, 04109 Leipzig, Germany

Motivated by the possibility of pressure-induced exciton condensation in intermediate-valence Tm[Se,Te] compounds we study the Falicov-Kimball model extended by a finite f-hole valence bandwidth. Within slave-boson mean-field theory we show that coherence between c- and f-states may be established at low temperatures, leading to an excitonic insulator (EI) phase. Thereby our vectorial slave-boson approach overcomes (i) the difficulties of the scalar slave-boson scheme by describing the EI state, and yields (ii) a substantial reduction of the critical temperatures in comparison to those of the standard Hartree-Fock approach. Analyzing the partial densities of states we find strong evidence that the EI typifies either a BCS condensate of electron-hole pairs (weak-coupling regime) or a Bose-Einstein condensate (BEC) of preformed excitons (strong-coupling regime), which points towards a BCS-BEC transition scenario as Coulomb correlations increase.

TT 27.45 Wed 14:00 Poster D1

Structural and Magnetic Properties of Fe Obtained by Dynamical Mean-Field Theory — •Ivan Leonov[1], Alexander I. Poteryaev[2], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia

We present an application of a novel *ab initio* approach to calculate the total energy of materials with correlated electrons [1,2]. It combines band structure and dynamical mean-field theory, and is implemented in terms of plane-wave pseudopotentials. Here we employ this computational scheme to study structural and magnetic properties of elemental Fe at finite temperatures. For this purpose we analyzed the energetics of the *bcc-fcc* lattice transformation in Fe using the Bain transformation path. We find that at ambient pressure the temperature of the *bcc-fcc* structural phase transition occurs at ∼200 K above the calculated Curie temperature. The structural optimization performed for paramagnetic Fe yields the correct lattice constants and predicts a 2 % shrinking of the volume at the *bcc-fcc* phase transition.

[1] I. Leonov, N. Binggeli, Dm. Korotin, V. I. Anisimov, N. Stojić, and D. Vollhardt, Phys. Rev. Lett. **101**, 096405 (2008).
[2] I. Leonov, Dm. Korotin, N. Binggeli, V. I. Anisimov, and D. Vollhardt, arXiv:0909.1283 (2009).

TT 27.46 Wed 14:00 Poster D1

Modified Fermi-liquid behavior of the Hubbard model at finite temperature within the dynamical mean-field theory — •Sebastian Schmitt — Lehrstuhl für Theoretische Physik II, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

The one-particle Green function of the Hubbard model is calculated within the dynamical mean field theory (DMFT) for various non-interacting density of states (DOS). The Fermi-liquid ground state usually observed within the DMFT reveals itself through the characteristic quadratic minimum in the imaginary part of the self-energy which develops already at finite temperature. In situations where the non-interacting DOS features van-Hove singularities in the vicinity of the Fermi level, this minimum at finite temperature is strongly modified and may even transform into a maximum. The presented findings are discussed in connection with non-Fermi liquid and pseudogap behavior usually encountered in non-local extensions of the DMFT.

TT 27.47 Wed 14:00 Poster D1

Projected excitations in a generalized Gutzwiller approximation — •Andrea Di Ciolo and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt am Main, Germany.

We extended the generalized Gutzwiller Approximation originally proposed in PRB 72, 144505 (2005) to study projected particle (hole) excitations for inhomogeneous systems with SDW and/or CDW.

This method allows to evaluate observables associated to a correlated state with one or more excitations: for single excitations, one can evaluate their tunnelling transition probabilities into the correlated state; for double excitations one can investigate the response of the system... This approach is conceptually very powerful, because it allows a model-independent analysis: this means that the results are due only to the physical properties of the trial state and not to the choice of a specifical Hamiltonian. The drawback is that the complete extension of the formalism is very challenging, because new Gutwiller factors arise beyond the standard ones, obtained for example in Supercond. Sci. Tech. 1, 36, (1988). In particular, one task is highly not trivial: the evaluation of the size of the Hilbert spaces associated to a physical correlated state and to auxiliary ones. In order to learn how to handle the subtleties of the extended scheme, we applied it first to the case of the AFM. These latter results can be compared to the experimental evidence for materials displaying a long-range AFM order.

TT 27.48 Wed 14:00 Poster D1

Influence of Spin Fluctuation on the Single and Two Particle Properties of Two Dimensional Correlated System — •B.D Napitu[1,2] and J Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik Heinrich-Damerow-Str.4 D-06120 Halle (Saale),Germany — [2]Max-Planck-Institut für Mikrostruk-

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We inspect the interplay between spin fluctuations and the local Coulomb repulsion in strongly correlated two dimensional systems using the Hubbard model. By employing a state-of-the-art extended dynamical mean field theory (EDMFT) that incorporates the non-local interaction in the conventional single site dynamical mean field theory (DMFT), the single particle spectral function, the dynamical spin susceptibility and two particle quantities are calculated. It is shown that the inclusion of spin fluctuation assists the formation of pseudogap in the single particle spectral function. Similarly, the particle-particle sector also shows a reduction of the spectral weight as the spin exchange interaction increases.

TT 27.49 Wed 14:00 Poster D1

Perturbative theory of isosbestic points — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

A family of non-monotonic curves, obtained by plotting a quantity $f(x, y)$ as a function of one of its variables (say, x) for different values of y, will in general intersect, leading to crossing points of the curves. In physics, chemistry and biology the crossing of a family of curves is the rule rather than the exception. Sometimes these crossing points are found to be confined to a remarkably narrow region, or are even located at a single point, thus leading to a conspicuous feature often called *isosbestic point*. Here we consider a perturbative expansion in the variable y. For an *exact* isosbestic point $x^\star$, the dependence of $f(x, y)$ on y is then described by the first term of the expansion in y. For *approximate* isosbestic points higher order terms are responsible for the finite width of the crossing region. This approach describes approximate isosbestic points in various unrelated quantities such as the optical conductivity $\sigma(\omega, n)$ in the Falicov-Kimball model, the photoemission spectra $A(\omega, T)$ of VO_2/TiO_2, the reflectivity $R(\omega, T)$ of $CaCu_3Ti_4O_{12}$, and the Raman response $\chi''(\omega, T)$ of $HgBa_2CuO_{4.16}$.

TT 27.50 Wed 14:00 Poster D1

Thermodynamic properties of the Hubbard model — •Patrick Haase[1], Sebastian Fuchs[1], Mark Jarrell[2], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37075 Göttingen, Germany — [2]Louisiana State Universtity, Baton Rouge, LA 70803, USA

We calculate the temperature dependence of the internal energy of the Hubbard model in the dynamical mean field approximation using continuous-time quantum Monte Carlo simulations. We fit the energy data with the density of states of a non-interacting system. With this density of states we are able to calculate thermodynamic properties like the entropy, which is not directly accessible by Monte Carlo simulations.

TT 27.51 Wed 14:00 Poster D1

High-frequency tails and the decay rate of high-energy excitations in correlated systems — •Matthias Sitte[1] and Lev Ioffe[2] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — [2]Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway NJ 08854 USA

For energies much larger than the bandwidth, the lifetime of a highly excited state becomes exponentially large. Similarly, the high-frequency tails of correlation functions decay exponentially. This response is due to a collective excitation of many discrete degrees of freedom. Such a many-particle scattering process describes, e.g., the decay of doublons (doubly occupied sites) in ultra-cold atom gases in optical lattices, or the NMR relaxation mechanism in large magnetic fields. Here, we investigate the shape of correlation functions at high frequencies. In particular, we consider the spin 1/2 Heisenberg XXZ chain, a paradigm model for strongly correlated systems, which can be realized, e.g., in spin chain systems and in ultra-cold atom gases using two-level systems. Using exact diagonalization methods we calculate the correlation function of the staggered magnetization in frequency space and compare to analytical approaches.

TT 27.52 Wed 14:00 Poster D1

Eigenexcitation of Anderson impurity model out of equilibrium — •Pei Wang and Stefan Kehrein — Arnold Sommerfeld Center, department of physics, LMU

We solve the Anderson impurity model out of equilibrium by searching for the eigenexcitation operator A, which is defined as [H,A]=EA. We express the fermion creation and annihilation operators by eigenexcitation operator to calculate the time evolution. Then we transform back to calculate the expectation value. This method is compared to the flow equation method. It is better for considering the correction to eigen energy.

TT 27.53 Wed 14:00 Poster D1

Non-equilibrium steady state in a periodically driven Kondo model — Markus Heyl and •Stefan Kehrein — Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 München

We investigate the Kondo model with time-dependent couplings that are periodically switched on and off. On the Toulouse line we solve the problem exactly by using bosonization and refermionization that are also suitable for the Kondo model out of equilibrium [1]. We derive exact analytical results for the spin dynamics in the steady state that builds up after an infinite number of switching periods. Remarkably, the algebraic long time behavior of the spin-spin correlation function remains completely unaffected by the driving. In the limit of slow driving the dynamics becomes equivalent to that of a single interaction quench. In the limit of fast driving one can show that the steady state cannot be described by some effective equilibrium Hamiltonian since a naive implementation of the Trotter formula gives wrong results. As a consequence, the steady state in the limit of fast switching serves as an example for the emergence of new quantum states not accessible in equilibrium.

[1] D. Lobaskin and S. Kehrein, Phys. Rev. B **71**, 193303 (2005).

TT 27.54 Wed 14:00 Poster D1

spatiotemporal formation of the Kondo screening cloud — •Alexander Hoffmann and Stefan Kehrein — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

The Kondo model is the paradigm for describing correlated quantum impuritites. Its equilibrium properties are well known, but its non-equilibrium behavior has recently attracted a lot of attention. We calculate the time dependent spin-spin correlation function between the impurity spin and the conduction band spin after a sudden switching on of the interaction. This amounts to studying the spatiotemporal formation of the Kondo screening cloud. To this end we bosonize the Kondo model and then refemionize it at the Toulouse point.

TT 27.55 Wed 14:00 Poster D1

Non-equilibrium magnetization dynamics of ferromagnetically coupled Kondo spins — •Andreas Hackl[1], Matthias Vojta[1], Stefan Kehrein[2], Walter Hofstetter[3], and David Roosen[3] — [1]Universität zu Köln — [2]Universität München (LMU) — [3]Universität Frankfurt

An analytical description of non-equilibrium phenomena in interacting quantum systems is rarely possible. Here we present one example where such a description can be achieved, namely the ferromagnetic Kondo model. In equilibrium, this model is tractable via perturbative renormalization-group techniques. We employ a recently developed extension of the flow-equation method to calculate the non-equilibrium decay of the local magnetization at zero temperature. The flow equations admit analytical solutions which become exact at short and long times, in the latter case revealing that the system always retains a memory of its initial state.

TT 27.56 Wed 14:00 Poster D1

Scaling approach to a time-dependent Kondo model: from adiabatic switching to an interaction quench — •Constantin Tomaras and Stefan Kehrein — LMU München, Department für Physik und Arnold-Sommerfeld-Center for Theoretical Physics, Theresienstraße 37, D-80333 München, Germany

The time-dependent quantum many-body problem has become of particular interest within the recent years [1]. Less is known about the transition from adiabatic turning on the interaction to an interaction quench in generic many-body systems. For the Hubbard model the quench physics were accessible with the help of flow equations [2], while the transition to an adiabatic switching procedure has been investigated by means of Keldysh perturbation theory [3]. Here we consider the isotropic ferromagnetic Kondo model, in which the interaction is switched on according to the time-dependent exchange couplings $J_{kk'}(t)$. Following [4,5], a convenient measure of the deviation of the impurity-spin z-component, from idealized adiabatic evolution is the ratio $\mu = \langle 0|S^z(t\to\infty) - S^z|0\rangle / \left(\langle\tilde{0}|S^z|\tilde{0}\rangle - \langle 0|S^z|0\rangle\right)$. $|\tilde{0}\rangle, |0\rangle$ are the

ground states of the interacting and non-interacting system. Applying some generalized renormalization scheme, the ratio μ is shown to interpolate continuously between its quenched and adiabatic value.

[1] M. Greiner et al. *Nature*, 419 (2002)
[2] M. Moeckel and S. Kehrein, *PRL*, 100 (2008)
[3] M. Moeckel and S. Kehrein, arXiv.org:0911.0875 (2009)
[4] A. Hackl, S. Kehrein, M. Vojta, arXiv.org:0908.3647 (2009) [5] A. Hackl et al. *PRL*, 102 (2009)

TT 27.57 Wed 14:00 Poster D1

Real-time simulations of nonequilibrium transport in the single-impurity Anderson model — •Fabian Heidrich-Meisner[1], Adrian Feiguin[2], Luis Dias Da Silva[3,4], George Martins[5], Carlos Busser[5], Enrique Anda[6], and Elbio Dagotto[3,4] — [1]LMU Munich, Germany — [2]University of Wyoming, USA — [3]ORNL, USA — [4]University of Tennessee, USA — [5]Oakland University, USA — [6]PUC Rio, Brazil

In this work, we consider the single-impurity Anderson model and use the adaptive time-dependent density matrix renormalization group (tDMRG) method to compute real-time currents out of equilibrium [1]. We first focus on the particle-hole symmetric point where Kondo correlations are the strongest and then extend the study of the nonequilibrium transport to the mixed-valence regime. As a main result, we present accurate data for the current-voltage characteristics of this model. As tDMRG is typically implemented with a real-space representation of the noninteracting leads, the Kondo regime, due to the emergent exponentially large Kondo screening length, is difficult to access. We therefore also apply tDMRG to Wilson leads [2], i.e., noninteracting leads with a logarithmic discretization as used in the numerical renormalization group method, and show that in the limit of small biases, perfect conductance can be obtained from tDMRG at much smaller Kondo temperatures than using a real-space representation of the leads.

[1] F. Heidrich-Meisner et al., Phys. Rev B 79, 235336 (2009)
[2] L.G.G.V. Dias da Silva et al., Phys. Rev. B 78 195317 (2008)

TT 27.58 Wed 14:00 Poster D1

Transport simulations in correlated one-dimensional systems — •Malcolm Einhellinger and Alex Cojuhovschi — Leibniz Universität Hannover, Germany

We develop a numerical approach for investigating transport properties in correlated low-dimensional solids and nanosystems. The time-evolving block decimation method is used to simulate the nonequilibrium dynamics in finite one-dimensional lattices. Stationary transport properties are then obtained by scaling the finite-system results. The method is illustrated with the conductance of correlated one-dimensional conductors (Luttinger liquids) such as the Hubbard model and the spinless fermion model. Comparisons with exact results confirm the validity of our approach.

TT 27.59 Wed 14:00 Poster D1

Quantum Dynamics of a spin-boson system close to a classical phase transition — •Lutz Bakemeier, Andreas Alvermann, and Holger Fehske — Institut für Physik, Universität Greifswald, Deutschland

The Rabi model of a spin 1/2 coupled to a harmonic oscillator features a classical phase transition in the limit of zero oscillator frequency. While no phase transition exists in the full quantum model, the existence of the classical transition leads to interesting dynamics in the 'adiabatic limit' of small oscillator frequency. We begin with the characterization of the groundstate. From a simple variational ansatz, which is in good quantitative agreement with exact data, we deduce the relevant effects at different ratios of spin and oscillator frequency. Only at large oscillator frequency the model properties are explained through simple renormalization of the spin dynamics. Based on the groundstate characterization we discuss the Rabi quantum dynamics, with particular emphasis on the signatures of the classical phase transition, e.g. a lock-in of spin and oscillator dynamics. Our contribution shows that the Rabi model is a kind of generic model for the physics of different time-scales. The relevance for general spin-boson models and the connection to a general concept of 'polaron' physics are discussed.

TT 27.60 Wed 14:00 Poster D1

Superperturbation solver for non-equilibrium — •Alexander Lieder, Sergej Brener, Alexander Chudnovskiy, Dmytro Grytskyy, Christoph Jung, and Alexander Lichtenstein — I. Institut für Theoretische Physik

We present a generalization of the recently developed Superperturbation solver for the Anderson impurity model for the non-equilibrium case. The idea is to solve a small reference system using exact diagonalization with its full time dependence on the Keldysh contour and to treat the neglected bath degrees of freedom perturbatively. The key point is to introduce new fermionic degrees of freedom via a Hubbard-Stratonovich transformation. In the space of these auxiliary fermions Wicks theorem is applicable and a perturbation theory with a renormalized interaction is possible.

TT 27.61 Wed 14:00 Poster D1

Strongly Correlated Steady-State Transport through a Quantum Dot — •Andreas Dirks[1], Philipp Werner[2], Mark Jarell[3], and Thomas Pruschke[1] — [1]Universität Göttingen, Institut für theoretische Physik — [2]ETH Zürich, Institut für theoretische Physik — [3]Louisiana State University, Baton Rouge/LA, USA

We investigate the application of continuous-time Quantum Monte Carlo algorithms to the imaginary-time formalism introduced by Han and Heary [1]. The analytic structure of the two-variable Green's functions is discussed, and an algorithm for the numerical analytic continuation is proposed.

[1] J. E. Han, and R. J. Heary, Phys. Rev. Lett. **99**, 236808 (2007)

TT 27.62 Wed 14:00 Poster D1

Matrix product state approach for a two-lead, multi-level Anderson model — •Andreas Holzner, Andreas Weichselbaum, and Jan von Delft — Lehrstuhl für Theoretische Festkörperphysik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany

We exploit the common mathematical structure of the numerical renormalization group and the density matrix renormalization group, namely matrix product states, to implement an efficient numerical treatment of a two-lead, multi-level Anderson impurity model. By adopting a star-like geometry, where each species (spin and lead) of conduction electrons is described by its own Wilson chain, instead of using a single Wilson chain for all species together, we achieve a very significant reduction in the numerical resources required to obtain reliable results, as illustrated for the occupation for a spinfull two-lead 4-level Anderson model. Moreover, we show that it is possible to find a new "optimal" lead basis, obtained via a unitary transformation of the type $c_{\alpha k\sigma} \to U_{\alpha\beta}c_{\beta k\sigma}$ (where α and β label distinct leads), in which lead degrees of freedom on *different* Wilson chains are effectively decoupled from each other for all but the first few sites of each chain. This new basis turns out to also diagonalize the scattering matrix for the leads. We demonstrate this for a spinless two-lead, 4-level Anderson model, presenting DMRG-results for the mutual information between two sites located far apart on different Wilson chains, and NRG results for the scattering matrix.

TT 27.63 Wed 14:00 Poster D1

Coupled qubits in a dissipative environment — •Etienne Gärtner and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Germany

In recent years Numerical Renormalization Group (NRG) methods have not only been applied to systems of pure fermionic degrees of freedom. The successful application of NRG-techniques to the spin boson model has led to important insights on several technicalities one has to handle e.g. when dealing with a bosonic Hilbertspace and its unavoidable truncation. In the present case we study a system of two coupled qubits interacting with a dissipative environment. The dissipation is mediated through a bath of harmonic oscillators, thus we use a two-spin boson model to describe the system. In case of ohmic damping we calculate the entropy in a wide range of the parameter space to extract information about the ground state and the phase diagram.

TT 27.64 Wed 14:00 Poster D1

Exact diagonalization studies of small spin clusters Kondo-coupled to one-dimensional tight-binding electrons — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld, Germany

Magnetic molecules are envisioned to store a single bit of information in future high-density information storage devices. For such an application it is necessary to graft the molecules on a substrate so that they can be individually addressed.

Motivated by the question of how the magnetic properties of a molecule are affected by the deposition on a surface, we study Kondo-Heisenberg model systems in which simple structures of exchange-coupled spins are interacting with one-dimensional tight-binding electrons. In particular, we focus on the magnetization of the spin cluster and examine, for different geometries, its dependence on an external magnetic field at finite temperatures. The effect of additional interaction terms like a single-ion anisotropy is also investigated.

In order to calculate the relevant thermodynamic observables, we perform a numerically exact, complete diagonalization of the model Hamiltonian. As the application of this method is limited to rather small systems, it is important to analyze the influence of finite-size effects. We investigate down to which temperatures reliable results, that adequately reflect the thermodynamic limit, can be obtained and how results for finite systems can be improved by e.g. boundary condition averaging.

TT 27.65 Wed 14:00 Poster D1

Thermal expansion and magnetostriction of the spin-$\frac{1}{2}$-chain compound $Cu(C_4H_4N_2)(NO_3)_2$ — •Jens Rohrkamp[1], Yvonne Sanders[1], Markus Garst[2], Matt D. Phillips[3], Mark M. Turnbull[3], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für theoretische Physik, Universität zu Köln, Germany — [3]Carlson School of Chemistry and Biochemistry, Clark University, USA

Compounds with magnetic subsystems representing simple model spin systems with weak magnetic coupling constants are ideal candidates to test theoretical predictions for the generic behavior close to quantum phase transitions. We present measurements of the thermal expansion and magnetostriction of the spin-$\frac{1}{2}$-chain compound copper pyrazine dinitrate $Cu(C_4H_4N_2)(NO_3)_2$. Of particular interest is the low-temperature thermal expansion close to the saturation field $H_c \approx 14\,\mathrm{T}$, which defines a quantum phase transition from the gapless Luttinger liquid state to the fully saturated state with a finite excitation gap. We find a sign change of the thermal expansion for the different ground states, and at the quantum critical point H_c the low-temperature expansion approaches a $1/\sqrt{T}$ divergence. Furthermore the magnetostriction data is compared to the spin-spin correlation function calculated via Bethe-Ansatz. This work was supported by the DFG through SFB 608.

TT 27.66 Wed 14:00 Poster D1

Magnetic Properties of the quasi-2D S=1/2 Heisenberg antiferromagnet $[Cu(pyz)_2(HF_2)]PF_6$ — •M. Ozerov[1], E. Čižmár[1,2], S.A. Zvyagin[1], R. Beyer[1], M. Uhlarz[1], Y. Skourski[1], J.L. Manson[3], J.A. Schlueter[4], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden - Rossendorf, Dresden, Germany — [2]Centre of Low Temperature Physics, P.J. Šafarik University, Košice, Slovakia — [3]Department of Chemistry and Biochemistry, Eastern Washington University, Cheney, WA, USA — [4]Materials Science Division, Argonne National Laboratory, Argonne, IL, USA

We report on ESR, magnetization, and specific-heat studies of $[Cu(pyz)_2(HF_2)]PF_6$ single crystals, identified as a quasi-two-dimensional spin-1/2 Heisenberg antiferromagnet. Our measurements revealed $J_{inter}/J_{intra} \leq 0.063$ and $A/J \sim 0.003$, where J_{inter}, J_{intra}, J are the interplane, intraplane and mean exchange interactions, respectively, and A is the anisotropy constant. It is argued that the magnetic properties of this material are strongly affected by two-dimensional spin fluctuations, despite of the onset of 3D long-range magnetic ordering at $T_N \approx 4.4$ K. The temperature-field phase diagram and ESR magnetic excitation spectrum in the 3D ordered phase of $[Cu(pyz)_2(HF_2)]PF_6$ will be discussed in detail.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043)

TT 27.67 Wed 14:00 Poster D1

ESR Studies of the Quantum Spin Dimer System $Ba_3Cr_2O_8$ — •D. Kamenskyi[1], J. Wosnitza[1], S.A. Zvyagin[1], J. Krzystek[2], A.A. Aczel[3], H.A. Dabkowska[3], and G.M. Luke[3] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden - Rossendorf, Dresden, Germany — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA — [3]McMaster University, Hamilton, Ontario, Canada

$Ba_3Cr_2O_8$ is a system of three-dimensionally coupled dimers, exhibiting a field-induced phase transition from a quantum-disordered to a long-range antiferromagnetically ordered state at $H_{c1} = 12.5$ T. We report tunable-frequency electron spin resonance (ESR) studies of $Ba_3Cr_2O_8$ single crystals performed in a frequency range between 50 and 700 GHz in fields up to 25 T (applied along the c axis). Two gaps in the magnetic excitation spectrum, $\Delta_1 = 564$ GHz and $\Delta_2 = 400$ GHz, were observed directly, confirming the spin-singlet ground state of $Ba_3Cr_2O_8$ below H_{c1}. The observation of singlet-triplet ESR transitions, which are normally forbidden in spin-1/2 dimer systems by selection rules, indicates the break-down of the axial symmetry in this compound. Details of the ESR excitation spectrum of $Ba_3Cr_2O_8$ across different regions of its phase diagram will be discussed.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043).

TT 27.68 Wed 14:00 Poster D1

Magnetic properties of epitaxially strained $Sr_{1-x}Ca_xRuO_3$ thin films — •Markus Wissinger, Dirk Fuchs, and Hilbert v. Löhneysen — Institut für Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany

The magnetic properties of epitaxially strained $Sr_{1-x}Ca_xRuO_3$ thin films were investigated with respect to lattice changes caused by i) chemical pressure due to the substitution by smaller Ca ions as well as by ii) epitaxial strain due to the growth on different lattice matched substrate materials.

Stoichiometric polycrystalline targets were produced via standard solid state reaction for $0 \leq x \leq 1$. Thin epitaxial films were deposited from the targets by pulsed laser deposition on various substrate materials. The structural and magnetic properties of the bulk and thin film samples were characterized by x-ray diffraction and superconducting quantum interference device magnetometry.

The lattice parameters a, b, and c of the bulk as well as the out-of-plane lattice parameter of the thin film samples were found to decrease with increasing Ca substitution. The Curie temperature T_c also decreases with increasing x. Tensile or compressive strain in epitaxial films results in a significant increase or decrease of T_c , respectively, in comparison to the bulk value. The critical concentration, x_c, where $T_c = 0$ therefore shifts to higher or lower concentrations with respect to the bulk where x_c amounts to 0.7. The sensitivity of T_c to chemical pressure and epitaxial strain will be compared and discussed in detail.

TT 27.69 Wed 14:00 Poster D1

Spinon localization in the heat transport of the spin-1/2 ladder compound $(C_5H_{12}N)_2CuBr_4$ — •Gerhard Kolland[1], Jens Rohrkamp[1], Beni Thielemann[2], Henrik M. Ronnow[3], Christian Rüegg[4], Karl Krämer[5], John A. Mydosh[1], Alexandr V. Sologubenko[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Lab. for Neutron Scattering, ETH Zürich & PSI Villigen, Switzerland — [3]Lab. for Quantum Magnetism, EPFL, Switzerland — [4]London Centre for Nanotech. and Dep. of Phys. and Astron., University College London, UK — [5]Dep. of Chem. and Biochem., University of Bern, Switzerland

Piperidium copper bromide $(C_5H_{12}N)_2CuBr_4$ is a two-leg spin-1/2 ladder system with comparatively weak antiferromagnetic exchange couplings along the legs and the rungs. Hence, this system has two experimentally accessible quantum phase transitions; from a gapped spin-singlet state to a gappless Luttinger-liquid state at $H_{c1} \simeq 7\,\mathrm{T}$ and from this state to a fully polarized state at $H_{c2} \simeq 14\,\mathrm{T}$. Here, we present experiments on the magnetic field-dependent thermal transport. The thermal conductivity is only weakly affected by the field-induced transitions at $H_{c1/c2}$, suggesting the absence of a direct contribution of the spin excitations to the heat transport. We observe, however, that the thermal conductivity is suppressed by the magnetic field deeply within the Luttinger-liquid state. These surprising observations are discussed in terms of localization of spinons within finite ladder segments and spinon-phonon umklapp scattering of the predominantly phononic heat transport. *Supported by the DFG through SFB 608.*

TT 27.70 Wed 14:00 Poster D1

Generalized t-J models derived systematically from Hubbard models in the doped case — •Simone A. Hamerla and Götz S. Uhrig — Technische Universität Dortmund,Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

Fermionic Hubbard models are mapped to generalized t-J models by a systematic change of basis using self-similar continous unitary transformations (s-CUTs) [1].

In the new basis, charge fluctuations affecting the number of double occupancies are eliminated. The mapping relies on the energetic separation of sectors with different numbers of double occupancies. Thus

this energy separation is calculated using the Liouville formalism. In this way we obtain the range of validity of the mapping for the first time in dependence of the doping.
Three different s-CUTs are investigated for various truncation schemes on linear chains and square lattices.

[1] A. Reischl, E. Müller-Hartmann, G. S. Uhrig, Phys. Rev. B 70, 245124

TT 27.71 Wed 14:00 Poster D1

Field-induced effects near the mysterious low-temperature phase transition in the proposed spin-liquid system κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ — •Rudra Sekhar Manna[1], Mariano de Souza[1], Andreas Brühl[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, SFB/TR 49, D-60438, Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

The charge-transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, a Mott insulator with a 2D triangular lattice structure, is considered as a likely candidate for a quantum-spin liquid. We have studied this material by measuring the uniaxial expansion coefficients α_i, the specific heat and magnetic susceptibility. The main observations are: (i) a pronounced in-plane (bc) anisotropy in α_i, implying significant T-dependent lattice distortions, and (ii) a pronounced phase-transition anomaly at 6 K. By employing a Grüneisen-scaling Ansatz, we have been able to separate the corresponding contribution to the specific heat. The entropy release suggests that the spin degrees of freedom alone cannot account for the phase transition [1]. While the 6 K transition is insensitive to the application of a magnetic field up to 10 T, the highest field accessible, distinct field dependencies have been found which set in at somewhat higher temperatures for magnetic fields along the b-axis of one particular high-quality crystal. Based on measurements as a function of temperature at constant field and isothermal field sweeps, an anomaly diagram was able to be constructed.

[1] R. S. Manna *et al.*, arXiv:0909.0718 (2009).

TT 27.72 Wed 14:00 Poster D1

Structural and magnetic properties of the mixed quantum antiferromagnet $Cs_2CuCl_{4-x}Br_x$ — •P. T. Cong, S. Belz, N. Krüger, F. Ritter, W. Assmus, B. Wolf, and M. Lang — Physikalisches Institut, Goethe-Universität, SFB/TR 49, D-60438 Frankfurt(M).

The two compounds, Cs_2CuCl_4 and Cs_2CuBr_4, have been classified as quasi-two-dimensional quantum antiferromagnets. Cs_2CuCl_4 shows long-range magnetic order, which can be described as a Bose-Einstein condensation of magnons, i.e., delocalized triplet excitations, whereas the iso-structural compound Cs_2CuBr_4, exhibits plateaus in the magnetization, indicating the localization of triplets. Here we present a systematic study of the magnetic properties in the $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$) mixed system. All crystals were synthesized by a solution-growth method. Two structural variants - an A-type orthorhombic and a B-type tetragonal - were detected in this system depending on the growth conditions. A detailed structural phase diagram has been constructed, based on X-ray Rietveld refinement, SEM and thermal analysis. χ(T) measurements of crystals near the end members of the series reveal a broad maximum at T_{max} indicative of quasi-2D short range correlations. While for the Cl^-rich system $0 \leq x \leq 0.8$, T_{max} slightly increases with increasing Br^-, a much stronger increase of T_{max}.is observed for the Br-rich system for $2.8 \leq x \leq 4.0$.

TT 27.73 Wed 14:00 Poster D1

Magnetic properties of the new low-dimensional spin magnet α-$Cu_2As_2O_7$ — •Yulieth Arango[1], Evgenia Vavilova[2], Olga Volkova[3], Mahmoud Abdel-Hafez[1], Matthias Weil[4], Alexander Vasiliev[3], Vladislav Kataev[1], Rüdiger Klingeler[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper und Werkstoffforschung IFW Dresden, Dresden, Germany — [2]Zavoisky Physical-Technical Institute of RAS, Kazan, Russia — [3]Physics Faculty, Moscow State University, Moscow, Russia — [4]Institute for Chemical Technology and Analytics, Vienna University of Technology, Vienna, Austria

The crystal structure of α-$Cu_2As_2O_7$ consists of two-dimensional infinite sheets (ab-plane) of [CuO_5] polyhedra stacked along the c-axis. The Cu^{2+} ($3d^5$, S=1/2) ions are connected via oxygen ligands in the Cu-O chains along the diagonal of the ab-plane. In this work we study the interplay between the crystal structure and magnetism of α-$Cu_2As_2O_7$ single crystals by measuring magnetic susceptibility, specific heat, high field electron spin resonance (HF-ESR), and nuclear magnetic resonance (NMR). The data reveal that in the spin sector Cu-O chains represent a realization of a quasi-one dimensional (1D) spin-1/2 anisotropic Heisenberg antiferromagnet with the nearest neighbor exchange constant $J \sim 160$ K. Due to residual 3D interactions α-$Cu_2As_2O_7$ orders antiferromagnetically at $T_N \simeq 11$ K. Below T_N two phases are identified: a collinear phase and a field B induced spin-flop phase at $B > B_C \simeq 1.8$ T.

TT 27.74 Wed 14:00 Poster D1

Electron spin resonance spectroscopy of a novel Ni based hybrid $S = 1$ chain — •F. Lipps[1], A. H. Arkenbout[2], A. Meetsma[2], T. T. M. Palstra[2], P. H. M. van Loosdrecht[2], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, Dresden, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

We present results of a multifrequency ESR and static magnetization study of single crystals of a new hybrid material that comprises arrays of one dimensional (1D) chains of $NiCl_6$ octahedra separated by a framework of organic molecules. The $Ni^{2+}(3d^8)$ ions in the $NiCl_6$ chain possess an integer spin $S = 1$. Thus, in case of the antiferromagnetic (AFM) coupling, such a chain may provide an experimental realization of a prominent 1D $S = 1$ Heisenberg model, the Haldane chain. In contrast to the $S = 1/2$ chain it has a nonmagnetic ground state and a gapped spectrum of spin excitations. The ESR response of the studied samples is characterized by a single well-defined lorentzian line with a g-factor of $g \simeq 2.2$. The T-dependence of the ESR intensity which is proportional to the static spin susceptibility as well as the bulk static magnetization reveal a low temperature maximum suggesting an AFM coupling of the order of ~ 24 K. In this low temperature regime the ESR signal broadens substantially which indicates a growth of the low-frequency AFM dynamic spin correlations. Remarkably, no indications of the development of the static local internal fields due to the long-range order are observed in the ESR spectra. We discuss a possible ground state and spin dynamics of the studied compound.

TT 27.75 Wed 14:00 Poster D1

Hole induced spin polarons in $LaCoO_3$ — •A. Alfonsov[1], E. Vavilova[1,2], V. Kataev[1], A. Podlesnyak[3], D.I. Khomskii[4], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Oak Ridge National Laboratory, P.O. BOX 2008 MS6494 Oak Ridge TN 37831-6494, USA — [4]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We report a comparative high field electron spin- (ESR), nuclear magnetic resonance (NMR) and static magnetization study of lightly hole-doped samples of $La_{0.998}Sr_{0.002}CoO_3$ and $La_{0.998}Ca_{0.002}CoO_3$. We have shown before [1] that small Sr doping of $LaCoO_3$ yields the spin-state polaron with a big spin value and large spin orbital coupling. The Ca^{2+} ion, in contrast to the Sr^{2+} ion, has almost the same ionic radii as the La^{3+} ion. Therefore, the substitution of Ca for La provides mainly a hole to the system without creating a sizeable crystal field distortion around the substituted Ca ion. This difference enables us to ascertain the roles of the introduced hole and the created crystal field distortion in the formation of the spin polarons. The data obtained on Ca and Sr doped $LaCoO_3$ samples provide experimental evidence that the introduced hole indeed plays the main role. We discuss a model of the formation of big spin polarons in $LaCoO_3$ due to a very small hole doping.

[1] A. Podlesnyak et al., Phys. Rev. Lett. 101, 247603 (2008)

TT 27.76 Wed 14:00 Poster D1

Magnetic anisotropy in the quasi one-dimensional Ising spin-1/2 chain system $BaCo_2V_2O_8$ — •Sandra Niesen, Gerhard Kolland, Martin Valldor, Oliver Heyer, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

$BaCo_2V_2O_8$ contains screw chains of CoO_6 octahedra which are running along the c axis of the tetragonal crystal structure and are separated by nonmagnetic Ba^{2+} und V^{5+} ions in the aa plane. Due to a compression of the octahedra along c the threefold degeneracy of the t_{2g} orbitals is lifted and the magnetic ground state can be described by an effective Ising spin-1/2 antiferromagnetic chain. Due to a finite inter-chain coupling, $BaCo_2V_2O_8$ shows long-range antiferromagnetic order below $T_N \simeq 5.5$ K with the spins oriented along c.
We have prepared single crystals of $BaCo_2V_2O_8$ by a spontaneous nucleation method. Here, we present measurements of the magnetization, the specific heat, the thermal expansion, magnetostriction, and the thermal conductivity in magnetic fields up to 17 T. Depending on

the field direction, the magnetic field influence is highly anisotropic. In case of H parallel c, the Néel order is strongly suppressed already for low fields, and changes into an incommensurate phase above about 4 T. For fields perpendicular to c, the field influence is much weaker. Besides, this expected Ising anisotropy, we have discovered a new magnetic anisotropy for fields applied within the aa plane. For magnetic fields applied along [110] T_N is only weakly suppressed, while for fields applied along [100] T_N is completely suppressed for fields above about 10 T. *This work is supported by the DFG through SFB 608.*

TT 27.77 Wed 14:00 Poster D1

Derivation of the effective microscopic models for the frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 from first principles — •Kateryna Foyevtsova, Ingo Opahle, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

The frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 have been attracting a lot of attention as low-dimensional quantum systems with a variety of unconventional properties, such as, for instance, the spin-liquid state in Cs_2CuCl_4 or magnetization plateaux in Cs_2CuBr_4.

In order to provide a theoretical insight to the on-going discussion of the Cs_2CuCl_4 and Cs_2CuBr_4 effective models, we perform a comprehensive Density Functional Theory (DFT) study of the electronic properties of Cs_2CuCl_4 and Cs_2CuBr_4 and derive the tight-binding (TB) and Heisenberg models' parameters for the two compounds. We find that in Cs_2CuCl_4 electronic correlations play an important role for the correct description of the crystal structure and discuss the implications of such results for DFT calculations with commonly-used approximations for the exchange-correlation functional.

TT 27.78 Wed 14:00 Poster D1

DMRG Study of Anisotropic Triangular Heisenberg Lattice — •Andreas Weichselbaum[1] and Steven R. White[2] — [1]Ludwig-Maximilians-Universität, 80333 München — [2]University of California, Irvine, CA 92697, USA

The anisotropic antiferromagnetic two-dimensional triangular Heisenberg lattice for spin 1/2 describes certain classes of transition-metal oxides (TMOs) and chalcogenides (TMCs), clearly supported by experimental data. The understanding of the ground state properties of this kind of system from a theoretical point of view, however, has remained an extraordinary challenge. In the model under consideration, quasi-one-dimensional Heisenberg chains of uniform intrachain coupling strength J interact with their neighboring chains via the interchain coupling J0. By varying the anisotropy ratio $j \equiv J'/J$ from $j = 0$ (decoupled Heisenberg chains) to $j = 1$ (uniform triangular lattice with finite Neel order like local magnetization), it was pointed out in previous studies [1] that, indeed, there appears to exist spin liquid properties up to remarkably high values of j of about 0.85. We given an update on our DMRG studies specifically optimized to reduce finite size effects [2].

[1] S. Yunoki et al., PRB 74, 014408 (2006).
[2] S. R. White et al., PRL 99, 127004 (2007).

TT 27.79 Wed 14:00 Poster D1

DMRG calculations for S=1 anisotropic Heisenberg antiferromagnetic chains — •David Peters[1], Ian P. McCulloch[2], and Walter Selke[1] — [1]JARA-SIM and RWTH Aachen, Institut für Theoretische Physik, Germany — [2]University of Queensland, Department of Physics, Brisbane, Australia

Using density matrix renormalization group calculations, for finite number of sites and in the thermodynamic limit, ground state properties of spin–1 Heisenberg chains with exchange and quadratic single-ion anisotropies in an external field are studied, for special choices of the two kinds of anisotropies [1,2]. In particular, the phase diagram includes antiferromagnetic, spin-liquid (or spin-flop), half magnetization plateau, and supersolid (or biconical) phases. Especially, generic features of the spin-liquid and supersolid phases as well as corresponding quantum phase transitions are discussed. Properties of the quantum chains are compared to those of corresponding classical spin chains.

Parts of the research has been funded by the excellence initiative of the German federal and state governments.

[1] D. Peters, I. P. McCulloch, W. Selke, Phys. Rev. B79, 132406 (2009); Journal of Physics: Conference Proceedings (in print)
[2] F. Heidrich-Meisner, I. P. McCulloch, A. K. Kolezhuk, Phys. Rev. B80, 144417 (2009)

TT 27.80 Wed 14:00 Poster D1

Dynamics of magnetic impurities in two-dimensional spin-1/2 antiferromagnets — •Björn Willenberg and Wolfram Brenig — Institut für Theoretische Physik, Technische Universität Braunschweig

Using Quantum Monte-Carlo methods based on the stochastic series expansion we investigate the dynamics of a single spin-1/2-degree of freedom coupled to a two-dimensional Heisenberg antiferromagnet (HAFM). Calculating imaginary time spin correlation functions and performing Maximum Entropy analysis we analyze the dynamical longitudinal and transverse local susceptibilities of the impurity. These quantities will be studied as a function of temperature and system size. Our findings will be compared to analytical results from stochastic Liouville equations. Finally we discuss the role of antiferro- versus ferromagnetic coupling of the impurity to the HAFM.

TT 27.81 Wed 14:00 Poster D1

Vacancies in non-collinear antiferromagnets — •Alexander Wollny, Lars Fritz, and Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany

2D quantum Heisenberg antiferromagnets provide a variety of interesting phenomena. The role of vacancies has been widely studied on the square lattice, e.g. in the context of cuprates, and is reasonably well understood.

For a system with geometrical frustration the situation is more difficult. Here a magnetically ordered state often displays non-collinear order which has a strong influence on the basic excitations of the system, the spin-waves. The simplest realization is the triangular lattice which shows a 120° spin structure. At the classical level, a vacancy induces a local distortion of the spin pattern which partially relieves the frustration.

We perform a classical Monte Carlo simulation which determines the structure of the distortion and shows that it declines exponentially. Thus, it does not correspond to a goldstone mode but can be interpreted as a local condensate of spin-waves. Taken this distortion into account, we study the spin-wave corrections to the classical ground state in linear order and discuss how the vacancy could be seen in a local susceptibility measurement.

TT 27.82 Wed 14:00 Poster D1

Manipulating magnetic structures in chiral metals by currents — •Karin Everschor[1], Markus Garst[1,2], Rembert Duine[3], and Achim Rosch[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str.77, 50739 Köln — [2]Physik Department T30c, Technische Universität München, 85747 Garching — [3]Institute for Theoretical Physics, Department of Physics and Astronomy Faculteit Betawetenschappen, Utrecht University, Leuvelaan 4, 3584 CE Utrecht, The Netherlands

A Skyrmion is a topologically stable field configuration, originally introduced by Tony Skyrme, a nuclear physicist, who interpreted a proton as a "knot" in pion fields. Recently, the two-dimensional version of such Skyrmions was visualized as a lattice of vortices in the magnetic structure of manganese silicide (MnSi) We investigate theoretically the interaction between the applied electrical currrents and the topological magnetic structure.

TT 27.83 Wed 14:00 Poster D1

Ground state phases of the spin-1/2 J_1–J_2–J_3 Heisenberg antiferromagnet on the square lattice — •Rachid Darradi[1], Johannes Reuther[2], Wolfram Brenig[3], Johannes Richter[4], and Peter Wölfle[5] — [1]Institute for Theoretical Physics Technical University Braunschweig Mendelssohnstr. 3 38106 Braunschweig Germany — [2]Institute for Condensed Matter Theory University Karlsruhe, Postfach 6980 76128 Karlsruhe Germany — [3]Institute for Theoretical Physics Technical University Braunschweig Mendelssohnstr. 3 38106 Braunschweig Germany — [4]Institute for Theoretical Physics, Otto-von-Guericke University Magdeburg, 39016 Magdeburg, Germany — [5]Institute for Condensed Matter Theory University Karlsruhe, Postfach 6980 76128 Karlsruhe Germany

We investigate the zero-temperature phase diagram of the spin-1/2 frustrated J_1–J_2–J_3 Heisenberg Antiferromagnet on the square lattice. Using high orders coupled cluster method (CCM), Series expansion based on the flow equation method, and functional renormalization group (FRG), we have calculated the ground state energy, triplet excitations, the magnetic order parameter, and generalized susceptibilities. We determine the quantum critical lines for the semiclassical Néel, spiral and collinear phase, comparing our complementary approaches and

contrasting our findings to other published results. Based on the susceptibilities which are related to valence-bond crystal order parameters we also discuss the nature of the quantum disordered phase separating the two semiclassical Néel and spiral phases.

TT 27.84 Wed 14:00 Poster D1

Consistent description of magnetic excitations and phase diagram of high-T_c cuprates within a strong-coupling approach — Sascha Brehm[1], •Enrico Arrigoni[2], Markus Aichhorn[3], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France

Magnetic excitations of the high-T_c cuprate superconductors (HTSC) are shown to be correctly reproduced within a two-dimensional Hubbard model in the appropriate strong-coupling regime. In particular, salient properties of the magnetic resonance mode, its intensity behavior in the underdoped regime and the "hour glass" dispersion display a good agreement with experiments. Our results are obtained in an essentially parameter-free theory based on an extension of the variational cluster approach (VCA) to treat two-particle excitations. When combined with earlier phase-diagram calculations using the VCA, it lends further support to a Hubbard-model description of the interplay of magnetism and superconductivity in the cuprate HTSC.

TT 28: FS: Time-Resolved Spectroscopy in Correlated Electron Systems: Experiment and Theory

Time: Thursday 9:30–13:00 Location: H18

Topical Talk TT 28.1 Thu 9:30 H18

Angle- and time-resolved photoelectron spectroscopy of charge density wave materials — •Uwe Bovensiepen — University Duisburg-Essen, Faculty of Physics, Duisburg, Germany

In charge density wave (CDW) materials a band gap opens at sufficiently low temperatures because the system gains energy by forming a new periodic arrangement of the ion cores, which modulates the electron charge density. As shown femtosecond time- and angle-resolved photoelectron spectroscopy (trARPES) monitors the phonon mode that couples to electrons at the Fermi level, which is a direct example of electron-phonon coupling. To achieve this the material is pumped by an IR femtosecond laser pulse ($h\nu = 1.5eV$). The response to this excitation is probed by a delayed UV laser pulse ($h\nu = 6.0eV$). The latter pulse generates photoelectrons which are analyzed regarding parallel momentum and kinetic energy. The tritelluride $TbTe_3$ responds by electron-hole pair excitation and two distinct coherent phonon modes that result in periodic variations of the respective photoemission lines at the phonon frequency. One of them presents a pronounced momentum dependent dynamics and is responsible for closing (and opening) of the band gap. Hence it represents the amplitude mode of the CDW. In the dichalcogenide 1T -TaS_2 the amplitude mode is also excited, however, it does not couple strongly to the band gap. Accordingly, electronic correlations might contribute to the gap formation. This is confirmed by a considerably faster and shortlived closing of the gap.

Experiments have been performed at the Freie Universität Berlin.

Invited Talk TT 28.2 Thu 10:00 H18

Many Body Theory for Time-Resolved Pump/Probe Photoemission and its Solution via Nonequilibrium Dynamical Mean-Field Theory — •James Freericks — Georgetown University, Washington, DC, USA

In this talk, I will present the exact many-body formalism for time-resolved pump/probe photoemission spectroscopy (PES). By using the sudden approximation and neglecting the energy and momentum dependence of matrix elements, one can reduce the PES response to a relative time Fourier transform of the (nonequilibrium) lesser Green's function in the presence of the pump and modulated by the probe envelope. We will apply this theory to a system that cannot be described by a quasiequilibrium approach with a time-dependent effective temperature: namely, the response of the system to a large dc electric field which generates damped Bloch oscillations in the system as it evolves to a nonequilibrium steady state. We will describe the interplay between the probe width and the ability to see temporal oscillations or sharp features in the spectra.

Recent references include: J. K. Freericks, H. R. Krishnamurthy and Th. Pruschke, Phys. Rev. Lett. **102**, 136401 (2009); J. K. Freericks, H. R. Krishnamurthy, Yizhi Ge, A. Y. Liu, and Th. Pruschke, phys. stat. sol. b **246**, 948 (2009); and B. Moritz, T. P. Devereaux, and J. K. Freericks, arXiv:0908.1807.

TT 28.3 Thu 10:30 H18

Electron-phonon interaction in 122-iron pnictides investigated by femtosecond time-resolved ARPES. — •Rocío Cortés[1], L. Rettig[1], S. Thirupathaiah[2], U. Bovensiepen[1,3], M. Wolf[1], H. A. Dürr[2], P. Gegenwart[4], T. Wolf[5], and J. Fink[2,6] — [1]Freie Universität Berlin, D-14195 Berlin — [2]Helmholtz-Zentrum Berlin, D-12489 Berlin — [3]Universität Duisburg-Essen, D-47048 Duisburg — [4]Georg-August-Universität Göttingen, D-37077 Göttingen — [5]Karlsruhe Institute of Technology, D-76021 Karlsruhe — [6]Leibniz-Institute for Solid State and Materials Research Dresden, D-01171 Dresden

The new class of FeAs based high-T_c superconductors exhibits a complex interplay between electronic, magnetic and lattice degrees of freedom. Here we report on electron-phonon coupling in $EuFe_2As_2$ and $BaCo_{0.15}Fe_{1.85}As_2$ investigated by femtosecond (fs) time- and angle-resolved photoelectron spectroscopy (trARPES). The samples were excited by 1.5 eV fs laser pulses, at 100 K equilibrium temperature. The temporal evolution of their electronic band structure after photoexcitation was probed by time-delayed 6 eV fs pulses. In this way a periodic oscillation of the electronic structure in the vicinity of the Fermi level was observed, which is attributed to coherent phonon modes and electron phonon-coupling. Comparison with Raman scattering results[1] allows to assign the mode with the highest frequency to the A_{1g} mode, which modifies the Fe-As distance and could be involved with the mechanism leading to superconductivity in these materials.

[1] A.P. Litvinchuk *et al.*, Phys. Rev. B **78**, 060503(R) (2008)

Topical Talk TT 28.4 Thu 10:45 H18

Time resolved photoemission and THz spectroscopy of high temperature superconductors — •Luca Perfetti — Laboratoire des Solides Irradiés, École Polytechnique, 91128 Palaiseau Cedex, France — Fachbereich Physik, Freie Universitaet, Arnimallee 14, 14195 Berlin, Germany

I will review some of the open questions concerning the mechanism of high temperature superconductivity. Our approach makes use of non-equilibrium techniques in order to disentangle electronic degrees of freedom from lattice modes. The time resolved photoemission technique and time resolved THz spectroscopy will be presented. These experiments provide novel information on the elementary interactions dressing the quasiparticles as well as on the calorimetry of the electrons. The relaxation time of the photoexcited state indicates that the electron-phonon coupling is too weak in order to provide the pairing interaction. Simple considerations based on the energy conservation allow for an extraction of the electronic specific heat over a wide temperature range. These results offer new insights on the phase diagram and the occurrence of a pseudogap in underdoped compounds.

15 min. break

Topical Talk TT 28.5 Thu 11:30 H18

Relaxation of strongly correlated electron systems: Insights from nonequilibrium dynamical mean-field theory — •Martin Eckstein — Theoretische Physik, ETH Zürich, 8093 Zürich, Schweiz

Pump-probe experiments with femtosecond time-resolution provide a unique way to observe the nonequilibrium dynamics of correlated electron systems after a strong laser excitation, before the electrons have equilibrated and the lattice dynamics becomes dominant. The bare timescales for the electronic relaxation are set by the Coulomb interaction and the hopping amplitude. However, the formation of

photo-excited states and the electronic thermalization are not well understood, and neither are the timescales involved in those processes. Nonequilibrium dynamical mean-field theory (DMFT) allows to address those fundamental questions. We have combined DMFT with a recently developed real-time Quantum Monte Carlo impurity solver to investigate the thermalization of correlated electrons in the Hubbard model [1]. We find that the relaxation behavior undergoes a qualitative change at an intermediate value of U. This transition, which coincides with a pronounced minimum in the thermalization time, occurs for rather general initial states, although the location of the transition depends on the initial state. We also discuss the possibility to observe similar relaxation phenomena in pump-probe experiments.

[1] M. Eckstein, M. Kollar, and P. Werner, Phys. Rev. Lett. 103, 056403 (2009); arXiv:0910.5674.

TT 28.6 Thu 12:00 H18

Quantum interference between photo-excited states in a solid-state Mott insulator — •Simon Wall[1,5], Daniele Brida[2], Stephen R. Clark[3,1], Dieter Jaksch[1,3], Arzhang Ardavan[1], Stefano Bonora[2], Giulio Cerullo[2], and Andrea Cavalleri[1,4] — [1]Department of Physics, Clarendon Laboratory, Oxford UK — [2]Dipartimento di Fisica, Politecnico di Milano, Italy — [3]Centre for Quantum Technologies, National University of Singapore — [4]Max Planck Research Group for Structural Dynamics, University of Hamburg-CFEL — [5]Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We show that, by measuring on an ultrafast timescale, the coherent quantum evolution of a correlated solid after photoexcitation can be observed during the first few femtoseconds. By using nearly-single-cycle, sub-10 fs IR pulses, we measure the time-dependent evolution of the optical conductivity in the quasi-1D organic ET-F2TCNQ after photoexcitation. By comparing our results to numerical calculations we are able to identify two regimes, one incoherent regime occurring on long timescales in which the dynamics are dictated by the electronic population in the excited state, and a second, coherent regime occurring within the first 40 fs, where interference effects between excited states dictates the dynamics. These experiments bridge the gap between fully coherent temporal evolution observed in optical lattices and the incoherent dynamics usually observed in condensed phase materials.

Topical Talk TT 28.7 Thu 12:15 H18

Two-Component Dynamics of the Order Parameter of High Temperature $Bi_2Sr_2CaCu_2O_{8+\delta}$ Superconductors Revealed by Time-Resolved Raman Scattering — •Michael Alexander Rübhausen — Institut für Angewandte Physik & Center for Free Electron Laser Science, Universität Hamburg

We study the dynamics of the superconducting order parameter in the high-T_c cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$ by employing a novel time-resolved pump-probe Raman experiment. We find two different coupling mechanisms that contribute equally to the pair-breaking peak. One coupling sets in very fast at 2 ps and relaxes slowly, while the other one is delayed and sets in roughly at 5 ps and relaxes fast. A model that couples holes through phonons is able to reproduce one part of the condensate dynamics; thus, we argue that hole-spin interactions are of importance as well.

I will also give an brief outlook on future options to perform time resolved inelastic light scattering experiments with table top and free electron laser sources.

In collaboration with: R. P. Saichu, I. Mahns, A. Goos, S. Binder, P. May, S. G. Singer, B. Schulz, A. Rusydi, J. Unterhinninghofen, D. Manske, P. Guptasarma, M. S. Williamsen, and M. Rübhausen

TT 28.8 Thu 12:45 H18

Ultrafast non-equilibrium dynamics in conventional and unconventional superconductors — •Andreas Schnyder and Dirk Manske — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We present simulations of the ultrafast dynamics of conventional and unconventional superconductors using density-matrix theory. In particular, we study how the optical conductivity evolves in response to ultrashort optical pulses in the frequency range of the superconducting gap, i.e., in the terahertz regime. The dominant relaxation process is assumed to be due to electron-phonon collisions. Employing a second order cluster expansion and assuming that the phonons remain equilibrated, Boltzmann type equations for the dynamics of the quasiparticle occupations and coherences are derived. We apply our theoretical model to the study of non-equlibrium dynamics in the two-gap superconductor MgB_2.

TT 29: TR: Nanoelectronics I: Quantum Dots, Wires, Point Contacts 1

Time: Thursday 9:30–13:00 Location: H19

TT 29.1 Thu 9:30 H19

Hyperfine-induced valley mixing and the spin-valley blockade in carbon-based quantum dots — •Andras Palyi and Guido Burkard — Department of Physics, University of Konstanz, Germany

Hyperfine interaction (HFI) in carbon nanotube and graphene quantum dots is due to the presence of ^{13}C atoms. We theoretically show [1] that in these structures the short-range nature of the HFI gives rise to a coupling between the valley degree of freedom of the electron and the nuclear spin, in addition to the usual electron spin-nuclear spin coupling. We predict that this property of the HFI affects the Pauli blockade transport in carbon-based double quantum dots. In particular, we show that transport is blocked only if both the spin and the valley degeneracies of the quantum dot levels are lifted, e.g., by an appropriately oriented magnetic field. The blockade is caused by four "supertriplet" states in the (1,1) charge configuration.

[1] A. Palyi and G. Burkard, Phys. Rev. B **80**, 201404(R) (2009)

TT 29.2 Thu 9:45 H19

AC-Conductance through an Interacting Quantum Dot — •Björn Kubala and Florian Marquardt — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, 80333 Munich, Germany

We investigate the linear ac-conductance for tunneling through an arbitrary interacting quantum dot in the presence of a finite dc-bias [1]. In analogy to the well-known Meir-Wingreen formula for the dc case, we are able to derive a general formula for the ac-conductance. It can be expressed entirely in terms of local correlations on the quantum dot, in the form of a Keldysh block diagram with four external legs. We illustrate the use of this formula as a starting point for diagrammatic calculations by considering the ac-conductance of the noninteracting resonant level model and deriving the result for the lowest order of electron-phonon coupling. We show how known results are recovered in the appropriate limits.

[1] Björn Kubala and Florian Marquardt, arXiv:0910.2844 (unpublished).

TT 29.3 Thu 10:00 H19

Nonequilibrium quantum transport through nanoscale junctions within the scattering-states numerical renormalization group approach — •Sebastian Schmitt and Frithjof B. Anders — Lehrstuhl für Theoretische Physik II, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

We employ the recently developed scattering-states numerical renormalization group approach to open quantum systems to study nonequilibrium Green functions and current-voltage characteristics of nanoscale junctions for intermediate and large values of the Coulomb interaction U. In particular, the influence of charge fluctuations when approaching the strong-coupling regime is discussed.

TT 29.4 Thu 10:15 H19

Non-equilibrium current and relaxation dynamics of a charge-fluctuating quantum dot — •Sabine Andergassen[1], Christoph Karrasch[1], Mikhail Pletyukhov[1], Dirk Schuricht[1], Laszlo Borda[2], Volker Meden[1], and Herbert Schoeller[1] — [1]Institut für Theoretische Physik A und JARA - Fundamentals of Future Information Nanotechnology, RWTH Aachen University — [2]Physikalisches Institut, Universität Bonn

We study the steady-state current in a minimal model for a quantum

dot dominated by charge fluctuations and analytically describe the time evolution into this state. The current is driven by a finite bias voltage across the dot. The Coulomb interaction of the localized dot electron with the lead electrons is treated using two complementary renormalization group methods. We find interesting non-equilibrium effects which can in general not be explained by simply considering the bias voltage as an additional infrared cutoff. The relaxation dynamics shows characteristic oscillations as well as an interplay of exponential and power-law decay.

TT 29.5 Thu 10:30 H19

Non-equilibrium transport through a two-level quantum dot: a renormalization-group analysis — •Sarah Müller[1], Sabine Andergassen[1], Verena Koerting[2], and Dirk Schuricht[1] — [1]Institut für Theoretische Physik A und JARA - Fundamentals of Future Information Nanotechnology, RWTH Aachen University — [2]Niels Bohr Institute, Universitetsparken 5, 2100 København Ø, Denmark

Transport through quantum dots is in general characterized by asymmetric couplings to the leads. In particular, in molecules and nanowires the coupling of each individual orbital level can be different. Motivated by recent experiments, we therefore study the effects of asymmetric hopping parameters on the non-equilibrium current and occupation probabilities of a two-level quantum dot. Starting from a two-level Anderson model, we perform a generalized Schrieffer-Wolff transformation to derive an effective Kondo model. A first perturbative analysis of the cotunneling current allows to determine a regime of negative differential conductance arising for couplings being both asymmetric with respect to the leads as well as to the quantum dot levels. Due to the non-equilibrium occupation of the levels inelastic cotunneling transitions are allowed not only from the ground state but from the excited state. The dependence of this cascade resonance on the magnetic field is discussed in detail. Since we expect the cotunneling lines to be measured experimentally for strong values of the couplings, we study the logarithmic enhancement of the ascribed signatures by means of a poor-man's renormalization-group treatment out of equilibrium.

TT 29.6 Thu 10:45 H19

Symmetry of the scattering states in defected metallic carbon nanotubes — •Leonhard Mayrhofer[1] and Dario Bercioux[2] — [1]Fraunhofer IWM, Wöhlerstraße 11, D-79108 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany

In the last decade, several STM experiments [1-3] on metallic carbon nanotubes have given the opportunity to study the properties of scattering states induced by tube ending and local defects. Of particular interest is the possibility of reconstructing the electronic spectrum via Fourier analysis. The experimental results show a lack of the electronic branches depending of the tube chirality and the nature of the defect. We have performed an in depth analysis of the properties of the scattering states as a function of the symmetry properties of single- and double-vacancy defects. Our results are based on the comparison of a numerically exact tight-binding procedure with an analysis of the carbon nanotube symmetry groups.

[1] M. Ouyang,*et al.*, Phys. Rev. Lett. **88**, 066804 (2002).
[2] J. Lee *et al.*, Phys. Rev. Lett. **93**, 166403 (2004).
[3] G. Buchs, *et al.*, Phys. Rev. Lett. **102**, 245505 (2009).

TT 29.7 Thu 11:00 H19

Crossover between the Kondo effect for quantum dots and the 0.7 conductance anomaly for quantum point contacts — •Jan Heyder, Florian Bauer, and Jan von Delft — Ludwig Maximilians Universitaet , Muenchen

It has been conjectured that the 0.7 conductance anomaly for transport through a quantum point contact (QPC) is closely related to the Kondo effect for transport through a quantum dot (QD) [1,2,3]. To study the relation between these two effects explicitly, we consider a 1-D quantum wire modeled by a tight-binding chain with short-ranged Coulomb interactions and a prescribed onsite potential, whose shape can be varied to mimick the smooth crossover from a double-barrier potential (QD geometry) to a single barrier potential (QPC geometry) as the bottom of the central valley is raised until the central valley disappears completely. We use the functional renormalization group to calculate the conductance, local density and local magnetization at zero temperature as a function of magnetic field, Coulomb interaction and potential shape. Our results reveal both striking similarities and striking differences between the parameter-dependencies of the 0.7 anomaly and the Kondo effect.

[1] Y. Meir, K. Hirose, N.S. Wingreen, Phys. Rev. Lett.,89, 196802 (2002).
[2] K. Hirose, Y. Meir, N. S. Wingreen, Phys. Rev.Lett.,90, 026804 (2003).
[3] T. Rejec, Y. Meir, Nature, 442, 900 (2006).

15 min. break

TT 29.8 Thu 11:30 H19

Spin-dependent transport through quantum-dot Aharonov-Bohm interferometers — •Bastian Hiltscher[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 adress the issue of coherence of transport through interacting quantum dots. For that purpose we consider an Aharonov-Bohm interferometer (ABI) with a single-level quantum dot embedded in one of the arms. For studying the role of spin we choose one lead to be ferromagnetic. We employ a diagrammatic real-time formalism where a perturbation expansion in the tunnel-coupling strength between dot and leads is performed, taking into account the Coulomb interaction non perturbatively [1].
Cotunneling through a quantum dot yields dephasing whenever the spin on the dot is flipped [2]. In the absence of Coulomb interaction transport is fully coherent and the total current is flux dependent. For an infinite interaction on the dot the AB oscillations are strongly influenced by the polarization and the transport direction. We discuss for different transport regimes which information the AB amplitude provides about coherence.

[1] König and Gefen, PRL **86**, 3855 (2001) and PRB **65**, 045316 (2002).
[2] Aikawa *et al.*, PRL **92**, 176802 (2004); Ihn *et al.*, NJP **9**, 111 (2007).

TT 29.9 Thu 11:45 H19

Transport properties of normal-quantum dot-superconductor hybrid structures — •Henning Soller and Andreas Komnik — Institut für Theoretische Physik, Philosophenweg 19, 69120 Heidelberg

We discuss the transport properties of a quantum dot coupled to normal as well as superconducting electrodes in the multi-terminal geometry. The system exhibits interesting effects already in the non-interacting case due to the energy-dependence of the superconducting density of states competing with the energy-dependent transmission through the resonant level. We analyze the full counting statistics of the system allowing for a possible inclusion of interactions and a magnetic field and provide explicit results for the current, noise and cross correlations.

TT 29.10 Thu 12:00 H19

Thermolelectric transport through strongly correlated quantum dots — •Theo Costi[1] and Veljko Zlatić[1,2] — [1]Institut für Festkörperforschung and Institute for Advanced Simulation (IAS), Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Institute of Physics, 10001 Zagreb, Croatia

We use the numerical renormalization group method to calculate thermoelectric transport through a strongly correlated quantum dot described by a single level Anderson impurity model attached to non-interacting leads[1]. We compare and contrast the results with the well known ones for the case of dilute magnetic impurities in non-magnetic metals. In the Kondo regime, we find significant differences in the height of the "charge-fluctuation" peak of the thermopower for these two different situations. The thermal conductivity for the quantum dot exhibits a richer behaviour than for the case of magnetic impurities. We discuss favourable conditions of gate voltage and temperature for achieving a large figure of merit for quantum dot systems.

[1] T. A. Costi and V. Zlatić, preprint (2009).

TT 29.11 Thu 12:15 H19

Two-Particle Dark States in the Transport through Quantum Dot systems — •Christina Pöltl, Clive Emary, and Tobias Brandes — Institut für Theoretische Physik, Hardenbergstr. 36, D-10623 TU Berlin, Germany

Dark states (DSs) are originally a quantum optic phenomenon discovered as a dark line in the fluorescence of sodium atoms. The concept of the Dark states has been generalized to mesoscopic transport as coherent superpositions that block current flow. The triple quantum dot (TQD) in a triangular geometry is a system where several transport

DS phenomena have been studied e.g. [1].

In this contribution, we apply bias such that both singly- and doubly- charged states participate in the transport through the TQD and focus on the formation of a two-electron DS [2].We discuss the conditions under which such a state forms and describe the signatures that it leaves in transport properties such as the differential conductance and shot noise. Our finite-bias calculations facilitate the experimental investigation of DS effects such as the break up of Coulomb blockade diamonds in the stability diagram of the TQD due to one- and two-electron DSs. However it shows that this two-electron DS is a product state of a spin-up and a spin-down single-particle DS. Therefore we also introduce a quantum dot system which allows to configure a spin entangled two-electron DS due to an exchange interaction between the electrons.

[1] B. Michaelis, et al. Europhys. Lett., 73, 677 (2006),
[2] C. Pöltl, et al. Phys. Rev. B 80, 115313 (2009)

TT 29.12 Thu 12:30 H19

Quantum Monte Carlo simulations for contacted quantum dots — •Lothar Mühlbacher[1] and Klaus Ferdinand Albrecht[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg, Germany — [2]Institut für theoretische Physik, Ruprecht-Karls-Universität, Heidelberg, Germany

Correlated transport through nanostructures can prototypically be studied in the framework of the Anderson impurity model. It comprises of a single, spin degenerate electronic level which couples via tunneling to two (or more) metallic electrodes. Although analytic solutions exist for many of its equilibrium properties, the non-equilibrium case, when the electrodes are subject to a finite voltage bias, is yet to be fully understood.

In recent years, real-time diagrammatic Monte Carlo (MC) techniques have emerged as a new and promising tool for a quantitative analysis of the non-equilibrium transport properties. For a large range of parameters, the transient as well as stationary transport properties can be calculated in a numerically exact way. Since diagrammatic MC schemes impose rather few restrictions with respect to the modeling of the electrodes, they also allow to include time-dependent tunneling couplings or to measure the quantum dot's spectral density via a three-terminal setup. Furthermore, in combination with path-integral techniques, diagrammatic MC methods are also capable of accessing the dynamics of a quantum dot coupled to a heat reservoir. Thus, in addition to electronic correlations, the influence of electron-phonon interactions on the transport properties can be studied as well.

TT 29.13 Thu 12:45 H19

Theory of the Topological Anderson Insulator — •Michael Wimmer[1], Christoph W. Groth[1], Anton R. Akhmerov[1], Jakub Tworzydło[2], and Carlo W. J. Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Institute of Theoretical Physics, Warsaw university, Poland

We present an effective medium theory that explains the disorder-induced transition into a phase of quantized conductance, discovered in computer simulations of HgTe quantum wells [1,2]. It is the combination of a random potential and quadratic corrections $\propto p^2\sigma_z$ to the Dirac Hamiltonian that can drive an ordinary band insulator into a topological insulator (having an inverted band gap). We calculate the location of the phase boundary at weak disorder and show that it corresponds to the crossing of a band edge rather than a mobility edge. Our mechanism for the formation of a topological Anderson insulator is generic, and would apply as well to three-dimensional semiconductors with strong spin-orbit coupling.

[1] J. Li *et al.* Phys. Rev. Lett. **102**, 136806 (2009).
[2] H. Jiang *et al.* Phys. Rev. B **80**, 165316 (2009)

TT 30: CE: Low-dimensional Systems - Models 1

Time: Thursday 9:30–13:00 Location: H20

TT 30.1 Thu 9:30 H20

Cluster Spin-DMFT for Quantum Spin Ladders — •Mukul Laad[1,2] and Kai Philliph Schmidt[2] — [1]Institut für Theoretische Physik, RWTH Aachen D-52056, Aachen, Germany — [2]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany

We introduce a new cluster-DMFT scheme for quantum spin models, with a view to accessing short-ranged dynamical spin correlations underlying spin liquid behavior in low-dimensional frustrated systems. Here, we present concrete results for spin S=1/2 two-leg ladder systems, with and without additional frustrating interactions. These show valence-bond-solid ground (VBS) states with rich excitation spectra consisting of elementary triplons, two-triplon bound states, and multiparticle scattering continuua. A wealth of earlier theoretical results allow us to benchmark cluster spin-DMFT.

TT 30.2 Thu 9:45 H20

Orbital currents and SU(2) spin rotational symmetry breaking in doped two-leg Cu-O Hubbard ladders. — •Piotr Chudzinski[1], Marc Gabay[2], and Thierry Giamarchi[1] — [1]DPMC-MaNEP, University of Geneva, Geneva, Switzerland — [2]LPS, Université Paris-Sud 11, Orsay Cedex, France

In the weak-coupling limit, we study, as a function of doping, two leg ladders with a unit cell containing both Cu and O atoms. For purely repulsive interactions, using bosonization and a novel RG scheme, we find that in a broad region of the phase diagram, the ground state consists of a pattern of orbital currents (OCP) defined on the top of an incommensurate density wave. We focus on this OCP and check what kind of changes in the phase diagram one may expect due to SU(2) spin-rotational symmetry breaking. We also investigate a single impurity problem (incl. OCP): we discuss the nature of impurity backscattering, check if Kondo physics is at play. This enables us to show the influence of SU(2) symmetry breaking on conductivity. We estimate the value of gap opened due to the OCP and discuss magnetic properties of a new phase. Finally we investigate the influence, on the phase diagram, of other possible SU(2) breaking mechanisms. The motivation comes from the fact that two-leg ladder Hamiltonian can be used to describe broader class of materials of interest for example zig-zag carbon nanotubes.

TT 30.3 Thu 10:00 H20

Quantum spin chains of Temperley-Lieb type with periodic boundary conditions: spectra, multiplicities and finite temperature — •Britta Aufgebauer and Andreas Klümper — Universität Wuppertal

We determine the spectra of a class of quantum spin chains of Temperley-Lieb type by utilizing the concept of Temperley-Lieb equivalence with the XXZ chain as a reference system. For open boundaries the spectra of these models differ from the spectrum of the associated XXZ chain only in the multiplicities of the eigenvalues. The periodic case is rather different. Here we show how the spectrum is obtained sectorwise from the spectra of globally twisted XXZ chains. As a spin-off, we obtain a compact formula for the degeneracy of the momentum operator eigenvalues. Further the representation theoretical results allow for the study of the thermodynamics by establishing a ' TL-equivalence at finite temperature and finite field'.

TT 30.4 Thu 10:15 H20

Hierarchy of edge-locking effects in one-dimensional quantum lattice models. — •Masud Haque — MPI-PKS, Dresden

In one-dimensional lattices with open boundary conditions, I will present a hierarchy of edge-locking (or edge localization) effects. I will show versions of the phenomenon for three classic condensed-matter models: (1) the Bose-Hubbard model; (2) the spinless fermion model with nearest-neighbor repulsion; (3) the XXZ spin chain.

The edge-locking effects will be demonstrated through far-from-equilibrium dynamics and spectral characteristics far from the ground state.

TT 30.5 Thu 10:30 H20

Zero Temperature Phase Diagram of the 1D t-J Model with Density Matrix Renormalization Group — •Alexander Moreno[1], Alejandro Muramatsu[1], and Salvatore Manmana[2] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institute of Theoretical Physics, Condensed Matter Theory, Lau-

sanne, Switzerland

We study the ground state properties of the one-dimensional t-J model using the Density Matrix Renormalization Group (DMRG), obtaining its phase diagram. We found at low densities that the phase separation region is shifted to higher values of J/t in comparison to previous results [1,2,3]. We confirmed also the results of M. Nakamura et al. [4] who claim, in contrast to other studies [2,3], that a spin gap region is present at densities higher than 0.25. We show that on going from the LL to the spin-gap phase, electrons form pairs visible in real space. The density in real shows also an evidence of the existence of a very small region of the phase diagram where a four electron bound state can be found, as was first suggested by M. Ogata et al. [1]

[1] M. Ogata, M. U. Luchini, S. Sorella, and F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).

[2] C. Y. Chen and T. K. Lee, Phys. Rev. B. **47**, 17 (1993).

[3] C. S. Hellberg and E. J. Mele, Phys. Rev. B. **48**, 1 (1993).

[4] M. Nakamura, K. Nomura, and Kitazawa, Phys. Rev. Lett. **79**, 3214 (1997).

TT 30.6 Thu 10:45 H20

Renormalization group study of Luttinger liquids with boundaries — •Stephan Grap and Volker Meden — Inst. Theo. Physik A RWTH Aachen

We use Wilsons weak coupling "momentum" shell renormalization group method to show that two-particle interaction terms commonly neglected in bosonization of one-dimensional correlated electron systems with open boundaries are indeed irrelevant in the renormalization group sense. Our study provides a more solid ground for many investigations of Luttinger liquids with open boundaries.

15 min. break

TT 30.7 Thu 11:15 H20

Family of exactly solvable models with ultimate co-operative paramagnetic ground state — •Kai Phillip Schmidt[1] and Mukul Laad[1,2] — [1]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany — [2]Institut für Theoretische Physik, RWTH Aachen, 52056 Aachen, Germany

We present a family of two-dimensional frustrated quantum magnets solely based on pure nearest-neighbor Heisenberg interactions which can be solved quasi-exactly. All lattices are constructed in terms of frustrated quantum cages containing a chiral degree of freedom protected by frustration. The ground states of these models are dimer analogs of ultimate co-operative paramagnets and exhibit an extensive entropy at zero temperature. We discuss the unusual and extensively degenerate excitations in such phases. Implications for thermodynamic properties as well as for decoherence free quantum computation are discussed.

TT 30.8 Thu 11:30 H20

Spin Phonon Interactions in triangular Antiferromagnets — Andreas Kreisel and •Peter Kopietz — Institut für Theoretische Physik, Goethe Universität Frankfurt, Max-von-Laue Strasse 1, D-60438 Frankfurt (M), Germany

The triangular lattice antiferromagnet has been recognized a long time ago to be an ideal system to study the effect of quantum fluctuations and frustration in reduced dimensions. If the exchange couplings are spatially anisotropic as in the compound Cs_2CuCl_4, one can observe an ordered phase at very low temperatures. A standard experimental technique to explore the phase boundary is the measurement of the ultrasound attenuation. In order to describe this process theoretically, we consider the exchange striction coupling between magnons and phonons in the ordered phase of the triangular lattice antiferromagnet and calculate the renormalization of the phonon excitations due to the coupling to the magnons.

TT 30.9 Thu 11:45 H20

Spin-liquid and magnetic phases in the anisotropic triangular lattice: the case of κ-$(ET)_2X$ — •Luca F. Tocchio[1], Alberto Parola[2], Claudius Gros[1], and Federico Becca[3] — [1]Institute for Theoretical Physics, Goethe-University Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main, Germany — [2]Dipartimento di Fisica e Matematica, Università dell'Insubria, Via Valleggio 11, I-22100 Como, Italy — [3]CNR-INFM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Beirut 2, I-34151 Trieste, Italy

The two-dimensional Hubbard model on the anisotropic triangular lattice, with two different hopping amplitudes t and t', is relevant to describe the low-energy physics of κ-$(ET)_2X$, a family of organic salts. The ground-state properties of this model are studied by using Monte Carlo techniques, on the basis of a recent definition of backflow correlations for strongly-correlated lattice systems.

The results show that there is no magnetic order for reasonably large values of the electron-electron interaction U and frustrating ratio $t'/t = 0.85$, suitable to describe the non-magnetic compound with $X=Cu_2(CN)_3$. On the contrary, Néel order takes place for weaker frustrations, i.e., $t'/t \sim 0.4 - 0.6$, suitable for materials with $X=Cu_2(SCN)_2$, $Cu[N(CN)_2]Cl$, or $Cu[N(CN)_2]Br$.

TT 30.10 Thu 12:00 H20

Adapted continuous unitary transformation to treat systems with quasiparticles of finite lifetime — Tim Fischer, Sebastian Duffe, and •Götz S. Uhrig — Lehrstuhl Theoretische Physik I, TU Dortmund, 44221 Dortmund

Generic physical systems display excitations of finite life time. Famous examples are Landau's Fermi liquid or rotons in ^{4}He. Diagonalization by unitary transforms usually aims at stable excitation of infinite life time. Here we introduce an improved generator for continuous unitary transformations which is particularly suited to describe systems with unstable quasiparticles of finite life time. The general properties of this generator are derived and discussed. To illustrate this approach we investigate the asymmetric antiferromagnetic spin-$\frac{1}{2}$ Heisenberg ladder which allows for spontaneous triplon decay. The resonance behavior of the decaying triplon is shown explicitly.

TT 30.11 Thu 12:15 H20

Optimized basis in continuous unitary transformations for symmetry-broken groundstates — •Nils A. Drescher, Tim Fischer, and Götz S. Uhrig — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

Continuous unitary transformations (CUTs) [1,2] are a method to systematically derive effective models for many-particle-systems of finite or infinite size. They allow us to separate Hilbert spaces of different numbers of quasiparticles. We use them to study dimerized, antiferromagnetic spin $\frac{1}{2}$ models. Our special interest is the quantum phase transition between spin liquid and long-range ordered phase with spontaneous staggered magnetization. To handle a spontaneously symmetry-broken groundstate with CUT, we modify the quasiparticle basis by introducing a continuous variation parameter. Even in the spin liquid phase, the optimal choice of this parameter leads to a significant gain of accuracy of magnetic properties. Results are shown for one and two dimensional systems.

[1] S. Dusuel and G.S. Uhrig, Journal of Physics A: Mathematics and General 37, 9275 (2004).

[2] C. Knetter, K.P. Schmidt, and G.S. Uhrig, Journal of Physics A: Mathematics and General 36(29), 7889 (2003).

TT 30.12 Thu 12:30 H20

Dynamical crossover in the fermionic Hubbard model — •Florian Goth and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We consider an implementation of the Diagrammatic Determinantal Quantum Monte-Carlo method on a Keldysh contour to study the realtime dependent evolution of the one-dimensional Hubbard model. The system is prepared in a thermal initial state, and the reaction to a sudden switching off of the Hubbard interaction is examined. The transition from an insulating thermal state at half-filling to metal like behaviour is studied on the basis of spin, charge and pairing correlation functions.

TT 30.13 Thu 12:45 H20

A new approach for the diagonalization of the Hubbard model using basis reordering — •Ralf Gamillscheg[1], Gundolf Haase[2], and Wolfgang von der Linden[1] — [1]Institute for Theoretical and Computational Physics, Graz University of Technology, Austria — [2]Institute for Mathematics and Scientific Computing, Karl-Franzens-University Graz, Austria

We present a new approach to obtain an effective Hamiltonian for many-particle systems which we call the Two-Subsystem Groundstate Approximation (TSGSA). The method was inspired by the so-called Automated Multilevel Substructuring Method (AMLS). Originally, it

relies on subdividing the physical space into several regions. In these sub-systems the eigenproblem is solved, and the regions are combined in an adequate way. We developed a method to partition the state space of a many particle system in order to apply similar operations on the partitions. The tensorial structure of the Hamiltonians of these many-body systems make them even more suitable for this approach.

The method allows to break down the complexity of large many-body systems to the complexity of two spatial sub-systems having half the size. Considering the exponential size of the Hilbert space with respect to the system size this represents a huge advantage.

We will show applications of this method for ground-state calculations and for determining dynamical observables like the single-particle Green's function.

TT 31: SC: Tunnelling, Josephson Junctions

Time: Thursday 9:30–13:00 Location: H21

TT 31.1 Thu 9:30 H21

Tuning superconductivity by carrier injection — •P. Müller[1], Y. Koval[1], X. Y. Jin[1], C. Bergmann[1], Y. Simsek[1], L. Özyüzer[1], H. B. Wang[2], G. Behr[3], and B. Büchner[3] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany — [2]National Institute for Materials Science (NIMS), Tsukuba, Japan — [3]IFW-Dresden, Germany

In layered high-temperature superconductors, like $Bi_2Sr_2CaCu_2O_{8+\delta}$, superconductivity is controlled by carrier doping of the conducting planes. Usually this is achieved by a non-stoichiometric composition. Normally, current flow inside superconductors is never expected to be able to change the material itself. However, we were able to show that by extensive current injection along the c-axis the superconducting properties of $Bi_2Sr_2CaCu_2O_{8+\delta}$ can be changed effectively and reversibly. By injecting current perpendicular to the planes, we show that critical temperature, c-axis resistivity and critical current of intrinsic Josephson junctions can be tuned in a large range from underdoping to extreme overdoping. Apparently, the insulating layers are charged by injected carriers, and work as a floating gate. The result is hole doping of the conducting layers. This flash memory concept seems to be a general property of layered materials where the insulating charge reservoir layers are separated from the conducting planes.

TT 31.2 Thu 9:45 H21

Spectral Features in Current-Voltage Characteristis of Terahertz Wave Emitting $Bi_2Sr_2CaCu_2O_{8+d}$ Mesas — •Lütfi Özyüzer[1], Yilmaz Simsek[2], Hasan Köseoglu[1], Fulya Türkoglu[1], Yasemin Demirhan[1], Zeynep Meric[1], Cihan Kurter[3], Ulrich Welp[3], Ken E. Gray[3], Takashi Yamamoto[4], Kazuo Kadowaki[4], Yuri Koval[2], Huabing Wang[5], and Paul Müller[2] — [1]Izmir Institute of Technology, Izmir, Turkey — [2]University of Erlangen-Nürnberg, Germany — [3]Argonne National Laboratory, USA — [4]University of Tsukuba, Japan — [5]National Institute for Materials Science, Japan

Terahertz electromagnetic radiations are more versatile in sensing, imaging, and spectroscopy applications across the physical and biological sciences. There is still lack of coherent, continuous, tunable and compact solid-state sources of electromagnetic wave at THz frequency range. Although Josephson junctions are potential candidate, the mechanism of terahertz waves from intrinsic Josephson junctions of layered high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+d}$ (Bi2212) mesas is still unresolved. Large area mesas ranging from 100x300 to 40x300 μm^2 with various heights were formed on Bi2212. Current-voltage (I-V) and THz emission characteristics were obtained at various temperatures. Spectral features in I-V curves were investigated to find a correlation between emission frequency and feature energy.

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TT 31.3 Thu 10:00 H21

Terahertz emission from intrinsic Josephson junction stacks in high-Tc superconductors: effects of fabrication technique — •Y. Simsek[1], L. Özyüzer[1,2], S. Preu[3], D. Ploss[3], S. Malzer[3], Y. Koval[1], H. B. Wang[4], and P. Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany — [2]Department of Physics, Izmir Institute of Technology, Izmir, Turkey — [3]Max Planck Institute for the Science of Light, Erlangen, Germany — [4]National Institute for Materials Science (NIMS), Tsukuba, Japan

It was found recently that large area $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) mesas show terahertz emission due to intrinsic Josephson junctions (IJJ). We have fabricated large and tall Bi2212 mesas by optical and electron beam lithography, and studied effects of fabrication technique on THz emission characteristics. Monitoring the emission was performed with a Si composite bolometer, while the applied current through the IJJ stacks was slowly swept by a function generator. Emission peaks were observed on I-V return branches while the bias current was decreasing. The frequency of emission was determined by a terahertz interferometer. The observed emission frequencies match the frequency calculated by the cavity resonance condition.

TT 31.4 Thu 10:15 H21

Macroscopic quantum tunneling of $Bi_2Sr_2CaCu_2O_{8+\delta}$ intrinsic Josephson junctions modified by current injection — •X. Y. Jin, Y. Koval, Y. Simsek, C. Bergmann, C. Steiner, and P. Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

The properties of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals can be changed in a wide range by current injection along the *c*-axis. As a result, experiments can be carried out repeatedly on the same sample, only with its critical current density and critical temperature tuned electronically. Macroscopic quantum tunneling experiments were performed on intrinsic Josephson junctions after modification by current injection. A systematic change of the thermal-to-quantum crossover temperature corresponding to the change of critical current density has been observed. Dielectric properties of insulating layers after injection were determined based on microwave spectroscopy experiments. Samples of different structures and geometry have been studied to clarify the current injection mechanism in detail.

TT 31.5 Thu 10:30 H21

Macroscopic quantum properties of Josephson junctions with ferromagnetic interlayer — •Georg Wild[1,2], Christian Probst[1], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]Physik-Department, Technische Universität München, Garching

Josephson junctions with ferromagnetic interlayer have attracted much interest due to their potential application as π-phase shift elements in flux qubits. However, up to now it is not clear whether magnetic excitations in the ferromagnetic interlayer induce noise and thus prevent the application of these junctions in quantum circuits. To elucidate this question we have fabricated π-coupled $Nb/AlO_x/NiPd/Nb$ superconductor/insulator/ferromagnet/superconductor Josephson junctions and investigated the escape rate out of the zero voltage state into the voltage state. At high temperatures this escape is dominated by thermal activation, while below the crossover temperature $T^\star$ it is due to quantum tunneling. In this work we compare the experimentally determined crossover temperature $T^\star_{\rm exp}$ to the theoretically expected value $T^\star_{\rm th}$ to clarify the question whether low-lying excitations in the junction influence its quantum properties. We analyze the only free parameter, the plasma frequency ω_p, by means of Fiske resonance studies and via microwave spectroscopy experiments at mK temperatures.

This work was supported by the DFG via SFB 631 and the Excellence Cluster NIM.

TT 31.6 Thu 10:45 H21

Optimization of Nb/Al-AlO_x/Nb Technology for the Investigation of Fluxon Dynamics in Long Josephson Junctions — •Johannes M. Meckbach[1], Christoph Kaiser[1], Konstantin Il'in[1], Michael Siegel[1], Kai Buckenmaier[2], Tobias Gaber[2], Uta Kienzle[2], Hanna Sickinger[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

Underdamped long Josephson junctions (LJJs) are ideal systems for the investigation of fluxon dynamics. In LJJs the Josephson phase may vary on the length scale of λ_J, the Josephson penetration depth, and thus is very sensitive to defects in the structure. Inhomogeneities in the barrier can lead to a locally suppressed critical current density and parasitic resonances in the microwave spectra of the JJ. We have developed and optimized the process for Nb/Al-AlO_x/Nb based LJJs exhibiting an exceptionally high quality. We show spectroscopic measurements which confirm the uniformity of the AlO_x barriers.

In very long linear JJs, the bias current peaks at the edges while the central part of LJJs is left almost unbiased. This results in unusual $I_c(H)$ dependences with reduced $I_c(0)$ and hampers the control of (semi)fluxons situated near the center of LJJs. To optimize the bias feed circuitry, we have investigated a variety of bias line geometries (multiple lines, resistors, etc.) measuring the scaling of the maximum critical current over the JJ length. We discuss advantages and drawbacks of these designs.

TT 31.7 Thu 11:00 H21

Spectroscopy of fractional Josephson vortex molecules — •Edward Goldobin, Tobias Gaber, Kai Buckenmaier, Uta Kienzle, Hanna Sickinger, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut – Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

Using tiny current injectors we create κ discontinuities of the Josephson phase in a long Josephson junction. The junction reacts at the discontinuities by creating fractional Josephson vortices of size λ_J pinned at them. Such vortices carry the flux Φ, which is a fraction of the magnetic flux quantum $\Phi_0 \approx 2.07 \times 10^{-15}$ Wb. Being pinned, a fractional vortex has an eigenfrequency (localized mode), which depends on κ and applied bias current, and which lays within the plasma gap. If one considers a molecule consisting of several coupled fractional vortices, the eigenfrequency will split into several modes. We report on spectroscopy of a fractional vortex molecule performed in the thermal regime.

15 min. break

TT 31.8 Thu 11:30 H21

Charge transport across a single-Cooper-pair transistor coupled to a resonant transmission line — •Juha Leppäkangas[1,3], Yuri Pashkin[2], and Erkki Thuneberg[3] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]NEC Nano Electronics Research Laboratories and RIKEN Advanced Science Institute, Tsukuba, Ibaraki 305-8501, Japan — [3]Department of Physical Sciences, University of Oulu, FI-90014 Oulu, Finland

We have investigated charge transport in ultrasmall superconducting single and double Josephson junctions coupled to a transmission-line resonator. The microstrip resonator is naturally formed by the on-chip leads and the sample holder. We observe equidistant peaks in the transport characteristics of both types of devices and attribute them to the process involving simultaneous tunneling of Cooper pairs and photon emission into the resonator. The experimental data is well reproduced with the orthodox model of Cooper pair tunneling that accounts for the microwave photon emission into the resonator.

TT 31.9 Thu 11:45 H21

Non-linear current-voltage characteristics of NS-tunnel junctions prepared by focused ion beam induced deposition — •Dirk Klingenberger, Oleksandr Foyevtsov, Fabrizio Porrati, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main.

We used a focused Ga-ion beam and the precursor W(CO)6 –injected into a vacuum chamber nearby the focal area of the beam– to create tungsten containing superconducting deposits with a critical temperature of about 5.2 K. The deposits were fabricated onto oxidized aluminum contacts pre-patterned by UV-photolithography. I-V- and V-dI/dV- measurements have been performed between 0.3 K and 6 K using a He3-cryostat. For selected beam energies used during deposition the samples show Josephson-junction like behaviour or tunneling of quasiparticles for temperatures below the superconducting transition of aluminum at about 2 K. In the temperature range between the superconducting transitions of the two electrodes Andreev-reflection was observed.

TT 31.10 Thu 12:00 H21

Analytical calculation of the excess current in the Octavio-Tinkham-Blonder-Klapwijk theory — •Gabriel Niebler[1,2], Gianaurelio Cuniberti[2], and Tomáš Novotný[1] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague 2, Czech Republic — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

We present an analytical derivation of the excess current in Josephson junctions within the Octavio-Tinkham-Blonder-Klapwijk theory for both symmetric and asymmetric barrier strengths. We confirm the result found numerically by Flensberg *et al.* for equal barriers [*Physical Review B* **38**, 8707 (1988)], including the prediction of negative excess current for low transparencies, and we generalize it for differing barriers. Our analytical formulae provide for convenient fitting of experimental data, also in the less studied, but practically relevant case of barrier asymmetry.

TT 31.11 Thu 12:15 H21

Small charge solitons in 1D arrays of Josephson junctions — •Alexander Shnirman[1], Stephan Rachel[2], Jens Homfeld[1], and Ivan Protopopov[1] — [1]Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Phyiscs, Yale University, New Haven, USA

We identify the new parameter regime within the Coulomb blockade (insulating) phase of a 1D array of coupled JJs. It is defined by the condition $\Lambda E_J > E_C > E_J$, where E_C and E_J are the charging and the Josephson energies of the junction, respectivly, and Λ is the bare screening length (measured in number of junctions). In this regime we investigate the dynamics of charge solitons and demonstrate two surprising features: i) flattening of the dispersion relation in the outer region of the Brillouin zone; ii) broadening of the soliton in the flat band regime in contrast to the expected and observed Lorenz contraction in the regime of regular dispersion relation.

TT 31.12 Thu 12:30 H21

Temporal dynamics of a chain of Josephson junctions in the Coulomb blockade regime. — •Jared Cole and Michael Marthaler — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany

Recent experiments have studied the transport of individual charge carriers through a one-dimensional array of small Josephson junctions, in the limit of small Josephson coupling. Modern time resolved charge detection techniques allow the direct measurement of temporal correlations between these carriers. We study such a system theoretical with the aim of understanding the transport properties within the array, in both the normal and superconducting regimes. Of particular interest are the effects of Coulomb repulsion between the carriers and the resulting transport through the array.

TT 31.13 Thu 12:45 H21

Dynamical bistability in driven Josephson circuits - the WKB limit and beyond. — •Vittorio Peano and Michael Thorwart — FRIAS Albert-Ludwigs-Universität, Freiburg, Deutschland

Driven and dissipative nonlinear quantum oscillators can be operated in a regime where a bistability is induced dynamically. Prominent examples are the Josephson bifurcation amplifier and the driven circuit QED set-up of the superconducting transmon qubit. Josephson circuits with their large quality factors and scalable nonlinearities are the perfect playground to explore this phenomenon from the classical limit down to the quantum scale. We show that the WKB approximation is an excellent tool in all these regimes. We explore its limit of validity, focusing thereby on the quantum Duffing oscillator and the driven circuit QED.

TT 32: MLT: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ... 2

Time: Thursday 14:00–18:00 Location: H18

TT 32.1 Thu 14:00 H18

Interaction Quenches of Fermi Gases — •Götz S. Uhrig — Lehrstuhl Theoretische Physik I, TU Dortmund, 44221 Dortmund

Progress in the manipulation of fermionic atoms in optical lattices makes it possible to switch interactions at will. So non-equilibrium issues gain increasing interest. It is shown that the jump in the momentum distribution of Fermi gases evolves smoothly for small and intermediate times once an interaction between the fermions is suddenly witched on. The jump does not vanish abruptly. Explicit calculations are possible for the Tomonaga-Luttinger model with and without spin. For general interacting models in arbitrary dimension the structure of the equations of motion in the Heisenberg picture is analyzed. It is found that the loci in momentum space where the jumps occur are those of the noninteracting Fermi sea. No relaxation of the Fermi surface geometry takes place.

TT 32.2 Thu 14:15 H18

Generalized Gibbs ensemble prediction of prethermalization plateaus in nearly integrable systems — •Marcus Kollar[1], F. Alexander Wolf[1], and Martin Eckstein[2] — [1]Theoretische Physik III, Universität Augsburg, 86135 Augsburg — [2]Theoretische Physik, ETH Zürich, 8093 Zürich, Schweiz

A quantum many-body system which is prepared in the ground state of an integrable Hamiltonian will not directly thermalize after a sudden small parameter change away from integrability. Instead, it first reaches a quasistable prethermalized state, which can be related to the perturbative ground state of the Hamiltonian after the quench [1]. We show that under certain conditions such prethermalization plateaus are predicted correctly by generalized Gibbs ensembles, which are the appropriate extension of standard statistical mechanics in the presence of many constants of motion. As a consequence, the relaxation behaviors of integrable and nearly integrable systems are continuously connected and described by the same statistical theory. For example, our result applies to the prethermalization plateau of the fermionic momentum distribution that is observed after a quench from zero to small Hubbard interaction [1,2].

[1] M. Moeckel and S. Kehrein, Ann. Phys. **324**, 2146 (2009).
[2] M. Eckstein, M. Kollar, and P. Werner, Phys. Rev. Lett. **103**, 056403 (2009); arXiv:0910.5674.

TT 32.3 Thu 14:30 H18

Prethermalization and nonequilibrium BCS dynamics in ultracold Fermi gases — •Michael Möckel[1] and Stefan Kehrein[2] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching — [2]Department für Physik and Arnold-Sommerfeld-Center, LMU München, Theresienstr. 37, 80333 München

Dynamical experiments with ultracold fermions in optical lattices are a growing field of research for which the time dependent (Fermi-) Hubbard model provides a paradigmatic description. Moreover, predictions on the nonequilibrium behavior of the BCS Hamiltonian have been made; the later describes effectively fermionic pair processes which are contained in the much richer structure of the Hubbard Hamiltonian. This newly motivates the question whether nonequilibrium BCS dynamics can be excited by a nonadiabatic switching of the Hubbard interaction without overheating the system.

Starting from an uncorrelated Fermi gas at zero temperature and in d>1 dimensions, we apply a nonadiabatic, linear and weak ramp of the Hubbard interaction. This allows us to investigate the nonequilibrium properties of a Fermi liquid beyond the adiabatic switching requirement of Landau's theory. We study the real-time evolution of the excited state after the ramping and observe that the relaxation time scales for the kinetic energy and the momentum distribution separate. Therefore a transient regime of prethermalization arises. During that regime the momentum distribution continues to show a discontinuity around the Fermi energy, indicating zero temperature. The delay of thermalization simplifies experimental observations.

Invited Talk TT 32.4 Thu 14:45 H18

Dispersion of the Excitations of Fractional Quantum Hall States — •Jurgen Smet[1], Igor Kukushkin[1,2], Vito Scarola[3,4], Vladimir Umansky[5], and Klaus von Klitzing[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Russia — [3]Department of Chemistry and Pitzer Center for Theoretical Chemistry, University of California at Berkeley, USA — [4]Theoretische Physik, ETH Zürich, Switzerland — [5]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel

The rich correlation physics in two-dimensional (2D) electron systems is governed by the dispersion of its excitations. In the fractional quantum Hall regime, excitations involve fractionally charged quasi particles, which exhibit dispersion minima at large momenta referred to as rotons. These rotons are difficult to access with conventional techniques because of the lack of penetration depth or sample volume. Our method overcomes the limitations of conventional methods and traces the dispersion of excitations across momentum space for buried systems involving small material volume. We used surface acoustic waves, launched across the 2D system, to allow incident radiation to trigger these excitations at large momenta. Optics probed their resonant absorption. Our technique unveils the full dispersion of such excitations of several prominent correlated ground states of the 2D electron system, which has so far been inaccessible for experimentation.

TT 32.5 Thu 15:15 H18

Massless Dirac-Weyl Fermions in a $\mathcal{T}_3$ Optical Lattice — •Daniel Urban[1,2], Dario Bercioux[1,3], Hermann Grabert[1,3], and Wolfgang Haeusler[1,4] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Departamento de Física de la Materia Condensada C-XII, Facultad de Ciencias, Universidad Autónoma de Madrid, E-28049, Madrid, Spain — [3]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [4]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

We propose an experimental setup for the observation of quasi-relativistic massless Fermions. It is based on a $\mathcal{T}_3$ optical lattice, realized by three pairs of counter-propagating lasers, filled with fermionic cold atoms. We show that in the long wavelength approximation the $\mathcal{T}_3$ Hamiltonian generalizes the Dirac-Weyl Hamiltonian for the honeycomb lattice, however, with a larger value of the pseudo-spin $S = 1$. In addition to the Dirac cones, the spectrum includes a dispersionless branch of localized states producing a finite jump in the atomic density. Furthermore, implications for the Landau levels are discussed.
Bercioux *et al.*, Phys. Rev. A (2009) *in press*, arXiv:0909.3035.

TT 32.6 Thu 15:30 H18

Resonant Superfluidity in an Optical Lattic — •Irakli Titvinidze[1], Michiel Snoek[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Institute for Theoretical Physics, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

We study a system of ultracold fermionic Potassium (^{40}K) atoms in a three-dimensional optical lattice in the neighborhood of an s-wave Feshbach resonance. Close to resonance, the system is described by a multi-band Bose-Fermi Hubbard Hamiltonian. We derive an effective lowest-band Hamiltonian in which the effect of the higher band is incorporated by a self-consistent mean-field approximation. The resulting model is solved by means of Generalized Dynamical Mean-Field Theory [1,2]. In addition to the BEC/BCS crossover we find on the BCS side of the resonance a phase transition to a fermionic Mott insulator at half filling, induced by the repulsive fermionic background scattering length. We also calculate the critical temperature of the BEC/BCS-state across the resonance and find it to be minimal at resonance.

15 min. break

TT 32.7 Thu 16:00 H18

Strongly correlated fermions in disordered lattices — •Denis Semmler[1], Krzysztof Byczuk[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany — [2]Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland

Strongly correlated fermions in a lattice exposed to a disorder potential are investigated by means of the Anderson-Hubbard model.

We employ the statistical dynamical mean-field theory, which incorporates both fluctuations due to disorder and local correlations due to interactions. In the case of binary disorder, the complete paramagnetic ground state phase diagram is obtained, which consists of disordered correlated metal, Anderson-Mott insulator and band insulator [1]. Binary disordered fermions can be realized by loading two species of atoms into an optical lattice of which one is immobile [2]. Furthermore, we investigate the effect of realistic speckle disorder in combination with hopping disorder, which is relevant for future experiments within the framework of ultracold atoms in optical lattices. [1] D. Semmler, K. Byczuk, and W. Hofstetter, arXiv:0911.0934.

[2] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock and K. Bongs, Phys. Rev. Lett. **96**, 180403 (2006).

TT 32.8 Thu 16:15 H18

Strong coupling expansion in the bosonic dynamical mean-field theory — •Anna Kauch[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, PL-00-681 Warszawa, Poland

The bosonic dynamical mean-field theory (B-DMFT), recently formulated by Byczuk and Vollhardt (Phys. Rev. B **77**, 235106 (2008)), 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 lattice bosonic problem is replaced by a single impurity coupled to two bosonic baths (corresponding to normal and condensed bosons, respectively). This yields a set of B-DMFT equations which have to be solved self-consistently. We propose here an approximate method to solve the B-DMFT equations for the bosonic Hubbard model by performing a strong-coupling perturbation expansion (linked-cluster expansion) around the atomic limit. We investigate the validity of this approach by comparing our results to the known phase diagram of the Hubbard model.

TT 32.9 Thu 16:30 H18

Multiflavour fermions in optical lattices — •Antonio Privitera[1], Irakli Titvinidze[1], Soon-Yong Chang[2], Andrew Daley[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, and IQOQI, A-6020 Innsbruck, Austria

We study the properties of three-flavor fermions [1,2] in a optical lattice with and without a (dynamically generated) large three-body repulsion. This can be induced in the form of a hard-core constraint by three-body losses [3]. We address the properties of this system by using dynamical mean-field theory and variational Monte Carlo technique. The phase diagram of the system is very rich and shows a strong interplay between magnetization and superfluidity. Without including the three-body repulsion, the system undergoes a quantum phase transition from a color superfluid to a trionic phase [4], which displays additional CDW modulation at half-filling. This transition is washed out when including a large three-body repulsion, in which case the system is always in the superfluid phase. In this latter case the color superfluid shows a strong tendency to fully polarize at strong coupling in marked contrast with the unconstrained case where the unpolarized trionic phase dominates.

[1] T.Ottenstein *et al.*, Phys. Rev. Lett. **101**, 203202 (2008)
[2] J. H. Huckans *et al.* Phys. Rev. Lett. **102**, 165302 (2009)
[3] A.Kantian *et al.*, arXiv:0908.3235
[4] A. Rapp *et al.*, Phys. Rev. B **77**, 144520 (2008)

TT 32.10 Thu 16:45 H18

Néel transition of fermionic atoms in an optical trap: real-space DMFT study — •Elena Gorelik and Nils Blümer — Institut für Physik, Universität Mainz, Mainz, Germany

We study theoretically the magnetic ordering transition for a system of repulsively interacting fermionic atoms harmonically trapped in a three-dimensional optical lattice. The real-space DMFT approach [1] combined with Hirsch-Fye quantum Monte Carlo (QMC) impurity solver is used to explore the temperature effects on the ordering phenomena, and to establish signatures of Néel transitions in experimentally accessible observables. We also provide estimates of the entropy for the calculated systems.

[1] M. Snoek et al., New Journal of Physics **10**, 093008 (2008).

TT 32.11 Thu 17:00 H18

Bose Josephson junction out of equilibrium — •Anna Posazhennikova[1], Mauricio Trujillo-Martinez[2], and Johann Kroha[2] — [1]Fachbereich Physik M703, Universitaet Konstanz, Konstanz, D-78457, Germany — [2]Physikalisches Institut adn Bethe Center for Theoretical Physics, Universitaet Bonn, Nussallee 12, D-53115 Bonn, Germany

We perform a detailed quantum dynamical study of nonequilibrium Josephson oscillations between interacting Bose-Einstein condesates confined in a double-well trap. We find, that the Josephson junction can sustain multiple undamped Josephson oscillations up to a certain characteristic time-scale, without quasiparticles being excited in the system. This might explain recent experimental data. Beyond the characteristic time scale the dynamics of the Josephson junction is governed by fast, quasiparticle assited Josephson tunneling as well as Rabi oscillations between the descrete quasiparticle levels. We predict, that an initially self-trapped state of the Bose Josephson junction will be destroyed by these fast oscillations.

TT 32.12 Thu 17:15 H18

Phonon-assisted currents of fermions in Bose–Fermi mixtures — •Martin Bruderer, Anna Posazhennikova, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We present an analysis of Bose–Fermi mixtures in optical lattices for the case where a static force is applied to the fermions, and the bosons (in the superfluid phase) are described by Bogoliubov phonons. Accordingly, the static force lifts the degeneracy of the energy levels in the lattice potential and the fermionic states form a Wannier–Stark ladder. We show that the Bogoliubov phonons enable hopping transitions between different Wannier–Stark states; these transitions are accompanied by energy dissipation into the superfluid and result in a net fermionic current along the lattice. We determine the dependence of the fermionic current on the static force and find that the phonon density of states strongly affects the emergent current. In particular, if the energy splitting between the Wannier–Stark states exceeds the width of the phonon band, then the current is strongly suppressed. This effect should be observable in a realistic experimental set-up.

TT 32.13 Thu 17:30 H18

Luttinger liquid of trimers in the asymmetric Fermi Hubbard model — •Giuliano Orso[1], Evgeni Burovski[2], and Thierry Jolicoeur[2] — [1]LMU Muenchen, Germany — [2]LPTMS, University of Paris South, France

We investigate attractive fermions in a one dimensional optical lattice with unequal tunneling rates [1]. Due to the mass asymmetry, the microscopic model is not integrable and multi-particle bound states appear. We focus on trimers, namely three-body bound state made of one light and two heavy fermions. We first present the exact solution of the three-body problem, yielding the binding energy and the effective mass of a single trimer. Based on DMRG simulations, we then show that trimers can open an energy gap at finite commensurate densities, leading to a suppression of superconducting correlations and topological changes in the grand-canonical phase diagram. [1] G. Orso, E. Burovski and T. Jolicoeur, arXiv:0907.1533

TT 32.14 Thu 17:45 H18

Universal Onset of Quantum Turbulence in Oscillating Flows and Crossover to Steady Flows — Risto Hänninen[1] and •Wilfried Schoepe[2] — [1]Helsinki University of Technology — [2]Regensburg University

The critical velocity v_c for the onset of quantum turbulence in oscillatory flows of superfluid helium is universal and scales as $v_c \sim \sqrt{\kappa \cdot \omega}$, where κ is the circulation quantum and ω is the oscillation frequency. This result can be derived from a general argument based on the "superfluid Reynolds number". Only the numerical prefactor may depend somewhat on the geometry of the oscillating object because the flow velocity at the surface of the object may differ from the velocity amplitude of the body. A more detailed analysis derived from the dynamics of the turbulent state gives $v_c \approx \sqrt{8\kappa\,\omega/\beta}$, where $\beta \sim 1$ depends on the mutual friction parameters. This universality is compared with the recently discovered universality of classical oscillatory flows. We also discuss the effect of remanent vorticity on the onset of quantum turbulence. Finally, by employing the "superfluid Reynolds number" again, we argue how v_c changes when the steady case $\omega = 0$ is approached. In that case v_c scales as κ/R, where R is the size of the object.

TT 33: TR: Nanoelectronics I: Quantum Dots, Wires, Point Contacts 2

Time: Thursday 14:00–18:00 Location: H19

TT 33.1 Thu 14:00 H19

Negative tunneling magneto-resistance in spin-polarized transport across carbon nanotubes — •Sonja Koller[1], Jens Paaske[2], and Milena Grifoni[1] — [1]Universität Regensburg — [2]Nano-Science Center, University of Copenhagen

From experiments on carbon nanotube single electron transistors with ferromagnetic, collinearly polarized leads, it is known that the tunneling magneto-resistance (a measure for the ratio of current in the parallel to current in the anti-parallel contact configuration) exhibits a strong dependence on the gate voltage. In particular, for certain gate regions, the anti-parallel current can even exeed the parallel one, leading to negative values of the tunneling magneto-resistance. The origin of this effect are tunneling induced level shifts, that we are able to calculate theoretically within a diagrammatic perturbation approach to transport across quantum dots, by inclusion and summation of certain diagram types to all orders. A qualitative agreement with the experiment is obtained.

TT 33.2 Thu 14:15 H19

Spin-Orbit Effects in Carbon-Nanotube Double Quantum Dots — •Stephan Weiss[1], Emmanuel Rashba[2,3], Ferdinand Kuemmeth[2], Hugh Churchill[2], and Karsten Flensberg[1] — [1]Niels Bohr Institute & Nano-Science Center, University of Copenhagen — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA — [3]Center for Nanoscale Systems, Harvard University, Cambridge, Massachusetts 02138, USA

We study the spectrum of a carbon nanotube double quantum dot with one and two electrostatically confined electrons in the presence of spin-orbit and Coulomb interactions [1]. Compared to GaAs dots the spectrum exhibits a richer structure due to the valley degree of freedom in nanotubes. Starting with the envelope function approach near the graphene Dirac point, we numerically diagonalize the two particle Hamiltonian and explain its spectrum in terms of spin and orbital singlets and triplets. We also show how spin-orbit effects compete with finite exchange Coulomb interactions at weak magnetic fields. Inspired by recent experiments that measured the relaxation and dephasing times of Kramers doublets in nanotube quantum dots, we investigate the transition between (02) $\leftrightarrow$ (11)-configurations as a function of the inter-dot detuning.

[1] S. Weiss, E.I. Rashba, F. Kuemmeth, H.O.H. Churchill, and K. Flensberg, in preparation

TT 33.3 Thu 14:30 H19

Vibration-assisted transport properties of suspended carbon nanotube quantum dots. — •Abdullah Yar, Andrea Donarini, Sonja Koller, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg,Germany

We investigate the transport properties of suspended armchair single-wall carbon nanotubes (SWNTs) weakly coupled to leads. In the low energy regime, such nano-electromechanical systems behave as quantum dot systems being highly sensitive to the influence of few vibrational modes. We performed a microscopic analysis of suspended metallic SWNTs and included Coulomb interaction effects beyond mean-field, by using bosonization techniques, yielding the spectrum and eigenfunctions of the isolated finite length SWNT. The theory predicts that strong electron-vibron coupling strongly suppresses the current flow at low biases, a collective behavior known as Franck-Condon blockade, in spite of the symmetric coupling to the leads. At larger values of the bias voltage interference between degenerate states can yield a characteristic current suppression.

TT 33.4 Thu 14:45 H19

Competing carbon nanotube quantum dots with different screening properties — •Karin Goss[1,3], Carola Meyer[1,3], Maarten R. Wegewijs[2,3], and Claus M. Schneider[1,3] — [1]Institute of Solid State Research (IFF-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Solid State Research (IFF-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA Jülich Aachen Research Alliance

We report quantum transport measurements on a carbon nanotube (CNT) quantum dot in the single electron tunneling regime. In addition to standard nanotube shell-filling effects, the stability diagram shows resonances in the Coulomb blockade regime. These resonances are not due to inelastic cotunneling through a single CNT as their finite slope and anomalous anticrossing with the diamond edges indicate. Instead, atomic force microscopy images suggest that the contacted device consists of a rope of nanotubes, based on the rather large diameter of ca. 7nm. In a constant interaction picture the observed transport phenomena can be attributed to two nanotubes acting as coupled quantum dots. The anticrossings of the additional resonances with the diamond edges indicate hybridization of states of the two dots. The difference of both the asymmetry of tunneling and screening properties between the two dots allows this hybridization to be probed.

TT 33.5 Thu 15:00 H19

Quantum Ratchets Driven by Tunnel Oscillations — •Sigmund Kohler and Michael Stark — Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

The ratchet 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. In the usual description, it is assumed that the ratchet is driven by a classical field, while the corresponding backaction can be ignored. Here we address the question whether the tunnel oscillations of a biased double quantum dot can be employed as driving source. Since such a driving source itself behaves quantum mechanically, its dynamics will be influenced by the ratchet and, thus, should be treated as a further degree of freedom. As a model, we use two capacitively coupled double quantum dots: a biased one that provides the ac force and an asymmetric, unbiased one that acts as ratchet in the predominantly coherent quantum regime. It turns out that the two-electron states of the coupled drive-pump Hamiltonian leave their fingerprints in the ratchet current.

TT 33.6 Thu 15:15 H19

High frequency pulsed-gate technique for the measurement of tunneling and relaxation rates in coupled quantum dots — •Daniel Harbusch[1], Stephan Manus[1], Peter Tranitz[2], Werner Wegscheider[3], and Stefan Ludwig[1] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, München, Germany — [2]Institut für Experimentelle Physik, Universität Regensburg, Regensburg, Germany — [3]Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland

Tunneling frequencies and charge relaxation rates in a double quantum dot (QD) are directly probed by pulsing control gates of the double QD and measuring average charge occupations using a nearby quantum point contact (QPC) as detector.

Our nano-devices are electrostatically defined in the two-dimensional electron system of a GaAs/AlGaAs heterostructure. All measurements are performed at an electron temperature about T $\approx$ 100 mK.

Our broadband sample holder is based on impedance matched micro strip lines optimized for pulsed gate experiments, covering the large bandwidth from dc to 18 GHz. We pulse individual gates of a double or triple QD occupied with only few electrons at pulse widths down to 150 ps and demonstrate a variety of applications. We directly measure tunneling and energy relaxation rates. Our results show the suitability of the setup for future experiments on the coherent charge transport of single electrons in a triple QD.

TT 33.7 Thu 15:30 H19

An electron avalanche amplifier in a two-dimensional electron system — •Daniela Taubert[1], Georg Schinner[1], Hans-Peter Tranitz[2], Werner Wegscheider[3], and Stefan Ludwig[1] — [1]Center for NanoScience and Fakultät für Physik, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [3]Solid State Physics Laboratory, ETH Zurich, 8093 Zurich, Switzerland

A biased quantum point contact - a device that is widely used as detector of single electrons in quantum dot circuits - and its back-action on the quantum dots can only be fully understood if the relaxation mechanisms of the excited hot electrons emitted into its leads are known. We therefore study the behavior of hot electrons in two-dimensional mesoscopic structures, thereby considering a wide range of electron

energies.

We observe scattering of excited charge carriers with the degenerate Fermi sea in a three-terminal device. Amplification of the injected electron current can be achieved by energetically separating the electrons excited from the Fermi sea from the conduction band holes they leave behind by means of a barrier. The observed amplification effect depends on the energy of the injected electrons, the injected current, and the height of the barrier used for separating electrons and holes. Our analysis is based on an energy-dependend electron-electron scattering length as well as neutralization of holes.

TT 33.8 Thu 15:45 H19

Adiabatic pumping through a double quantum dot with Coulomb interaction — •Roman-Pascal Riwar and Janine Splettstoesser — Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany

We consider adiabatic pumping through a double quantum dot coupled to normal metal or ferromagnetic contacts by means of a real-time diagrammatic approach, performing a rigorous expansion in the weak coupling regime. The electrons in the serially aligned dots, which are subject to Coulomb repulsion, are pumped by alternating the left and right dot energy levels. In the case of weak inter-dot coupling we observe tunnel-induced renormalisation effects due to a coherent superposition of pseudospin states. Real spin effects are seen when arbitrarily polarised ferromagnets are attached to the double dot, where we investigate the limit of strong inter-dot coupling. In particular, we study the spin valve effect which can be reversed in the pumping current.

15 min. break

TT 33.9 Thu 16:15 H19

Thermopower of a Cooper pair splitter — •Jens Siewert[1,2] and Evgeny Ya. Sherman[1,2] — [1]Departamento de Química Física, Universidad del País Vasco , Apdo. 644, 48080 Bilbao, Spain — [2]Ikerbasque, Basque Foundation for Science, Alameda Urquijo 36, 48011 Bilbao, Spain

A Cooper pair splitting device has been realized recently by connecting two quantum dots (formed by InAs nanowires [1] and single-wall carbon nanotubes [2]) to a single superconducting source electrode and two normal-conducting drain electrodes. The electrostatic potentials of the dots can be tuned by means of gate voltages. The dominant transport process at low temperatures and bias voltages is coherent Cooper-pair tunneling ('Andreev tunneling'). We study transport in this device at finite temperatures in the framework of a simple tunneling Hamiltonian model taking into account an extra tunneling term between the two quantum dots and possible asymmetries between the tunneling rates to the leads. We calculate the thermopower and address the question whether it provides a possibility to experimentally access the contribution of the crossed Andreev reflection process.

[1] L. Hofstetter, S. Csonka, J. Nygard, and C. Schönenberger, Nature **461**, 960 (2009).

[2] L.G. Herrmann, F. Portier, P. Roche, A. Levy Yeyati, T. Kontos, and C. Strunk, e-print arxiv0909.3243 (2009).

TT 33.10 Thu 16:30 H19

Two-Particle Nonlocal Aharonov-Bohm Effect from Two Single-Particle Emitters — •Janine Splettstoesser[1,3], Michael Moskalets[2], and Markus Buttiker[3] — [1]Institut für Theoretische Physik A, RWTH Aachen University, D-52074 Aachen — [2]Department of Metal and Semic. Physics, NTU Kharkiv Polytechnic Institute, 61002 Kharkiv, Ukraine — [3]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

High-frequency single-particle emitters have been realized experimentally in the integer quantum Hall effect regime [1]. These tools allow for the implementation of complex interferometers in mesoscopic systems showing two-particle interference effects. In the work presented here we explore the entanglement production from two uncorrelated sources. We therefore propose a mesoscopic circuit in the quantum Hall effect regime comprising two independent single-particle sources and two distant Mach-Zehnder interferometers with magnetic fluxes. This and the tunability of the single-particle sources allow in a controllable way to produce orbitally entangled electrons [2]. Two-particle correlations appear as a consequence of erasing of which-path information due to collisions taking place at distant interferometers and in general at different times. The two-particle correlations manifest themselves as an Aharonov-Bohm effect in the noise. In an appropriate time-interval the concurrence reaches a maximum, proving the existence of time-bin entanglement.

[1] G. Fève, et al., Science 316, 1169 (2007).

[2] J. Splettstoesser, M. Moskalets, and M. Buttiker, Phys. Rev. Lett. 103, 076804 (2009).

TT 33.11 Thu 16:45 H19

Tunneling into Nonequilibrium Luttinger Liquid with Impurity — •Stéphane Ngo Dinh[1,2], Dmitry A. Bagrets[3], and Alexander D. Mirlin[1,2,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

We evaluate tunneling rates into/from a quantum wire containing a weak backscattering defect and biased by a voltage U. Interacting electrons in such a wire constitute a true *nonequilibrium* state of the Luttinger liquid (LL). This state is created due to inelastic electron backscattering leading to the emission of nonequilibrium plasmons with typical frequency $\hbar\omega \leq eU$. Using a real-time instanton approach we show that the tunneling rates are split into two edges. The tunneling exponent at the Fermi edge E_F is *positive* and equals that of the equilibrium LL, while the exponent at the side edge $E_F - eU$ is *negative* if Coulomb interaction is not too strong. We also calculate the nonequilibrium dephasing rate that governs the smearing of the power-law singularities.

The approach developed here will be useful for the analysis of tunneling and interference in a broad class of nonequilibrium LL structures with impurities and/or tunneling couplings.

TT 33.12 Thu 17:00 H19

Anisotropic exchange coupling in double quantum dots — •Fabio Baruffa[1], Peter Stano[2], and Jaroslav Fabian[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]Institute of Physics, Slovak Academy of Science, Bratislava, Slovak Republic

The electron spins in quantum dots are one of the candidates as a qubit for quantum computation [1]. In coupled quantum dots, the two-qubit quantum gate is realized by manipulating the exchange coupling which is due to the Coulomb interaction and the Pauli principle. The presence of the spin-orbit couplings change the magnitude of the exchange and lead to new term due to the lack of the spin-rotational symmetry, the anisotropic exchange [2]. We propose an accurate effective spin Hamiltonian for modeling spin-orbit-induced spin dynamics in the presence of the magnetic field [3]. We have also performed numerically exact calculations of the isotropic and anisotropic exchange coupling in realistic two-electron GaAs coupled quantum dots in the presence of both Dresselhaus and Bychkov-Rashba spin-orbit interactions [4]. The numerics allow us to establish the goodness of our model and to see the limits of previous statements. Furthermore we find that in zero magnetic field the second-order spin-orbit effects are absent at all interdot couplings. This work was supported by the DFG GRK 638.

[1] D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998)
[2] K. V. Kavokin, Phys. Rev. B 64, 075305 (2001)
[3] F. Baruffa, P. Stano and J. Fabian, cond-mat/0908.2961
[4] J. Fabian et al., Acta Phys. Slov. 57, 565 (2007)

TT 33.13 Thu 17:15 H19

Spin Relaxation in Silicon based Quantum dots — •Martin Raith[1], Peter Stano[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Physics, Slovak Academy of Sciences, 84511 Bratislava, Slovak Republik

Recent progress in manufacturing top-gated quantum dots based on Si/SiGe or Si/SiO_2 systems emphasized the importance of silicon as a possible host material for the creation of spin qubit arrays and the associated idea proposed by Loss and DiVincenzo (1998) for the realization of a quantum computer. Silicon is of special interest because of its small spin-orbit coupling and the availability of isotopes with zero nuclear spin. Therefore silicon based quantum dots imply long spin lifetimes and yield promising candidates for quantum information processing. We provide quantitative results of the characteristic energies in the presence of spin-orbit coupling and phonon-induced spin relaxation times for realistic silicon based single and double dot sys-

tems using analytical models and numerical methods. This work is supported by the DFG SPP 1285.

TT 33.14 Thu 17:30 H19

Control of Spin Blockade by AC Magnetic Fields in Triple Quantum Dots — •Maria Busl[1], Rafael Sánchez[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales Madrid, CSIC, 28049 Cantoblanco Madrid, Spain — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We analyze theoretically transport through a triangular triple quantum dot (TQD) determined by the interplay of coherent phenomena coming from dc and ac magnetic fields. A dc magnetic field applied perpendicularly to the dot area induces a flux Φ. In triangular TQDs with one extra electron, it was shown [1, 2] that current can be blocked when the electron drops into an eigenstate that is decoupled from transport, a so-called dark state. This blocking in turn can be destroyed by the flux piercing the TQD. We show that in a triangular TQD with two extra electrons, current will be blocked either by the formation of a two-electron dark state or by Pauli spin blockade, depending on the flux Φ. Spin blockade can be broken by ac magnetic fields, and a finite current can be generated [3]. Unexpectedly however, we demonstrate that an ac magnetic field is not only able to break spin blockade but also to induce it again, at a particular field frequency ω. Hence applying an ac magnetic field is a way of *controlling* spin blockade in a TQD [4].

[1] C. Emary, Phys. Rev. B **76**, 245319 (2007).
[2] M. Busl *et al.*, Physica E (in press).
[3] F.H.L. Koppens *et al.*, Nature **442**, 766 (2006).
[4] M. Busl *et al.*, arXiv:0907.0182.

TT 33.15 Thu 17:45 H19

Generation and detection of spin-polarized currents via double quantum dot structures — •Stefan Maier[1], Jan P. Dahlhaus[1,2], and Andreas Komnik[1] — [1]Ruprecht-Karls-Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We propose a setup for generation and detection of spin-polarized currents. The structure we use is a double quantum dot with parallel topology. The filtering mechanism is based on the anti-resonance structure in the transmission coefficient. We show that the device remains fully operable also in the case of not too strong inter- as well as intradot electronic correlations. We discuss how the coupling asymmetry and finite temperature may affect the efficiency of the device and present estimations for the relevant device parameters necessary for its experimental realization.

TT 34: SC: Iron-Based Superconductors - 122

Time: Thursday 14:00–17:30 Location: H20

TT 34.1 Thu 14:00 H20

Photoemission in Ferropnictides — •Klaus Koepernik and Helmut Eschrig — IFW Dresden, Germany

High resolution angle resolved photoemission spectroscopy yields the most direct and most detailed information on the electronic structure of solids. This opens the opertunity to really compare theoretical band structures with experiment. However, the method is surface sensitive. For the ferro-pnictides highly resolved data are available, which are re-evaluated on the basis of density functional calculations.

TT 34.2 Thu 14:15 H20

Superconductivity induced anomalies in the dielectric response of $Ba_{0.68}K_{0.32}Fe_2As_2$ identified by spectral ellipsometry. — •Aliaksei Charnukha, Paul Popovich, Yulia Matiks, Oleg Dolgov, Alexander Yaresko, Dunlu Sun, Chengtian Lin, Bernhard Keimer, and Alexander Boris — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, Stuttgart, 70569 Deutschland

Spectroscopic ellipsometry was used to study the dielectric function of a hole-doped $Ba_{0.68}K_{0.32}Fe_2As_2$, with a sharp ($\Delta T < 0.6$ K) transition to the SC state below $T_c \approx 38.5$ K, in the spectral range $0.012 - 6.5$ eV at temperatures $7 - 300$ K. The optical conductivity spectra are dominated by a series of interband transitions, which all agree well with the predictions of LDA calculations. Our results provide clear evidence of SC gap formation in the far-infrared optical conductivity spectra, $2\Delta_{SC} \approx 5.5-6.5\ k_BT_c$. We find the penetration depth to be 1600 Å in close agreement with the values determined by other techniques. The data also provide detailed information about the evolution of the optical self-energy in the normal and SC states. The frequency and temperature dependencies of the SC gap formation speak for the extended $s_\pm-$wave pairing symmetry with strong coupling to the intermediate boson mode centered at $\approx$ 25meV. Examination of the conductivity in the optical spectral range uncovered superconductivity-induced suppression of interband transitions at energies more than $200\Delta_{SC}$.

TT 34.3 Thu 14:30 H20

Band and momentum dependent electron dynamics in superconducting $Ba(Fe_{1-x}Co_x)_2As_2$ — •Bernhard Muschler[1], Wolfgang Prestel[1], Rudi Hackl[1], Thomas P. Devereaux[2], Jiun-Haw Chu[3], James G. Analytis[3], and Ian R. Fisher[3] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching — [2]SIMES, SLAC, Menlo Park, CA 94025, USA — [3]GLAM, Stanford University, CA 94304, USA

We report results of electronic Raman scattering (ERS) experiments on high quality single crystals of $Ba(Fe_{1-x}Co_x)_2As_2$ in the normal and superconducting states. With a light penetration depth of approximately 30 nm ERS is bulk sensitive. ERS highlights different regions in the Brillouin zone (BZ) for different combinations of the incoming and outgoing photon polarizations. Since the bands of the iron pnictides lie at high symmetry points in the BZ we can predominantly project out the hole (α) and electron (β) bands in A_{1g} and B_{1g} symmetry, respectively. We find a strong polarization dependence of the spectra which indicates band dependent carrier dynamics. In the superconducting state the presence of spectral weight down to the lowest accessible Raman shifts supports very small gaps. While true nodes with a sign change of the gap are unlikely, the spectra are compatible with accidental nodes, which may be lifted by doping and/or disorder. In the normal state we find Raman relaxation rates being almost constant and strongly temperature dependent on the α and β bands, respectively. This work is supported by the DFG under Grant No. Ha2071/3-4 in the Research Unit FOR538.

TT 34.4 Thu 14:45 H20

Direct observation of superconducting energy gap in the conductivity spectra of iron-pnictide films — •Dan Wu[1], Boris Gorshunov[1,2], Philipp Kallina[1], Martin Dressel[1], A-Voronkov[2], Kazumasa Iida[3], Silvia Haindl[3], Fritz Kurth[3], Ludwig Schultz[3], and Bernhard Holzapfel[3] — [1]1. Physikalisches Institut, Universiät Stuttgart, Germany — [2]Prokhorov Institute of General Physics, Russian Academy of Sciences, Russia — [3]IFW Dresden, Germany

The optical reflection, transmission and phase shift of a $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin film with a superconducting transition temperature $T_c = 20$ K was measured over a wide frequency range. The evaluated optical conductivity and permittivity show a clear evidence of the complete opening of superconducting gap $2\Delta/(2\pi\hbar c) = 30$ cm^{-1}. The behavior agrees very well with the BCS prediction for an *s*-wave superconductor with no nodes in the order parameter or additional state in the gap. The normal state conductivity shows a incoherent-like background up to mid-infrared range, which is very similar to the spectra obtained from single crystals, confirming the intrinsic property of this broad contribution in 122 pnictide systems.

TT 34.5 Thu 15:00 H20

Optical studies on iron pnictides under pressure — •Johannes Ferber, Hunpyo Lee, Yu-Zhong Zhang, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt

The recent discovery of superconductivity in the iron pnictides draws high attention to the investigation of their properties. In particular, the measurement of the optical response provides experimental access

to the electronic structure and the presumably important correlation effects. We examine the optical properties of different iron-based pnictides under pressure. Various 1111 and 122 systems are analyzed and compared using DFT and DMFT techniques.

15 min. break

TT 34.6 Thu 15:30 H20

Lattice dynamics of 122 pnictides from first principles — •Rolf Heid and Klaus-Peter Bohnen — Karlsruher Institut für Technologie, Institut für Festkörperphysik

The pnictide superconductors exhibit a complex interplay of structural and magnetic degrees of freedom, which also has a significant impact on the lattice dynamics properties. Here, we present a first-principles study of the phonon dispersion of 122 pnictides using linear-response theory within a mixed-basis pseudopotential approach. We focus on the dependence of the phonon spectra on structural parameters and magnetic order, and also consider the impact of pressure and doping. The accuracy and potential shortcoming of this first-principles approach are discussed in the light of experimental phonon measurements on $CaFe_2As_2$ (both at ambient pressure and in the collapsed phase [1,2]) and on $BaFe_2As_2$ (both pure and doped [3]).

[1] Mittal *et al.*, Phys. Rev. Lett. **102**, 217001 (2009)
[2] Mittal *et al.*, arXiv0911.1665 (2009)
[3] Reznik *et al.*, arXiv0908.4359 (2009)

TT 34.7 Thu 15:45 H20

Phonon anomalies in pure and doped $R_{1-x}K_xFe_2As_2$ (R=Ba, Sr) investigated by Raman light scattering — •Martin Rahlenbeck[1], Mathieu Le Tacon[1], Guoli Sun[1], Dunlu Sun[1], Chengtian Lin[1], Bernhard Keimer[1], and Clemens Ulrich[1,2,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia — [3]The Bragg Institute, Australian Nuclear Science and Technology Organization, Lucas Heights, New South Wales 2234, Australia

We present a detailed temperature dependent Raman light scattering study of optical phonons in superconducting and non-superconducting $R_{1-x}K_xFe_2As_2$ (R=Ba, Sr) single crystals. In all samples we observe a strong continuous narrowing of the Raman-active Fe and As vibrations upon cooling below the spin-density-wave transition T_s. We attribute this effect to the opening of the spin-density-wave gap. The electron-phonon linewidths inferred from these data greatly exceed the predictions of ab-initio density functional calculations without spin polarization, which may imply that local magnetic moments survive well above T_s. A first-order structural transition accompanying the spin-density-wave transition induces discontinuous jumps in the phonon frequencies. These anomalies are increasingly suppressed for higher potassium concentrations. We also observe a pronounced splitting of the E_g modes at this transition temperature. At the superconducting transition temperature T_c we observe subtle phonon anomalies with a behavior qualitatively similar to that in the cuprate superconductors.

TT 34.8 Thu 16:00 H20

Self-energy effects, el-ph coupling and non FL behavior in Fe-As superconductors — •Peter Lemmens[1], Kwang-Yong Choi[1], Dirk Wulferding[1], Vladimir Gnezdilov[2], Ilya Eremin[3], Helmuth Berger[4], Chengtian Lin[5], Shigeru Kasahara[6], and Yuji Matsuda[6] — [1]IPKM, TU-BS, Braunschweig — [2]ILTP, Kharkov, Ukraine — [3]ITP, Univ. Bochum — [4]EPFL, Lausanne — [5]MPI-FKF Stuttgart — [6]GSS, Univ. Kyoto, Japan

Raman scattering experiments of the undoped Sr-122 and the doped, superconducting pnictides show anomalies of a B_{1g} phonon induced by SC and SDW transitions. We give estimates of the electron-phonon coupling related to this renormalization. We follow the cross over from Fermi to non-Fermi liquid behavior with P-doping. In addition, we observe a pronounced quasi-elastic Raman response and a weak renormalization of an electronic continuum. Work supported by DFG.

TT 34.9 Thu 16:15 H20

Calorimetric studies of hole-doped $Ba_{0.68}K_{0.32}Fe_2As_2$ multiband superconductor — •P. Popovich, A. V. Boris, O. V. Dolgov, D. L. Sun, C. T Lin, R. K. Kremer, and B. Keimer — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We report on the determination of the low temperature specific heat of hole-doped $Ba_{0.68}K_{0.32}Fe_2As_2$ single crystals with a sharp (< 0.6 K) anomaly at $T_c \approx 38.5$ K. The jump at T_c is $\Delta C/T \approx 120$ mJ/molK^2. The low residual electronic specific heat (< 2 mJ/molK^2) shows that the amount of the non-superconducting impurities in our single-phase samples is less than 3%. In order to investigate the electronic part of the specific heat we subtracted a phonon background. As a background we used either our experimental specific heat data on a non-superconducting non-magnetic isostructural substance or a set of Einstein modes. Both models give qualitatively the same result. The α-model with two superconducting gaps fits well to the SC-induced electronic specific heat. Our findings imply that the superconducting properties of $Ba_{0.68}K_{0.32}Fe_2As_2$ can be well described in a framework of the strong-coupling model.

TT 34.10 Thu 16:30 H20

Magnetic fluctuations and superconductivity in Fe pnictides probed by Electron Spin Resonance — •Nikola Pascher[1], Joachim Deisenhofer[1], Hans-Albrecht Krug von Nidda[1], H. S. Jeevan[2], P. Gegenwart[2], and Alois Loidl[1] — [1]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany — [2]I. Physik. Institut, Georg-August-Universitaet Goettingen, D-37077 Goettingen, Germany

The electron spin resonance absorption spectrum of Eu^{2+} ions serves as a probe of the normal and superconducting state in $Eu_{0.5}K_{0.5}Fe_2As_2$. The spin-lattice relaxation rate $1/T_1^{ESR}$ obtained from the ESR linewidth exhibits a Korringa-like linear increase with temperature above T_C evidencing a normal Fermi-liquid behavior. Below 45 K deviations from the Korringa-law occur which are ascribed to enhanced magnetic fluctuations upon approaching the superconducting transition. Below T_C the spin lattice relaxation rate $1/T_1^{ESR}$ follows a $T^{1.5}$-behavior without the appearance of a coherence peak.

TT 34.11 Thu 16:45 H20

Evidence of Two-Band Superconductivity in K- and Co-doped 122 Barium Iron Pnictides from Point-Contact Spectroscopy — •Michael Marz[1], Oliver Berg[1], Samuel Bouvron[1], Thomas Wolf[2], Hilbert v. Löhneysen[1,2], and Gernot Goll[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe

Point-contact spectroscopy (PCS) experiments on superconducting iron pnictides were performed to investigate the structure of the superconductive energy gap. We investigated K- and Co-doped $BaFe_2As_2$ single crystals in the superconducting state in the temperature range from $T = 2$ K to $T = 30$ K. We measured the differential conductance vs. voltage in superconductor/normal-metal point contacts using platinum as a normal-metal counterelectrode. Measurements were carried out with $I \perp c$ ('edge-to-edge' method) and $I \parallel c$ ('needle-anvil' geometry) to determine a possible orientation dependence. In all cases do the obtained spectra reveal signatures which we ascribe to the occurrence of two-band superconductivity in this material, in line with a recent analysis of high-resolution specific-heat measurements [1]. For a quantitative determination of the gap values, the spectra were analyzed within a modified BTK theory to describe two-band superconductivity.

[1] F. Hardy *et al.*, archiv cond-mat **0910.5006**.

TT 34.12 Thu 17:00 H20

Point-contact spectroscopy on doped and undoped 122 barium iron pnictides in the normal-conducting state — •Oliver Berg[1], Michael Marz[1], Thomas Wolf[2], Hilbert v. Löhneysen[1,2], and Gernot Goll[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe

Point-contact spectroscopy (PCS) measurements in the superconducting state of K- and Co-doped $BaFe_2As_2$ single crystals exhibit, in addition to features due to superconductivity, an unexpected, weakly temperature-dependent voltage-dependence of the differential conductance dI/dV in both the superconducting and in normal states. To clarify the origin of this behavior we have investigated PCS of doped and undoped Ba-122 single crystals up to $T = 200$ K. In additon to this ubiquitous voltage dependence, undoped $BaFe_2As_2$ crystals reveal a significant zero anomaly (ZBA) of the differential conductance that is common to antiferromagnetic materials. Our observation that the ZBA is absent in the doped, i. e., superconducting samples supports this assignment because doping of $BaFe_2As_2$ with K or Co is known to suppress the antiferromagnetic ordering. The spectra can be described with two Lorentzian functions for the the

different contributions. These doped samples ($Ba_{0.68}K_{0.32}Fe_2As_2$ and $Ba(Fe_{0.935}Co_{0.065})_2As_2$) exhbit at $T < T_c$ the dI/dV spectra expected of Andreev reflection for two-band superconductors.

TT 34.13 Thu 17:15 H20

J_c anisotropy in 122 and 1111 pnictide thin films — •Jens Hänisch, Kazumasa Iida, Martin Kidszun, Sivia Haindl, Thomas Thersleff, Alexander Kauffmann, Fritz Kurth, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box: 270116, 01171 Dresden, Germany

We have successfully grown epitaxial, superconducting films in two families of iron pnictides, $Ba(Fe_{1-x}Co_x)_2As_2$ (122) [1] and $LaFeAs(O_{1-x},F_x)$ (1111) [2]. Detailed investigations of their critical current density J_c with respect to temperature as well as both the applied magnetic field magnitude and orientation will be shown in this contribution. Both films grow very clean and without observable correlated defects parallel to the c-axis, as confirmed by TEM. This is also reflected in the absence of a c-axis peak in $J_c(\theta)$. In contrast to cuprate high-T_c superconductors such as YBCO or even Bi2223, the pnictides have very low anisotropies in their $J_c(\theta)$ behaviour as well as in their characteristic and critical fields, such as H_{irr} and H_{c2}. Both families show the same anisotropy behaviour, 122 having slightly lower anisotropies.

[1] K. Iida, J. Hänisch, R. Hühne, F. Kruth, M. Kidszun, S. Haindl, J. Werner, L. Schultz and B. Holzapfel, Appl. Phys. Lett. 95, 192501 (2009).

[2] M. Kidszun, S. Haindl, E. Reich, J. Hänisch, K. Iida, L. Schultz and B. Holzapfel, Supercond. Sci. and Techn., in print.

TT 35: TR: Nanoelectronics III: Molecular Electronics 1

Time: Thursday 14:00–17:45 Location: H21

TT 35.1 Thu 14:00 H21

On-chip optoelectronic functionalization of CNTs with photosynthetic proteins and CdTe nanocrystals — •Frederik Hetsch[1], Simone M. Kaniber[1], Matthias Brandstetter[1], Fritz C. Simmel[2], Itai Carmeli[3], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching, Germany — [2]Physik Department, Technische Universität München, James Franck Straße 1, D-85748 Garching, Germany — [3]Department of Chemistry and Biochemistry, Tel-Aviv University, 69978 Tel-Aviv, Israel

We examine carbon nanotube (CNT) based hybrid systems by optoelectronic transport spectroscopy. CNTs are functionalized on-chip both with the "photosystem I" (PSI) and CdTe nanocrystals according to different chemical routes. PSI is a protein complex located in the thylacoid membrane of plants, algae and cyanobacteria which mediates the light-induced electron transfer in the photosynthetic pathway. The efficient energy conversion in the PSI and the adjustable optical properties of colloidal semiconductor nanocrystals, together with a nano-sized dimension, make both systems to promising candidates for applications in nano-optoelectronic devices. We will discuss the optoelectronic properties of PSI-CNT and CdTe-CNT hybrids.

TT 35.2 Thu 14:15 H21

Exact master equation for nano-systems: applications to charge transport through DNA oligomers — •Matisse Wei-Yuan Tu, Myeong Lee, Stanislav Avdoshenko, Daijiro Nozaki, Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

We present a formally exact master equation derived with the help of the Feynmann-Vernon's influence functional theory and a time-dependent electrical current formula derived from it [1,2]. We study charge transport through a DNA 15-mer connected to electrodes, when a single base mismatch is introduced into it. The electronic structure of the molecule is mapped onto an effective linear tight-binding chain with time-fluctuating electronic parameters drawn from snapshots along molecular dynamics trajectories. By exploring the real-time charge propagation and the dynamical current, we analyse the statistical properties of the current for matched and mismatched DNA oligomers.

[1] Matisse Wei-Yuan Tu and Wei-Min Zhang, Phys. Rev. B **78**, 235311(2008).

[2] Jinshuang Jin, Matisse Wei-Yuan Tu, Wei-Min Zhang and YiJin Yan, arXiv:0910.1675.

TT 35.3 Thu 14:30 H21

Charge transfer characteristics of dsDNA with base mismatch in a solvent — •Myeong H Lee, Stanislav M Avdoshenko, Daijiro Nozaki, Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062, Dresden, Germany

We present charge transfer characteristics of DNA by evaluating the electronic parameters in the presence of water and counterions. Motivated by the recent experiment by Guo *et al.* [1], we investigate three types of dsDNA oligomers; a well matched 15 base pair sequence and single mismatched base pairs (GT, CA) in sequence. Charge transfer parameters are obtained using a fragment orbital approach [2] on the coarse-grained level, where a fragment consists of a pair of nucleotides from each DNA strand. In order to fully take into account the effect of dynamical fluctuations [3] the electronic structure calculation is performed using a hybrid QM/MM method for each snapshot along the MD trajectory. From the electronic structure parameters the current is obtained for both coherent and incoherent transport [4] contribution to see the effect of single base pair mismatch.

[1] X. Guo *et al.*, Nature Nanotech. **3**, 163 (2008).

[2] D. G. Fedorov *et al.*, J. Phys. Chem. A **111**, 6904 (2007).

[3] R. Gutierrez, *et al.*, Phys. Rev. Lett. **102**, 208102 (2009); P. B. Woiczikowski *et al.*, J. Chem. Phys. **130**, 215104 (2009); P. B. Woiczikowski *et al.*, J. Phys. Chem. B **112**, 7937 (2008).

[4] J. L. D'Amato *et al.*, Phys. Rev. B **41**, 7411 (1990).

TT 35.4 Thu 14:45 H21

Conductance Through a Redox System in the Coulomb Blockade Regime: Many-Particle Effects and Influence of Electronic Correlations — •Sabine Tornow and Gertrud Zwicknagl — Institut fuer Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany

We investigate the transport characteristics of a redox system weakly coupled to leads in the Coulomb blockade regime. The redox system comprises a donor and acceptor separated by an insulating bridge in a solution. It is modeled by a two-site extended Hubbard model which includes on-site and inter-site Coulomb interactions and the coupling to a bosonic bath. The current voltage characteristics is calculated at high temperatures using a rate equation approach. For high voltages exceeding the Coulomb repulsion at the donor site the calculated transport characteristics exhibit pronounced deviations from the behavior expected from single-electron transport. Depending on the relative sizes of the effective on-site and inter-site Coulomb interactions on one side and the reorganization energy on the other side we find negative differential resistance or current enhancement.

TT 35.5 Thu 15:00 H21

Ab-initio based modeling of electron-vibron effects in single-molecule junctions — •Dmitry A. Ryndyk and Klaus Richter — Institute for Theoretical Physics, University of Regensburg, Germany

We develop an approach for quantum transport in single-molecule junctions, combining an ab initio based many-body model and the techniques of nonequilibrium Green functions. In particular, we use DFT to determine relaxed molecular junction geometry and relevant vibronic modes, and semi-empirical or ab initio (Hartree-Fock based) atomistic calculations for relevant electronic states and the coefficients of electron-vibron interaction. Finally, this effective model is used for transport calculations. As an example, we apply the method to Pt-H_2(O)-Pt junctions and Pt-oligophenyl-Pt junctions. We focus on the interplay of electron-vibron interaction and coupling to the leads, and on the effects of nonequilibrium vibrons. The results are compared with DFT+NGF approach and available experiments.

TT 35.6 Thu 15:15 H21

Transport properties of CuPc based devices — •Cosima Schus-

ter — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Electronic structure and transport properties of copper phthalocyanine (CuPc), an organic semiconductor, are investigated using density functional theory and scattering theory combined with the nonequilibriums Green's function formalism. Mainly, we discuss the electronic structure of CuPc attached to gold chains – a prototypical one-dimensional molecular device, which shall serve as model system for CuPc in transistors. There, electron and hole transport with different tranport properties is observed depending on the geometry and material of the contacts.

We determine, in particular, the charge density of the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital). Attached to leads, electrons are transfered to/from the leads, respectively, depending on the contact geometry. For a planar contact, the electron transport properties are intrinsic properties of the molecule and do not depend on the contact material. On the other hand, molecules contacted in perpendicular geometry, become hole doped. The transmission through the molecules does not only depend on the density of states of the device but also on the spatial overlap of molecular orbitals and leads in transport direction. Molecular orbitals localized on the Cu thus do not contribute to the transport in planar geometry, but provide the transmitting channel in perpendicular contact geometry.

TT 35.7 Thu 15:30 H21

Dynamical bi-stability in single-molecule junctions: the case of PTCDA on Ag(111) — •Thomas Brumme[1], Olga Neucheva[2], Cormac Toher[1], Rafael Gutiérrez[1], Stefan Tautz[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]Institute for Bio- and Nanosystems-3 and JARA-Fundamental of Future Information Technology, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

A broadly observed phenomenon in experiments on molecular junctions is time dependent switching of the tunneling current. In many cases such behavior involves different current states which are attributed to the transfer of single atoms or functional groups in a molecule between different stable configurations. We describe here the investigation of the current switching observed in a molecular junction formed by a PTCDA molecule between an STM tip and an Ag(111) surface, which is believed to be due to the carboxylic oxygen atom switching between the surface and the tip. The switching process displays a strong dependence on the applied bias voltage between tip and surface, but a much weaker sensitivity to the bias polarity. We analyse the experimental data in terms of a minimal model Hamiltonian approach describing the coupling between an adsorbate level (a relevant PTCDA molecular orbital) to local vibrations excited by the tunneling electron. The switching rates as a function of the applied bias could be fitted with a physically reasonable parameter set.

15 min. break

TT 35.8 Thu 16:00 H21

Spin degrees of freedom in single-molecule junctions — •Stefan Wagner[1], Stefan Ballmann[1], Daniel Secker[1], Frank Schramm[2], Mario Ruben[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, D-91058 Erlangen, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

We report on transport measurements on single molecules with spin degrees of freedom.

Fe^{2+}-bis(pyrazolyl)pyridine is known as a spin transition compound, in which the Fe^{2+} atom carries either no spin or $S = 2$, depending on its local environment. We find qualitatively different zero bias anomalies at very low temperatures, in particular a Kondo feature, but also an unconventional dip-like feature in $\mathrm{d}I/\mathrm{d}V$. The anomalies and their behavior in magnetic fields are explained by singlet-triplet transitions and magnetic anisotropy.

In addition, a Bis(Co^{2+})bipyrimidine-wire is investigated, with two Co^{2+} ions. Here, we see two states in the low-bias anomaly, referring to a singlet and multiplet states of the ion pair.

TT 35.9 Thu 16:15 H21

Single-molecule Junctions with C_{60} Fullerene-based Anchoring Groups — •Christian Seiler[1], Alexei Bagrets[2], Velimir Meded[2], and Ferdinand Evers[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

We investigate electronic structure and recently measured [1] ballistic transport properties of the 1,4-bis(fullero[c]pyrrolidin-1-yl)benzene (BDC60) molecule with gold contacts using Density Functional Theory and the Landauer-Büttiker formalism. We study the potential of C_{60} fullerenes as anchoring groups from a theoretical point of view. Because the high symmetry of C_{60} leads to a large HOMO-LUMO gap, it behaves like a band insulator, casting doubts on its suitability as an anchoring group. We analyze the effect of symmetry breaking in the presence of electrodes and discover that the electronic level splitting of C_{60} is small, not mitigating the issue. Moreover, electronic structure calculations of BDC60 reveal that its current-carrying HOMO is a state originating from the internal benzene ring with an energy in the gap of the anchoring C_{60}. Its hybridization is low which we attribute to the π-systems of C_{60} and the internal benzene ring being nearly orthogonal. We conclude that this creates an additional tunneling barrier which is in agreement with the low conductance values found in [1].

[1] Christian A. Martin et al., JACS, 130(40):13198-13199, 2008

TT 35.10 Thu 16:30 H21

Atomistic control and stability of molecular junctions: *ab initio* **structure prediction via transport observables** — •Florian Pump, Cormac Toher, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

The electronic transport properties of molecular junctions are very sensitive to the molecular structure and the contact configuration. We present, using the nonequilibrium Green function formalism in combination with DFT [1], the results of our calculations related to recent experiments investigating the interplay of contact structure and electronic transport characteristics of molecular systems. We focus on STM-experiments involving single PTCDA [2] and fullerene molecules and on investigations of the long-term behavior of the transport properties of terphenylene and terthiophene molecules in mechanically controllable break-junctions [3]. The STM-setup allows for an enhanced control over the contact geometry using the tip as one of the electrodes which enables the investigation of both the electronic and geometric structure of the junction. Our calculations allow for the systematic investigation of the effect of the contact geometry and the molecular configuration on the transport properties of molecular junctions, which should in turn improve the agreement between theory and experiment.

[1] A. Pecchia and A. Di Carlo, Rep. Prog. Phys. **67**, 1497 (2004).
[2] F. Pump *et al.*, Appl. Phys. A **93**, 335 (2008).
[3] D. Dulic, F. Pump, S. Campidelli, P. Lavie, G. Cuniberti, and A. Filoramo, Ang. Chem. Int. Ed. **48**, 8273 (2009).

TT 35.11 Thu 16:45 H21

Influence of substituents on the transport properties of molecular junctions — •Falco Hüser[1], Fabian Pauly[1], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

We study by DFT-based methods the correlation between the Hammett constant and the transport properties of single-molecule junctions, i.e. their conductance and thermopower [1]. Motivated by recent experiments [2,3,4], we focus on a large variety of benzenediamines [2] and of benzene-alkane-dithiols [3].

Electron-donating side-groups shift the conducting molecular orbitals up and increase the conductance and thermopower for the hole-conducting molecules, while electron-accepting side-groups have the opposite effect. By means of a single-level model, we relate these effects to properties of the isolated molecules. Relative variations are found to be in good agreement with the measurements.

Going beyond the experiments, we show how the influence of the substituents can be diminished by alkyl spacers and reestablished by alkenyl spacers.

[1] F. Hüser, F. Pauly, G. Schön (submitted).
[2] L. Venkataraman *et al.*, Nano Lett. **7**, 502 (2007).
[3] E. Leary *et al.*, Chem. Commun. **38**, 3939 2007.
[4] K. Baheti *et al.*, Nano Lett. **8**, 715 (2008).

TT 35.12 Thu 17:00 H21

Investigating Electron Correlation Effects in Transport in

Molecular Junctions — •Cormac Toher, Florian Pump, and Gianaurelio Cuniberti — Institute for Materials Science, TU Dresden, D-01062 Dresden, Germany.

The use of theoretical and computational methods to understand molecular electronics experiments has been hindered by the fact that the geometric structure of the molecular junction is usually not very well understood. This problem can be overcome by using an STM tip to form one of the electrodes of the junction [1,2], and hence taking advantage of the STM's imaging capabilties to characterize the junction. Here we present the results of recent calculations related to a set of STM experiments studying PTCDA on metallic surfaces, using the non-equilibrium Green function formalism in combination with DFT [3, 4]. This comparison demonstrates that DFT based transport calculations are insufficient to accurately describe such systems, even when the geometric configuration is well-controlled. This is due to the failure of approximate exchange-correlations to describe phenomena such as the derivative discontinuity and the Kondo effect.

[1] F. Pump, R. Temirov, O. Neucheva, S. Soubatch, S. Tautz, M. Rohlfing, and G. Cuniberti, Appl. Phys. A 93, 335 (2008).

[2] R. Temirov, A. Lassise, F.B. Anders, and F.S. Tautz, Nanotechnology 19, 065401 (2008).

[3] J.M. Soler et. al., J. Phys. Cond. Matter 14, 2745 (2002).

[4] A.R. Rocha et. al., Phys. Rev. B 73, 085414 (2006).

TT 35.13 Thu 17:15 H21

Controlling AC transport in graphene-based Fabry-Perot devices using magnetic fields — •Claudia Gomes da Rocha[1], Luis E. F. Foa Torres[2], Andrea Latge[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]FaMAF, Universidad Nacional de Cordoba, Ciudad Universitaria 5000 Cordoba, Argentina — [3]Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói-RJ, Brazil

We report on a theoretical study of the effects of time-dependent fields on electronic transport through graphene nanoribbon devices. The Fabry-Perot interference pattern is modified by an ac gating in a way that depends strongly on the shape of the graphene edges. While for armchair edges the patterns are found to be regular and can be controlled very efficiently by tuning the ac field, samples with zigzag edges exhibit a much more complex interference pattern due to their peculiar electronic structure. These studies highlight the main role played by geometric details of graphene nanoribbons within the coherent transport regime. We also extend our analysis to noise power response, identifying under which conditions it is possible to minimize the current fluctuations as well as exploring scaling properties of noise with length and width of the systems. Finally, the response of the system under the presence of an external magnetic field is also analysed in which both DC and AC Fabry-Perot patterns and energy gaps can be efficiently tuned by such controlling parameter.

TT 35.14 Thu 17:30 H21

The dark side of benzene: interference vs. interaction — Dan Bohr[1] and •Peter Schmitteckert[2] — [1]Department of Physics, University of Basel, Switzerland — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), Germany

We present the study of the linear conductance vs. applied gate voltage for an interacting six site ring structure, which is threaded by a flux of π and coupled to a left and a right lead. This ring structure is designed to have a vanishing conductance for all gate voltages and temperatures provided interactions are ignored. Therefore this system is an ideal testbed to study the interplay of interaction and interference. First we find a Kondo type resonance for rather large hopping parameter. Second, we find additional resonance peaks which can be explained by a population blocking mechanism. To this end we have to extend the Kubo approach within the Density Matrix Renormalization Group method to handle degenerate states.

TT 36: TR: Poster Session

Time: Thursday 14:00–18:00 Location: Poster A

TT 36.1 Thu 14:00 Poster A

Lithographically fabricated mechanically controlled break junctions (MCBJ) made of Platinum — •Florian Strigl, Reimar Waitz, and Elke Scheer — Department of Physics, University of Konstanz, 78475 Konstanz, Germany

We present the fabrication scheme and electrical transport properties of lithographically fabricated platinum break junctions for adjusting atomic-size platinum contacts. Platinum atomic contacts are interesting for contacting individual molecules [1] as well as for studying photo-assisted transport [2, 3]. Because of the high melting point of platinum the standard electron beam lithography process for lithographic MCBJs [4] cannot be applied, but a procedure using subtractive dry etching of the platinum layer has to be used. We present here the first electronic transport properties of atomic size contacts produced from these MCBJs under ambient conditions as well as at cryogenic vacuum. We study the conductance as a function of the contact size and calculate histograms from these data. Furthermore we study the current-voltage characteristics of single-atom contacts. Our preliminary data yields a preferred conductance of the single-atom contact in the order of 1.6 to 2 G_0 in agreement with results obtained on "classical" MCBJs [5].

[1] Nature 419 (2002) 906

[2] Phys. Rev. Lett. 99 (2007) 086801

[3] Phys. Rev. B 75 (2007) 075406

[4] Rev. Sci. Instrum. 67 (1996) 108-11,

[5] Phys. Rev. B, 67 (2003) 245411

TT 36.2 Thu 14:00 Poster A

Nonequilibrium transport through a correlated quantum dot with magnetic impurity — •Daniel Becker[1], Stephan Weiss[2], Jens Eckel[3], Michael Thorwart[3], and Daniela Pfannkuche[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Niels Bohr Instituttet, Nano-Science Centret, Universitetsparken 5, DK-2100 Copenhagen, Denmark — [3]FRIAS, Albert-Ludwigs-Universität Freiburg, Albertstr.19, 79104 Freiburg, Germany

The iterative summation of path integrals (ISPI)[1] is adopted to a single-level quantum dot, in which a quantum spin-1/2 magnetic impurity interacts with the dot-electron spins. For two electrons on the dot, Coulomb interaction is taken into account. Based on a generating function, the tunneling current at finite bias voltages and the orientation of the impurity spin are calculated numerically. The scheme is deterministic by construction and non-perturbative and allows to study real-time nonequilibrium transport for strong electron-impurity and Coulomb interaction, even at low temperatures and for a wide range of bias voltages. Of particular interest is the mutual influence between tunneling current and the impurity spin dynamics in the presence of the Coulomb interaction and a magnetic field.

[1] S. Weiss et al., Phys. Rev. B 77, 195316 (2008)

TT 36.3 Thu 14:00 Poster A

Transport through a vibrating quantum dot: Polaronic effects — •Thomas Koch[1], Jan Loos[2], Andreas Alvermann[1], Alan Bishop[3], and Holger Fehske[1] — [1]Institute of Physics, Ernst-Moritz-Arndt University Greifswald, 17487 Greifswald, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, 16200 Prague, Czech Republic — [3]Theory, Simulation and Computation Directorate, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We present a Green's function based treatment of the effects of electron-phonon coupling on transport through a molecular quantum dot in the quantum limit. Thereby we combine an incomplete variational Lang-Firsov approach with a perturbative calculation of the electron-phonon self energy in the framework of generalised Matsubara Green functions and a Landauer-type transport description. Calculating the ground-state energy, the dot single-particle spectral function and the linear conductance at finite carrier density, we study the low-temperature transport properties of the vibrating quantum dot sandwiched between metallic leads in the whole electron-phonon coupling strength regime. We discuss corrections to the concept of an anti-adiabatic dot polaron and show how a deformable quantum dot can act as a molecular switch.

TT 36.4 Thu 14:00 Poster A

Modification of the electronic transport in Au by prototypical impurities and interlayers — •Mohamed Fadlallah[1,2], Cosima Schuster[1], Udo Schwingenschlögl[3], and Ulrich Eckern[1] — [1]Universität Augsburg, 86135 Augsburg, Germany — [2]Benha University, Benha, Egypt — [3]KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

Electronic tranport calculations using the Smeagol code based on density functional theory and the non-equilibrium Green's functions method are presented. We study the modifications of the transport through Au due to prototypical impurities and interlayers. Our results demonstrate that non-metallic impurities (S or Si) act upon transport similar to vacancies, since they do not contribute to the electronic states at the Fermi energy. On the other hand, metallic impurities and interlayers (Cu or Ni) can have drastic effects on the transport, in particular when the Au *sd* hybridized states at the Fermi energy are perturbed. For Au/nAg/Au heterostructures the conductance decreases as the interlayer thickness increases but no saturation is found up to n=8 interlayers. The formation of an interface alloy is also considered. The transmission through a two component interlayer system can be described as a superposition of the effects of the individual layers.

TT 36.5 Thu 14:00 Poster A

A Real-Time Path Integral Approach for a Dissipative Nonequilibrium Quantum Dot — •Klaus Ferdinand Albrecht[1,2], Lothar Mühlbacher[1], and Andreas Komnik[2] — [1]Physikalisches Institut, Universität Freiburg — [2]Institut für Theoretische Physik, Universität Heidelberg

Based on a recently developed real-time path integral approach, we apply a diagrammatic Quantum Monte Carlo method to study the nonequilibrium dynamics of a contacted quantum dot coupled to a phonon environment, which consists of either one or several phonon modes. The timescales reached by this exact method are long enough to exploit transient behavior as well as transport properties of the system.

TT 36.6 Thu 14:00 Poster A

Dephasing in a mesoscopic ring connected via arms to leads — •M. Treiber[1], O. M. Yevtushenko[1], F. Marquardt[1], J. von Delft[1], and I. V. Lerner[2] — [1]Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham, B15 2TT, UK

We recently considered dephasing by electron interactions in an almost isolated ring using a model of homogeneous electron dissipation [1]. We showed that the amplitude of the Altshuler-Aronov-Spivak (AAS) oscillations crosses over to 0D behavior ($\Delta g_{\rm AAS} \sim T^{-2}$) when the temperature T drops below the Thouless energy. In the 0D regime, dephasing is dominated by large energy transfers, only restricted by T due to Pauli blocking. Therefore, the observation of this hitherto elusive crossover would allow quantitative tests of the role of T as UV-cutoff in the theory of dephasing. We discussed in [1] that by filtering $\Delta g_{\rm AAS}$ from its nonoscillatory background, the influence of the leads, which may mask the predicted crossover, can be substantially reduced.

In this presentation, we consider a "lead-arm-ring-arm-lead" geometry, which is closer to the experimental situation. We assume absorbing leads and ballistic (not tunneling) contacts between arm and ring, having different numbers of conducting channels at both sides. We study the T dependence of the dephasing time, analyze in detail arm-ring cross contributions, which were neglected in [1], and discuss the possibility for an experimental observation of 0D dephasing in this model.

[1] M. Treiber et al., Phys. Rev. B **80**, 201305(R) (2009).

TT 36.7 Thu 14:00 Poster A

Quantum transport through magnetic quantum dots — •Benjamin Baxevanis and Daniela Pfannkuche — I. Institute for Theoretical Physics, University of Hamburg, D-20355 Hamburg, Germany

The non-equilibrium transport of charge carriers through magnetic quantum dots is studied theoretically. A single-level quantum dot with a coupling of the electron spin to a local spin 1/2 of a magnetic impurity represents the underlying model. The Coulomb interaction of two electrons as well as the interaction between electrons and the spin impurity are taken into account in a numerically exact manner by means of the recently proposed real-time version of the diagrammatic Monte Carlo method [1]. This approach is applied to investigate the transient dynamics in the system subject to external parameters. In particular, the effects due to the mutual interplay between charge carriers and the impurity spin are examined.

[1] P. Werner, T. Oka, and A. J. Millis, Phys. Rev. B **79**, 035320 (2009)

TT 36.8 Thu 14:00 Poster A

Nonequilibrium cotunneling in quantum dots: Building the bridge between the T-matrix approach and exact perturbation theory — •Georg Begemann[1], Sonja Koller[1], Milena Grifoni[1], and Jens Paaske[2] — [1]Universität Regensburg — [2]Nano-Science Center, University of Copenhagen

Using a T-matrix based rate equation approach, it is possible to perform fast calculations on fourth order transport, i.e. on the cotunneling regime of transport across quantum dots. However, there is the long standing question about the quality of such calculations in comparison to exact, but numerical costly perturbation theory results. In this poster, we present the exact perturbation theory and show the fundamental relation which exists between the two. We can pinpoint to which approximations to the exact method the T-matrix approach corresponds and give a detailed comparison between results on transport across quantum double dots. We also show how an effective Kondo Hamiltonian can be derived in the deep Coulomb blockade regime for Coulomb diamonds with odd filling and that it is equivalent to the fourth order T-matrix contributions.

TT 36.9 Thu 14:00 Poster A

Non-Equilibrium Dynamics of Electron Transport through Interacting Quantum Dots — •Alexander Croy and Ulf Saalmann — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

The transport of electrons through nanoscale devices, including quantum dot systems, has been a subject of intense research in the past decades. The study of time-resolved phenomena is of particular interest in this regard. This interest is driven not only by the prospect of realizing quantum computers using such systems, but also by the rapid experimental progress in this field.

In this context we study theoretically the *time-resolved* electric currents flowing through single and double quantum dots that are subject to a voltage pulse. Our numerical calculations are based on a recently developed propagation scheme for non-equilibrium Green functions [1]. This scheme relies on an efficient auxiliary-mode expansion of the Fermi function [2] and facilitates the study of arbitrary time-dependencies. We also present an extension of this scheme which allows treating interacting electrons for energies above the Kondo temperature. The results are compared to quantum master equations for the many-body density matrix describing the state of the quantum dot system.

[1] A. Croy and U. Saalmann, PRB, in print (2009), arXiv:0908.2936
[2] A. Croy and U. Saalmann, PRB 80, 073102 (2009)

TT 36.10 Thu 14:00 Poster A

Transmission through metallic chains: Role of distortions and contact geometry — •Thomas Wunderlich, Berna Akgenc, Cosima Schuster, and Ulrich Eckern — Institus für Physik, Universität Augsburg, 86135, Germany

We present results of electronic structure and transport calculations for metallic chains, based on density functional theory and scattering theory combined with the the non-equilibrium Green's function technique. Starting from a simple model system of monovalent metallic chains we investigate the influence of distortions on the electronic structure and the transport properties of H and Li chains. Furthermore we calculate the electronic structure of Au chains which are contacted to leads via different geometries, and study the influence of the contact geometry on the transmission coefficient. In particular, we compare chains, pyramides and planes in the contact region. A comparison with analytical results is given.

TT 36.11 Thu 14:00 Poster A

Transport characteristics of carbon nanotube devices with spin-orbit coupling and parallel magnetic field — •Miriam del Valle, Magdalena Marganska, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93 053 Regensburg, Germany

Spin-orbit interaction was long thought to be negligible in carbon nanotubes (CNTs) due to the low atomic mass of carbon. However, recent experiments on CNT devices have shown a clear signature of spin-orbit coupling, originating in the curvature of the nanotube. We present here the calculations of density of states and transport characteristics of CNT devices including spin-independent curvature effects, spin-orbit coupling and the presence of a parallel magnetic field.

The calculations are done both with an effective model in reciprocal space and a real space tight-binding Hamiltonian with one p_z orbital per atom. The results allow us to interpret experimental data, throwing light onto the role of curvature and spin-orbit coupling in CNT systems. Among their most interesting effects is the possibility of highly spin-polarized currents close to the charge neutrality point, which may be useful in spintronics devices.

TT 36.12 Thu 14:00 Poster A

Controlled ballistic electron beam propagation in a Rashba spin orbit split two dimensional electron gas — •Mathias J. Mühlbauer, Christoph Brüne, Elena G. Novik, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg, Germany

For spintronic applications, systems with high spin orbit (SO) coupling strength provide a promising environment. There it should be possible to observe the electronic analogue of the birefringent effect for polarized light as proposed by M. Khodas et al. [1]. The beam polarization takes place at a junction between regions with different SO splitting. HgTe/HgCdTe quantum wells are the material of choice. Electron beam injection and detection can be provided by quantum point contacts (QPCs). However, the realization of QPCs in HgTe/HgCdTe structures is not trivial due to the narrow band gap and the presence of the Quantum Spin Hall Effect (QSHE) [2]. Here, we demonstrate that it is possible to fabricate QPCs using electron beam lithography and dry etching techniques and to control its transmission with a top gate electrode. The functionality of the devices is confirmed by measurements of conductance and electron beam collimation effect. The quantized conductance is the first demonstration for a HgTe based structure. We would like to note that the conductance sequence shows steps of e^2/h indicating the influence of the Rashba SO splitting. We will present and discuss measurements on these devices.

[1] M. Khodas et al.,Phys. Rev. Lett. 92, 086602 (2004).
[2] M. König et al.,Science, 318, 766, (2007).

TT 36.13 Thu 14:00 Poster A

Micromagnetic properties of narrow PdFe and PdNi strips — •Daniel Steininger, Dominik Preusche, Maurice Ziola, Günther Bayreuther, and Christoph Strunk — Institut für Angewandte und Experimentelle Physik, Universität Regensburg

We present an investigation of submicron ferromagnetic strips from PdFe and PdNi intended to act as contact electrodes to carbon nanotube-based spin devices.

Various strips are studied for their magnetic properties with respect to coercive fields, ferromagnetic transition temperature and micromagnetic structure depending on their aspect ratio and material composition.

Magnetic hysteresis measurements on $Pd_{0.95}Fe_{0.05}$-, $Pd_{0.83}Ni_{0.17}$- and $Pd_{0.3}Ni_{0.7}$ using a magneto optical Kerr magnetometer were performed on arrays containing strip widths from 100nm to 2.5μm. For further investigation of the spontaneous magnetization we measured the anisotropic magnetoresistance on individual $Pd_{0.3}Ni_{0.7}$ strips and performed wide angle x-ray scattering to examine the lattice texture of $Pd_{0.3}Ni_{0.7}$-Films. Atomic- and magnetic force microscopy confirm independently the micromagnetic structure of $Pd_{0.3}Ni_{0.7}$ electrodes.

TT 36.14 Thu 14:00 Poster A

Transport through a Molecular Bridge: Comparison of Different Truncation Schemes for Non-Equilibrium Green Functions — •Brendan Coughlin, Sabine Tornow, and Gertrud Zwicknagl — Institut fuer Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany

We present a detailed model study of electron transport through a molecular bridge using analytical methods. Employing an extended Hubbard model for the molecular bridge which is contacted to leads we calculate non-equilibrium Green functions. A scheme of coupled equation of motion is set up with the help of computer algebra systems. To calculate the conductivity higher order decoupling schemes in different parameter regimes are systematically tested and compared with numerical methods.

TT 36.15 Thu 14:00 Poster A

Multiple-charge transfer and trapping in DNA dimers — •Sabine Tornow[1], Ralf Bulla[2], Frithjof Anders[3], and Gertrud Zwicknagl[1] — [1]Institut fuer Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institut fuer Theoretische Physik, Universitaet zu Koeln, 50937 Koeln, Germany — [3]Theoretische Physik II, TU Dortmund, 44221 Dortmund, Germany

We investigate the transfer characteristics of multiple charges in a DNA base-pair dimer using a model Hamiltonian approach. It comprises different Coulomb matrix elements which where calculated recently by Starikov [E. B. Starikov, Phil. Mag. Lett. 83, 699 (2003)] as well as the dissipative environment which is modeled by a bosonic bath. In the nuclear tunneling regime we employ the Numerical Renormalization Group method whereas in the thermal activation regime a scheme of kinetic equations and Marcus rates is used to calculate the time-dependent population probabilities. We find that the mobility of two excess charges depends strongly on the Coulomb-matrix elements which differ for the different base pairs. Starting with two electrons on the donor, the Coulomb matrix elements determine, if, e.g, both electrons are self-trapped, transferred as a pair or only one of the electrons is transferred. The latter can be even activation-less when the difference of the on-site and inter-site Coulomb matrix element is equal to the reorganization energy which is the case in a GC-GC dimer. Whereas two excess electrons in AT-AT, dependent on the temperature and spectral function of the environment, are either self-trapped or are oscillating as a pair.

TT 36.16 Thu 14:00 Poster A

Interference in transport through single molecules in a STM set-up — •Sandra Kolmeder, Andrea Donarini, and Milena Grifoni — Institute of Theoretical Physics, University of Regensburg, Germany

We theoretically study the transport properties of single molecules in a STM configuration. The focus is on STM experiments, which measure electronic properties of individual molecules deposited on ultrathin insulating films on metal substrates. The insulating film allows to electronically decouple the molecule from the matallic surface. We model this geometry as a double-barrier tunneling set-up where we account for angular momentum selection rules governing tunneling processes from the tip to the molecule and from the molecule to the substrate. In turn this might lead to interference effects in transport, like selective conductance and current blocking, because of involved orbitally degenerate states.

TT 36.17 Thu 14:00 Poster A

Electrical contacting of vertical nanostructures — •Matthias Wieser[1], Jochen Grebing[1], Marcel Höwler[1], Kerstin Bernert[1], Artur Erbe[1], Jürgen Fassbender[1], and Bertram Schmidt[2] — [1]Forschungszentrum Dresden-Rossendorf e. V., D-01328 Dresden — [2]Otto-von-Guericke-Universität Magdeburg, D-39106 Magdeburg

The aim of this new approach is the contacting and characterization of small vertical nanostructures. Therefore, in contrast to conventional lateral contacting a vertical pillar with a height of about 70nm and an elliptic size of 100nm × 150nm is contacted using a bottom electrode, a via with the same height as the pillar and two top electrodes for tip-contacting of measurement devices. The structuring of the different layers is done using electron beam lithography (EBL). A resist layer is used as an insulator between the bottom and the top electrodes. In the center of the pillar an Al_2O_3 tunnel barrier will be integrated. The current voltage (IV) characteristics of the system will be investigated and compared to the direct tunneling and the Fowler-Nordheim tunneling model. Using this technique we will characterize the electrical properties of oxides with varying thickness.

TT 36.18 Thu 14:00 Poster A

Nonequilibrium quantum transport in the local Holstein model — •Roland Hützen[1], Stephan Weiss[2], Michael Thorwart[3], and Reinhold Egger[1] — [1]Heinrich-Heine Universität Düsseldorf — [2]Niels Bohr Institute & Nano-Science Center, University of Copenhagen — [3]FRIAS, Albert-Ludwigs Universität Freiburg

The local Holstein model serves as a basic model to study quantum transport through a single molecule. We employ the Keldysh path integral formalism to describe the system under nonequilibrium conditions. Free fermionic fields are integrated out and the coupling between the dot electron and the phonon mode is disentangled exactly

by introducing auxiliary spin fields ($S_j = 0, \pm 1$) on every Trotter slice. Those interact with each other over finite memory times, whereas free bosonic fields are integrated out as well. The remaining functional integration over the discrete spins is performed by means of the deterministic ISPI method [1]. We calculate the generating function for the tunneling current at finite bias voltages. For small electron-phonon coupling strengths λ we have checked our results against perturbation theory at finite temperature. In addition we have studied the regime of slow and fast phonon modes.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, Phys. Rev. B **77**, 195316 (2008).

TT 36.19 Thu 14:00 Poster A

Formation of metallic electrodes for molecular transport measurements by electromigration — •Birgit Kiessig[1,2], Wanyin Cui[1,2], Kai Grube[1], Regina Hofmann[2], Dominik Stöffler[2], and Roland Schäfer[1] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — [2]Karlsruher Institut für Technologie, Physikalisches Institut, Wolfgang-Gaede-Straße 1, 76128 Karlsruhe

Molecular transport measurements require the fabrication of conductive electrodes spaced only a few nm apart. Electromigration of metallic nanostructures is a tool to achieve this aim which by now has been approved by several groups around the world.

We report on our own experience with electromigration of various materials, namely Au, Al and AuPd, using a feedback controlled electromigration process.

A dependence of the size of the resulting gaps on substrate and structure material as well as ambient temperature is observed. We mainly attribute this to different mechanisms and magnitude of heat transport from the nanostructures to the surroundings which results in different temperature profiles in the devices.

Furthermore we monitore structure thinning during electomigration in situ with a scanning electron microscope. At the same time resistance is measured and a simple model is used to explain the observed dependence of resistance on geometry.

TT 36.20 Thu 14:00 Poster A

Inter-System Crossing in a Dissipative Three-Spin System — •Sabine Tornow[1], Frithjof Anders[2], and Gertrud Zwicknagl[1] — [1]Institut fuer Mathematische Physik, TU Braunschweig, 38106 Braunschweig, Germany — [2]Theoretische Physik II, TU Dortmund, 44221 Dortmund, Germany

We present an extended Hubbard model with dissipation (dissipative Hubbard model) for analyzing the spin and electron dynamics of a donor-acceptor system representing a chromophore coupled to a radical in a solvent. The latter is modeled by a bosonic bath. After photoexcitation, the initial local singlet state on the chromophore can perform a transition to a local triplet state (inter-system crossing) dependent on the coupling to the dissipative environment, Coulomb interactions, exchange interactions, on-site-energies and hopping parameters. We investigate the rate of local triplet formation and calculate the time-dependent population probabilities of all electronic states with the Time-Dependent Numerical Renormalization Group. The investigation of the role of different parameters can help to tailor appropriate molecules and solvents, to study fundamental questions about controlling molecular spin-systems.

TT 36.21 Thu 14:00 Poster A

Electron Transport through Molecular Junctions — Dirk Brossell, •Ole Pfoch, and Barbara Sandow — Freie Universität Berlin, Institut für Experimentalphysik, Arminallee 14, 14195 Berlin

Molecular switches with characteristic conductance attributes are highly favoured as new generation of nanoelectronic devices. Switching between stable isomers occurs by interaction with light, by current and magnetic field. Using mechanically controllable break junction we can fabricate stable metal-molecule-metal junctions. We present our newly developed break junction experiment which has been used to study the transport and switching properties of a gold-molecule-gold junction or a copper-molecule-copper junction, i.e. with a molecular switch like azobenzene.

TT 36.22 Thu 14:00 Poster A

Inelastic Electron Tunneling Spectroscopy of a Single-Molecule Break Junction — •Youngsang Kim[1], Hyunwook Song[2], Hans-Fridtjof Pernau[1], Takhee Lee[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, Gwangju 500-712, Korea

We report the inelastic electron tunneling (IET) spectra of an 1,6-hexanedithiol (HDT) single-molecule junction using a mechanically controllable break junction (MCBJ) technique. We measure the completely assigned IET spectra of the HDT junction. All of the spectral features are attributable to vibrational modes associated with the molecular species, providing a clear evidence of the existence of the component molecule through which tunneling is occurring. In addition, we discuss the effect of the junction elongation by changing the separation between two electrodes in MCBJ, which gives rise to changes in the configuration in the single-molecule junction.

TT 36.23 Thu 14:00 Poster A

Entanglement transfer from electrons to photons in quantum dots: An open quantum system approach — •Jan Carl Budich and Björn Trauzettel — Institut für Theoretische Physik, 97074 Würzburg, Deutschland

We investigate entanglement transfer from a system of two spin-entangled electron-hole pairs, each placed in a separate single mode cavity, to the photons emitted during their recombination process. Dipole selection rules and a splitting between the light-hole and the heavy-hole subbands are the crucial ingredients establishing a one-to-one correspondence between electron spins and circular photon polarizations. To account for the measurement of the photons as well as dephasing effects, we choose a stochastic Schrödinger equation and a conditional master equation approach, respectively. The influence of interactions with the environment as well as asymmetries in the coherent couplings on the photon-entanglement is analyzed for two concrete measurement schemes. The first one is designed to violate the Clauser-Horne-Shimony-Holt (CHSH) inequality, while the second one employs the visibility of interference fringes to prove the entanglement of the photons. Because of the spatial separation of the entangled electronic system over two quantum dots, a successful verification of entangled photons emitted by this system would imply the detection of nonlocal spin-entanglement of massive particles in a solid state structure.

TT 36.24 Thu 14:00 Poster A

Experiments with Double-SQUID Qubits — •Bernhard Dörling[1], Stefano Poletto[1], Maria Gabriella Castellano[2], Fabio Chiarello[2], and Alexey V. Ustinov[1] — [1]Karlsruher Institut für Technologie — [2]Instituto Fotonica e Nanotecnologie - CNR, Roma, Italy

A double-SQUID qubit (flash-qubit) allows the manipulation of quantum states by very short pulses of magnetic flux, without using microwaves [1]. It consists of an rf-SQUID with a dc-SQUID replacing the single Josephson junction.

The energy potential profile is controllable by dc bias fluxes threading the two loops. The initial qubit state in a double well is prepared by applying a dc flux pulse to one loop, thereby tilting the double well so that only one of the two states remains stable. To manipulate the state of the qubit a dc flux pulse is applied to the other loop to change the potential into a single well, where coherent Larmor oscillations between the two lowest eigenstates take place. Reading out the state is once again performed in the double well situation, where our readout dc-SQUID is able to discriminate between the two computational states due to their flux difference.

We hope to present measurements done on a new sample, fabricated using shadow evaporation of aluminium and silicon nitride as the dielectric.

[1] Stefano Poletto et al., New J. Phys. **11**, 013009 (2009)

TT 36.25 Thu 14:00 Poster A

Dissipative dynamics of a qubit coupled to a nonlinear undriven or driven oscillator — •Carmen Vierheilig, Johannes Hausinger, and Milena Grifoni — Universität Regensburg, 93040 Regensburg, Germany

Coupling a qubit to a nonlinear readout device, for example a DC-SQUID in the nonlinear regime or a Josephson junction bifurcation amplifier, lead to advantages in several measurement schemes and to new physical observations. In this poster we consider the case of a qubit coupled to a nonlinear, driven or undriven, oscillator. The oscillator is in turn coupled to a thermal bath, which thus indirectly induces dissipation and dephasing in the qubit's dynamics.

In the undriven situation focus is on the regime where the frequency

of the linear oscillator nearly equals the qubit's energy splitting. This yields a multiplicity of quasi-degenerate states of the coupled qubit-nonlinear oscillator system, reflected in a complex dynamics of the qubit towards equilibrium [1].

When an additional ac-field is included, resonant transitions between the multiplets can be induced.

[1] C. Vierheilig, J. Hausinger, and M. Grifoni, Phys. Rev. A **80**, 052331 (2009)

TT 36.26 Thu 14:00 Poster A

Bifurcation Readout of a Josephson Phase Qubit — •Tobias Wirth, Jürgen Lisenfeld, Alexander Lukashenko, and Alexey V. Ustinov — Karlsruhe Institute of Technology (KIT), Physikalisches Institut, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

The standard method to read out a Josephson phase qubit is using a dc-SQUID to measure the state-dependent magnetic flux of the qubit by switching to the non-superconducting state. This process generates heat directly on the qubit chip and quasi-particles in the circuitry. Both effects require a relatively long cool-down time after each switching event. This, together with the time needed to ramp up the bias current of the SQUID limits the repetition rate of the experiment. In our ongoing experiments we replace the standard readout scheme by a SQUID shunted by a capacitor. This nonlinear resonator is operated close to its bifurcation point between two oscillating states which depend on the qubit flux. The measurement is done by detecting either the resonance amplitude or phase shift of the reflected probe signal. We verified that our SQUID resonator works as linear resonator for low excitation powers and observed the periodic dependence of the resonance frequency on the externally applied magnetic flux. For higher excitation powers the device shows a hysteretic behavior between the two oscillating states. Current experiments are focused on a pulsed rf-readout to measure coherent evolution of the qubit states. We hope to achieve longer coherence times, perform faster measurements, and test non-destructive measurement schemes with Josephson phase qubits.

TT 36.27 Thu 14:00 Poster A

Galvanic coupling of two superconducting microwave resonators — Thomas Weissl[1], •Elisabeth Hoffmann[1], Frank Deppe[1], Edwin P. Menzel[1], Achim Marx[1], Rudolf Gross[1], David Zueco[2], Georg M. Reuther[2], Juan J. Garcia-Ripoll[3], and Enrique Solano[4] — [1]Walther-Meissner-Institut and TU München, Garching, Germany — [2]Universität Augsburg, Augsburg, Germany — [3]Instituto de Fisica Fundamental, CSIC, Madrid, Spain — [4]Universidad del País Vasco-Eurskal Herriko Unibertsitatea, Spain

Thermal entanglement, e.g. in a system of two degenerate coupled superconducting microwave resonators, is achieved just by lowering the temperature below a critical temperature T_c and can be detected via suitable correlation measurements. T_c depends on the coupling strength of the two resonators. To obtain a critical temperature of about 100 mK in an actual experiment, a coupling strength of the order of 1 GHz is required. For superconducting flux quantum circuits, such a large coupling can be realized by making use of the kinetic inductance: the circuits have to be galvanically connected and form a single entity. Nevertheless, the physics can often be described by two separate modes with an enhanced coupling constant. Our experiments show that the mode structure of two coupled superconducting microwave resonators changes discontinuously when connecting them galvanically instead of just placing them very close to each other. This is explained within a simple toy model. This work is supported by the DFG within SFB 631 and NIM.

TT 36.28 Thu 14:00 Poster A

Dual-path measurements of the noise properties of Josephson parametric amplifiers — •Alexander Baust[1], Edwin P. Menzel[1], Matteo Mariantoni[1], Frank Deppe[1], Miguel Angel Araque Caballero[1], Elisabeth Hoffmann[1], Thomas Niemczyk[1], Achim Marx[1], Rudolf Gross[1], Enrique Solano[2], Kunihiro Inomata[3], Tsuyoshi Yamamoto[3,4], and Yasunobu Nakamura[3,4] — [1]Walther-Meissner-Institut and TU München, Garching, Germany — [2]Universidad del Pais Vasco and Ikerbasque Foundation, Bilbao, Spain — [3]RIKEN, Wako, Japan — [4]NEC Corporation, Tsukuba, Japan

Phase sensitive amplifiers, e.g. Josephson parametric amplifiers (JPA), in principle allow for the amplification of one signal quadrature without adding noise. In practice however, internal losses introduce noise. In experiments, the JPA output signal usually is further amplified by HEMT amplifiers, which obscure the noise properties of the JPA by their much larger noise. We show that splitting the signal and utilizing two amplification chains allows one to eliminate the noise contribution of the HEMT amplifiers. In this way, the first two signal moments can be analyzed by correlation measurements. We study two possible applications of our dual-path method. First, we investigate the noise properties of a superconducting JPA. Second, we address the measurement of squeezed states generated by the latter and discuss to what extent squeezing can be observed in our samples.

We acknowledge support from SFB631, NIM, UPV/EHU Grant GIU07/40 and European project EuroSQIP.

TT 36.29 Thu 14:00 Poster A

Back-action on the flux-qubit from a driven non-linear detector — •Vicente Ancelmo Leyton Ortega[1], Vittorio Peano[1], Michael Thorwart[1], and John Henrry Reina[2] — [1]Freiburg Institute for Advanced Studies (FRIAS), Albert-Ludwigs Universität Freiburg, 79104 Freiburg — [2]Universidad del Valle, Departamento de Física, A.A. 25360, Cali-Colombia.

We consider a superconducting flux qubit inductively coupled to a driven SQUID, acting as a detector, in presence of weak dissipation and close to the optimal working point. We study the nonlinear response of the detector to the drive and the population difference of the qubit state. By varying the external magnetic field piercing the SQUID, we access two different regimes: i) For vanishing external flux, the SQUID acts as a Josephson bifurcation amplifier, however, operated here with few energy quanta rather than in its classical regime. In this regime, we show that the back-action of the detector on the qubit is small, rendering the driven SQUID an ideal detector. ii) When the external flux is close to half a flux quantum, the combined qubit-oscillator system implements the two-photon Jaynes-Cummings model. We study multiphoton (anti-)resonances in the two-photon transition regime.

TT 36.30 Thu 14:00 Poster A

Characterization of non-Gaussian quantum noise via dephasing of qubits — •Stefan Kessler and Florian Marquardt — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr 37, D-80333 München, Germany

Until now, a major restriction of solid state qubits as quantum memories is their small coherence times due to the unavoidable coupling to their noisy environment. On the other hand the decoherence of the qubit can be used as unique probe for the time correlations of the environmental noise fluctuations.

While most of the previous work on decoherence has been based on environments modeled by Gaussian fluctuators or ensembles of classical fluctuators, we address here genuine quantum non-Gaussian noise. Features of quantum non-Gaussian noise have been observed in recent experiments in mesoscopic physics, where strong coupling between the system and few environmental fluctuators is dominant.

In this work, we consider the pure dephasing of a two level system due to its quantum environment and introduce an effective quantum noise spectrum based on the time evolution of the qubit coherence. We show that this spectrum provides a convenient way to distinguish experimentally between Gaussian and non-Gaussian noise and can be used to characterize the non-Gaussianity of the noise. The results are illustrated by different models of non-Gaussian environments. We discuss the implications for experimental setups measuring quantum noise.

TT 36.31 Thu 14:00 Poster A

Gradiometric superconducting flux qubit with tunable gap — •Manuel Johannes Schwarz[1], Tomasz Niemczyk[1,2], Frank Deppe[1], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Str. 8, 85748 Garching — [2]Physics Department, TU München, 85748 Garching

One promising candidate for the implementation of scalable quantum information processing is a superconducting flux qubit. In its gradiometric version, it consists of two galvanically coupled superconducting loops with three or four nanoscale Josephson junctions, one of them being slightly smaller than the others, placed on the shared line. In principle, the qubit transition frequency can be controlled by applying an external flux to the loop. However, in order to maintain long phase coherence time, the qubit must be operated at a certain optimal flux bias. Nevertheless, tunability can be obtained by replacing the smaller junction with a DC SQUID loop acting as an effective junction, whose critical current can be varied via an additional flux line without chang-

ing the flux bias in the qubit loop [1]. Using electron beam lithography, two-angle shadow evaporation and Al technology, we have fabricated such a device together with a readout SQUID. At 30 mK, we observe a clear qubit signature in the switching current of the readout SQUID. Furthermore, we show the results of spectroscopic measurements and discuss to which extent an additional flux through the small SQUID loop affects this data. This work is supported by the DFG via SFB631 and NIM.

[1] F.G. Paauw et al., Phys. Rev. Lett. 102, 090501 (2009)

TT 36.32 Thu 14:00 Poster A

Multiplexing Qubit Readout using Microwave Resonators — •Markus Jerger, Stefano Poletto, and Alexey V. Ustinov — Physikalisches Institut, Karlsruher Institut für Technologie (KIT), Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

We investigate the coupling of quantum bits to transmission line resonators. A set of resonators around 10 GHz with short decay times is used for a fast measurement of the qubit states. Distinct resonances enable frequency-domain multiplexing readout of several qubits. An additional resonator with a long decay time is used to entangle the states of selected qubits and transfer information between them. We explore situations where the coupling is dominated by either the magnetic or the electric fields of the resonators.

The qubit we use is a Josephson phase qubit, consisting of a superconducting loop interrupted by a Josephson junction with a well-defined phase difference across the junction. Under certain conditions, the loop forms a two-level system with eigenfrequencies in the gigahertz range that evolves according to the laws of quantum mechanics.

In this session we will present our latest measurements.

TT 36.33 Thu 14:00 Poster A

Towards Quantum Experiments in Electromechanical Systems — •Fredrik Hocke[1], Stefan Weis[2], Xiaoqing Zhou[2], Thomas Niemczyk[1], Edwin P. Menzel[1], Georg Wild[1], Hans Huebl[1], Achim Marx[1], Tobias Kippenberg[2,3], and Rudolf Gross[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Max Planck Institut für Quantenoptik, Garching , Germany — [3]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

During the last years optomechanics has developed into a wide playground, allowing the study of quantum mechanics in a literal sense. Here, a light field is coupled to the mechanical motion of a resonator and exploited to cool down the mechanical mode eventually to its quantum mechanical ground state. In our case, the light field is realized in form of microwave photons in a superconducting on-chip cavity and the mechanical oscillator as freely suspended, nanometer-sized beam. This on-chip layout allows implementing experiments at low temperatures in a straightforward way. We present first experimental results on the characterization of nanometer-sized beams and beam-resonator hybrids. This work is supported by the Excellence Cluster "Nanosystems Initiative Munich (NIM)".

TT 36.34 Thu 14:00 Poster A

Feedback and Rate Asymmetry of the Josephson Junction Noise Detector — •Daniel Urban[1] and Hermann Grabert[1,2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany

The Josephson junction noise detector measures the skewness of non-Gaussian noise via the asymmetry of the rate of escape from the zero-voltage state upon reversal of the bias current. The feedback of this detector on the noise generating device is investigated in detail [1]. Concise predictions are made for a second Josephson junction as noise generating device. The strong nonlinearity of this component implies particularly strong feedback effects, including a change of sign of the rate asymmetry as the applied voltage approaches twice the superconducting gap.

[1] D. F. Urban and H. Grabert, Phys. Rev. B **79**, 113102 (2009).

TT 37: MLT: Poster Session

Time: Thursday 14:00–18:00 Location: Poster A

TT 37.1 Thu 14:00 Poster A

Superconductor-insulator transition in TiN films — •David Kalok[1], Ante Bilušić[1,2], Tatyana Baturina[3], Mikhaïl Baklanov[4], Valerii Vinokur[5], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Department on Physics, University of Split, Croatia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia — [4]IMEC, Leuven, Belgium — [5]Materials Science Division, Argonne National Laboratory, USA

In the past years, several unusual features of the insulating state terminating superconductivity in strongly disordered superconducting films have been revealed. We investigate low-temperature transport properties of thin TiN films on the insulating side of the superconductor-insulator transition (SIT). At higher temperature, $T \geq 50\ mK$, we observe a thermally activated conductance with activation energy $E_A/k_b = 0.5\ K$. At lower temperatures, IV measurements show a threshold voltage V_T, below which the conductance is orders of magnitudes lower. Activation energy E_A and threshold V_T depend in a non-monotonic way on magnetic field and moreover on the orientation of the magnetic field. The influence of electron heating on the switching mechanism is investigated. We explore the B-Field driven SIT in parallel and perpendicular field.

TT 37.2 Thu 14:00 Poster A

Search for quantum phases in frustrated systems — •Ansgar Kalz, Andreas Honecker, Sebastian Fuchs, and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We use quantum Monte-Carlo simulations to analyse phase diagrams of spin models on two-dimensional lattice geometries with competing interactions. The frustration suppresses the classically ordered phases and we expect the emergence of phases which originate by quantum fluctuations like superfluidity or dimer ordering.

For the square lattice with nearest and next-nearest neighbour interaction the magnetically ordered states are the Néel state and the collinear state. The phase transitions for these classically ordered phases tend towards zero temperature for increasing quantum fluctuations. In a certain region of frustration and quantum fluctuations the classical phases vanish completely and new groundstates appear. We analyse the nature of these new groundstates by calculating correlations of multiple spin interactions.

We present the behaviour of the classical and quantum mechanical order parameters like staggered magnetisation, superfluid density and dimer-dimer correlations in temperature and parameter space. We show finite and zero temperature phase diagrams and look at the properties of the emerging phase transitions.

TT 37.3 Thu 14:00 Poster A

Anomalous diffusion of strongly correlated fermions in an optical lattice — •Stephan Mandt[1], David Rasch[1], Theo Costi[2], and Achim Rosch[1] — [1]Institute of Theoretical Physics, Cologne, Germany — [2]Forschungszentrum Jülich, Germany

We study the expansion of a cloud of strongly correlated fermionic atoms in an optical lattice. Initially, the cloud has a narrow Gaussian density profile but it spreads apart after being released from an additional confining potential. In experiment, it is observed that the particles at the edge of the cloud move ballistically. This ballistic motion is governed by the cubic symmetry of the lattice which is reflected in the characteristic shape of the expanding cloud. In contrast, the atoms at the center of the cloud are dominated by interparticle collisions and behave diffusively. Modelling the system in the framework of the Boltzmann equation, we describe the spatial crossover from ballistic to diffusive dynamics and recover the experimental observations made by the group of Immanuel Bloch.

TT 37.4 Thu 14:00 Poster A

Low temperature dielectric properties of $^{88}Sr^{48}TiO_3$ — •F. Aslan[1], T. Peichl[1], G. Fischer[1], S. Schöllhammer[2], W. Menesklou[2], and G. Weiss[1] — [1]Physikalisches Institut — [2]Institut für Werkstoffe der Elektrotechnik, KIT 76128 Karlsruhe

It is well established that the behavior of amorphous solids at low temperatures is governed by atomic two-level tunneling systems with properties as detailed in the phenomenological tunneling model. However, this genuine tunneling model fails to explain the recently measured magnetic field dependence of the low temperature dielectric properties of glasses. Extensions of the tunneling model that include a coupling of the lateral motion of the atoms to the orientation of their nuclear quadrupole moment could explain at least some of the observed magnetic field effects. In our studies, we try to directly demonstrate this idea by comparing the dielectric behavior of $SrTiO_3$-ceramics made of isotopes of natural abundance with that of samples enriched with the isotopes ^{88}Sr and ^{48}Ti which have no nuclear quadrupole moment. In contrast to the expectation, the magnetic field effects of the dielectric constant of $^{88}Sr^{48}TiO_3$ were not smaller but even 4.5 times larger than those of SrTiO3 with natural components. SQUID-magnetometer measurements revealed that our $^{88}Sr^{48}TiO_3$-material contains about 6 times more ferromagnetic and two orders of magnitude more paramagnetic impurities than our natural $SrTiO_3$. Although ruled out by other authors, this again rises the question whether the sensitivity to magnetic fields of the dielectric properties of glasses at low temperatures is caused by magnetic impurities.

TT 37.5 Thu 14:00 Poster A

Low temperature vibrating reed measurements of Zr based metallic glasses — •C. Adler, W. Mohr, T. Peichl, and G. Weiss — Physikalisches Institut, Karlsruher Institut für Technologie 76128 Karlsruhe

The low temperature thermal and acoustic behavior of glasses, dielectric or metallic, is dominated by two-level systems caused by the tunneling of small groups of atoms between two almost equivalent sites. Specific distributions of the relevant parameters are suggested by the well established tunneling model. Acoustic measurements of various superconducting metallic glasses demonstrate that conduction electrons not only drastically change the dynamics of tunneling systems as compared to insulating glasses but also seem to influence the apparent density of states of the tunneling systems. The advent of bulk metallic glasses (BMG) considerably facilitates acoustic experiments. Our vibrating reed measurements of the BMG $Zr_{59}Ti_3Cu_{20}Ni_8Al_{10}$ and the splat cooled metallic glass $Zr_{65}Al_{7.5}Cu_{27.5}$ reveal interesting differences in the internal friction which presumably reflect the quite different cooling rates in the preparation procedures of the two metallic glasses.

TT 37.6 Thu 14:00 Poster A

Investigation of mechanical losses in bulk materials for gravitational wave detectors — •Christoph Heilmann[1], Daniel Heinert[1], Christian Schwarz[1], Andreas Tünnermann[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Straße 15, 07745 Jena, Germany

One of the dominating noise sources in gravitational wave detectors is thermal noise of the optical components. The Brownian motion of the bulk sample's surface is directly coupled to the mechanical loss of the substrate material.

We present measurements of the mechanical loss for different substrate materials in a temperature range from 5 K to 300 K. Thereby, we focus on monocrystalline samples of calcium fluoride, silicon and sapphire. Silicon – as a low loss material – is the most promising candidate material for the use in gravitational wave detectors. We demonstrate mechanical losses as low as 1.8×10^{-9} at a temperature of 5.6 K. We present a summary of possible damping mechanisms in the different materials and compare them to the experimental values obtained from our cryogenic loss spectroscopy.

This work is supported by the DFG under contract SFB TR7.

TT 37.7 Thu 14:00 Poster A

Dielectric spectroscopy on magnetically doped relaxor ferroelectrics — •Daniel Niermann and Joachim Hemberger — 2. Physikalisches Institut, Universität zu Köln

Materials showing a mutual dependence between magnetization and electric polarization in external fields got into the focus of recent research during the last years, not at least due to possible technical applications. It was recently shown that magnetoelectric behaviour can not only be observed in materials exhibiting long-range ferromagnetic and ferroelectric orders, so called multiferroics, but also in disordered multiglasses with two different glassy states. We performed Fe-doping on the B-sites (Ti^{4+}) of the host crystal $SrTiO_3$, while adjusting the over-all valency by simultaneous doping of non-magnetic La^{3+}-ions on the A-sites. For increased doping a transition from quantum-paraelectric to relaxor-ferroelectric behaviour is expected. Polycrystalline samples of $Sr_{1-x}La_xTi_{1-x}Fe_xO_3$ (x = 0.01, 0.05, 0.10) were prepared by a standard ceramic process and characterized by x-ray diffractometry, REM-EDX and measurements of magnetic susceptibility. Relaxor-states and field dependent dielectric properties of the sample-compound were studied by broadband dielectric spectroscopy. The measurements were performed down to low temperatures using an impedance-analyser and a standard two electrode parallel-plate capacitor geometry.

TT 37.8 Thu 14:00 Poster A

Finite-density corrections to the Unitary Fermi gas: A lattice perspective from DMFT — •Antonio Privitera[1,2], Massimo Capone[1], and Claudio Castellani[1] — [1]CRS SMC, CNR-INFM and Dipartimento di Fisica, Universita di Roma La Sapienza, Piazzale Aldo Moro 2, I-00185 Roma, Italy — [2]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany

We investigate the approach to the universal regime of the dilute unitary Fermi gas as the density is reduced to zero in a lattice model [1]. To this end we study chemical potential, superfluid order parameter and internal energy of the attractive Hubbard model in three different lattices: a cubic lattice, a Bethe lattice with a semicircular DOS, and a lattice gas with parabolic dispersion and a sharp energy cutoff. The model is solved using Dynamical Mean-Field Theory, that treats directly the thermodynamic limit and arbitrarily low densities, eliminating finite-size effects. The evolution to the low-density limit is smooth and it does not allow to define an unambiguous low-density regime. Such finite-density effects are significantly reduced using the lattice gas, and they are maximal for the cubic lattice. Even though DMFT is bound to reduce to the more standard static mean field in the limit of zero density due to the local nature of the self-energy and of the vertex functions, it compares well with accurate Monte Carlo simulations down to the lowest densities accessible to the latter [2].

[1]A. Privitera *et al.*, arXiv:0909.1298

[2] A. Bulgac *et al.*, Phys. Rev. A **78**, 023625 (2008)

TT 37.9 Thu 14:00 Poster A

Lattice small polaron theory for Bose-Fermi mixtures — •Antonio Privitera, Mohammad Reza Bakhtiari, and Walter Hofstetter — Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany

We present a generalization of small polaron theory describing polaronic effects in strongly imbalanced Bose-Fermi mixtures in the case where both Bosons and Fermions are trapped in the same optical lattice [1]. This allows us to estimate how the hopping of a single Fermionic impurity immersed in a large BEC is renormalized for different temperatures and coupling regimes. The presence of a lattice strongly affects the properties of the Bogolubov modes, which play the same role as phononic excitations in the context of condensed matter physics. We show that these lattice effects cannot be simply included within a mass renormalization, even at zero temperature. Finally we discuss the limits of validity of the approach and compare our results with recent experiments on strongly imbalanced Bose-Fermi mixtures.

[1] T. Best *et al.*, Phys. Rev. Lett. **102**, 030408 (2009)

TT 37.10 Thu 14:00 Poster A

Canted Antiferromagnetic Order of Imbalanced Fermi-Fermi Mixtures in Optical Lattices: a Dynamical Mean-Field Perspective — •Irakli Titvinidze[1], Michiel Snoek[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Institute for Theoretical Physics, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

We investigate antiferromagnetic order of repulsively interacting fermionic atoms in two- and three-dimensional optical lattices by means of Dynamical Mean-Field Theory. Special attention is paid to the case of an imbalanced mixture, in which case the antiferromagnetism is canted, i.e. the staggered component perpendicular to the applied field. We take into account the presence of the underlying harmonic trap, both within a local density approximation and by performing full Real-Space DMFT [1] calculations. No Stoner instability towards a ferromagnetic phase is found. Phase separation is only observed for large repulsion and strong imbalance.

TT 37.11 Thu 14:00 Poster A

Local mean-field theory for quantum phase transitions in disordered Bose-Hubbard systems — •Astrid Elisa Niederle and Heiko Rieger — Theoretical Physics, Saarland University, D-66041 Saarbrücken

The Bose-Hubbard model represents a theoretical approach to study Bose-Einstein condensates in diverse kinds of optical lattices. We focus on the influence of disorder in these systems and especially the phase transitions in dependence of the system parameters and study the properties of a Bose-Einstein condensate in an optical trap with an equally distributed disorder in the on-site energies. We develop a local mean-field approach to investigate the transitions between the three competing phases (superfluid, Mott insulator, Bose glass), which can be observed in dependence of the system parameters. Beside the global changes of the phase diagram in dependence of the geometry, finite size effects are discussed.

TT 37.12 Thu 14:00 Poster A

Variational Cluster Approach for Bosonic Systems — •Stephan Filor and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen

We propose a variational cluster ansatz to bosonic systems which is based on Potthoff's self-energy functional approach. To find a suitable cluster approximation it takes advantage of certain properties of the Baym-Kadanoff formalism which treats the grand canonical potential as a functional of the Green's function respectively the self-energy.

In our ansatz the bosonic operators are used within the Nambu formalism to allow for a condensed phase, for which we additionally introduce a reservoir coupled to the cluster sites as a variational parameter. The approach is tested for simple lattices.

TT 37.13 Thu 14:00 Poster A

Dynamical mean-field theory for bose-fermi mixtures in optical lattices — •Krzysztof Byczuk[1] and Dieter Vollhardt[2] — [1]Institute of Theoretical Physics, University of Warsaw*, ul. Hoza 69, PL-00-681 WARSZAWA — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism*, Institute of Physics, University of Augsburg*, D-86135 Augsburg, Germany

We derive a dynamical mean-field theory for mixtures of interacting bosons and fermions on a lattice (BF-DMFT) [1,2]. The BF-DMFT is a comprehensive, thermodynamically consistent framework for the theoretical investigation of Bose-Fermi mixtures and is applicable for arbitrary values of the coupling parameters and temperatures. It becomes exact in the limit of high spatial dimensions d or coordination number Z of the lattice. In particular, the BF-DMFT treats normal and condensed bosons on equal footing and thus includes the effects caused by their dynamic coupling. Using the BF-DMFT we investigate two different interaction models of correlated lattice bosons and fermions, one where all particles are spinless (model I) and one where fermions carry a spin one-half (model II). In model I the local, repulsive interaction between bosons and fermions can give rise to an attractive effective interaction between the bosons. In model II it can also lead to an attraction between the fermions.

[1] K. Byczuk and D. Vollhardt, Phys. Rev. B 77, 235106 (2008)
[2] K. Byczuk and D. Vollhardt, Ann. Phys. (Berlin) 18, 622 (2009)

TT 37.14 Thu 14:00 Poster A

Phase diagrams for spin-1 bosons in an optical lattice — •Ming-Chiang Chung — National Center for Theoretical Sciences, Hsinchu, Taiwan

In this talk, the phase diagrams of a polar spin-1 Bose gas in a three-dimensional optical lattice with linear and quadratic Zeeman effects both at zero and finite temperatures are obtained within mean-field theory. The phase diagrams can be regrouped to two different parameter regimes depending on the magnitude of the quadratic Zeeman effect Q. For large Q, only a first-order phase transition from the nematic NM phase to the fully magnetic FM phase is found, while in the case of small Q, a first-order phase transition from the nematic phase to the partially magnetic PM phase, plus a second-order phase transition from the PM phase to the FM phase is obtained. If a net magnetization in the system exists, the first-order phase transition causes a coexistence of two phases and phase separation: for large Q, NM and FM phases and for small Q, NM and PM phases. The phase diagrams in terms of net magnetization are also obtained.

TT 37.15 Thu 14:00 Poster A

Multiple condensed phases in interacting Bose systems — •Michael Männel[1], Klaus Morawetz[2,3], Pavel Lipavský[4,5], and Michael Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany — [3]International Center of Condensed Matter Physics, University of Brasilia, 70904-970, Brasilia-DF, Brazil — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [5]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 unphysical processes in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature. For attractive interaction, an Evans-Rashid transition occurs between a quasi-ideal Bose gas and a BCS-like phase with a gaped dispersion. The gap decreases with increasing density and vanishes at a critical density where the single-particle dispersion becomes linear for small momenta indicating Bose-Einstein condensation. The investigation of the pressure shows however, that the mentioned quantum phase transitions might be inaccessible due to a preceding first order transition.

TT 37.16 Thu 14:00 Poster A

Three-body interacting cold polar molecules in one dimension — •Gregor Foltin[1], Andreas Läuchli[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany — [2]Max Planck Institut für Physik komplexer Systeme, Nöthnitzerstrasse 38, 01187 Dresden, Germany

It has been proposed recently [1] that cold polar molecules in an optical lattice can be tuned to a regime of strong three-body interactions. It is therefore an interesting question what kind of quantum phases are stabilized in a system of hardcore bosons interacting via two- and three-body forces. The effects of pure but longer range three-body interactions has been studied on the square lattice giving a cascade of solid and also supersolid phases [2]. The leading two- and three-body term has been investigated in one dimension [3] and on the honeycomb model [4]. Here we are interested in the effects of subleading terms for the one-dimensional case. To this end we use a classical approach, fermionic mean-field theory, and exact diagonalizations in order to map out the zero-temperature phase diagram.

[1] H.P. Büchler, A. Micheli, P. Zoller, Nature Physics 3, 726 (2007).
[2] K.P. Schmidt, J. Dorier, and A. Läuchli, Phys. Rev. Lett. 101, 150405 (2008).
[3] B. Capogrosso-Sansone, S. Wessel, H.P. Büchler, P. Zoller, G. Pupillo, Phys. Rev. B 79, 020503(R) (2009).
[4] L. Bonnes, H.P. Büchler, and S. Wessel arXiv:0911.0312.

TT 37.17 Thu 14:00 Poster A

Vortices in rotating quantum droplets — •Henri Saarikoski[1,4], Ari Harju[2], Matti Manninen[3], and Stephanie Reimann[1] — [1]Mathematical Physics, Lund University, SE-22100 Lund, Sweden — [2]Department of Applied Sciences and Helsinki Institute of Physics, P.O. Box 4100, FI-02015 HUT, Finland — [3]Nanoscience Center, Department of Physics, FI-40014 University of Jyväskylä, Finland — [4]Present address: University of Regensburg, 93040 Regensburg

The structure of rotating quantum systems is fundamentally determined by how these systems carry angular momentum. A priori very different systems share some basic properties that appear universal. Examples are the reduced dimensionality due to rotation and formation of vortices, as well as composites of particles and vortices. These phenomena may occur both in bosonic and fermionic systems and regardless of the form of the interparticle potential. Due to this universality, rotating quantum liquids can be described theoretically by using similar concepts and analogous vocabulary.

Our review work aims to give a unified view of the progress in the fields of finite rotating quantum systems, setting the emphasis on the structural properties of the many-body state. The focus will be on the theoretical results and development of many-body techniques used in this context. We highlight the similarities between rotating bosonic and fermionic systems, taking the analogy between electronic states in quantum dots, and bosonic states in rotating Bose-Einstein condensates as a recurring example.

TT 37.18 Thu 14:00 Poster A

Exploring magnetic solitons using DMRG — Anton Wöllert and •Andreas Honecker — Institut für theoretische Physik -

Friedrich Hund Platz 1, Göttingen, Germany

We study the anisotropic ferromagnetic frustrated Heisenberg spin-1/2 chain out of equilibrium. The aim is to find solitonic structures using the adaptive time dependent density matrix renormalization group (t-DMRG). This should be achieved by quenching the system from an excited state and examining the real time evolution. Especially parts of the phase diagram are analyzed, where solitons can be observed in the classical model.

TT 37.19 Thu 14:00 Poster A

Quenches in three dimensional ultracold bosonic systems — •Akos Rapp and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, 50937 Köln

Ultracold atoms provide clean systems to study phenomena related to the competition between kinetic, interaction and confinement energies under flexible experimental conditions. Confinement leads to phases which are absent in a homogeneous system, and the "Mott cake" structure in a strongly repulsing bosonic system is probably the most spectacular example. We study the bosonic Hubbard model in a three dimensional harmonic trap combining rapid quenches with adiabatic changes of the system parameters. Using a combination of the bosonic Gutzwiller approximation and high-temperature expansions we analyze how much entropy is generated during the quenches and investigate which phases can be stabilized in the trap.

TT 37.20 Thu 14:00 Poster A

Probing Local Relaxation of Cold Atoms in Optical Superlattices — •Andreas Flesch[1,2], Marcus Cramer[3], Ian P. McCulloch[4], Jens Eisert[3,5], and Ulrich Schollwöck[1,6] — [1]Institut für Theoretische Physik C, RWTH Aachen University, 52056 Aachen — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungzentrum Jülich, 52425 Jülich — [3]Institute for Mathematical Sciences, Imperial College London, SW7 2PE London — [4]School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072 — [5]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam — [6]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, 80333 München

Ultracold atoms in optical superlattices are a promising candidate for the experimental investigation of relaxation processes in coherent non-equilibrium dynamics of quenched quantum systems. We study the evolution of a particular initial state prepared in a superlattice structure under a Bose-Hubbard Hamiltonian in the entire range of interaction strengths using mainly a t-DMRG approach [1,2]. By the investigation of certain correlation functions, we show that the proposed setup allows to experimentally probe signatures of local relaxation of subsystems in non-equilibrium dynamics. First experimental results [3] are in a very good agreement with the theoretical predictions.

[1] M. Cramer et al., PRL 101, 063001 (2008)
[2] A. Flesch et al., PRA 78, 033608 (2008)
[3] S. Trotzky and I. Bloch, private communication

TT 37.21 Thu 14:00 Poster A

Spin Coherence in Graphene — •Matthias Droth and Guido Burkard — Universität Konstanz, 78464 Konstanz, Germany

Spin relaxation in a quantum dot can occur due to interaction with nuclear spins or phonons. Since $\mu_N \ll \mu_{e^-}$ the former coupling is supressed for typical magnetic fields slightly above the mT regime such that phonon coupling is the dominant effect. For a rectangular dot on a graphene nano ribbon we calculate T_1 assuming the relaxation to occur via spin-orbit and electron-phonon interaction as proposed in [1]. In order to obtain the spectrum and density of states of the relevant acoustic phonons we start from a continuum model and derive the dispersion relations for in-plane and out-of-plane acoustic phonons. Due to open boundary conditions at the ribbon edges the usual q^2 dependence for out-of-plane modes in bulk is cut off at the zone center where we find a linear dispersion. The transverse and longitudinal sound velocities of the in-plane modes match well with literature values [2].

[1] A. V. Khaetskii, Y. V. Nazarov; Physical Review B **64**, 2001
[2] L. A. Falkovsky; arXiv:0802.0912v1

TT 37.22 Thu 14:00 Poster A

Signatures of Klein tunneling in the Aharonov-Bohm effect in graphene rings — •Jörg Schelter[1], Dan Bohr[2], and Björn Trauzettel[1] — [1]Department of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Department of Physics and Astronomy, University of Basel, CH-4056 Basel, Switzerland

We numerically investigate the effect of Klein tunneling on the Aharonov-Bohm oscillations in graphene rings using a tight-binding model with nearest neighbor couplings. In order to introduce Klein tunneling into this system, we apply an electrostatic potential to one of the arms of the ring, such that this arm together with the two adjacent leads form either a $nn'n$- or npn-junction. The former case corresponds to normal tunneling and the latter case to Klein tunneling.

We find that the transmission properties strongly depend on the smoothness of the two pn-junctions in series. In particular, for sharp junctions the amplitude profile is symmetric around the charge neutrality point in the gated arm, whereas for smooth junctions the Aharonov-Bohm oscillations are strongly suppressed in the Klein tunneling regime.

TT 37.23 Thu 14:00 Poster A

Work function engineering and doping of graphene — •Burkhard Sachs[1], Tim Wehling[1], Alexander Lichtenstein[1], and Mikhail Katsnelson[2] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

Realistic graphene samples are always subject to external perturbations, e.g., impurities, adsorbates or strains. We investigate doping effects on graphene originating from molecular adsorbates and strains by using density functional theory calculations. The impact of work function variations on real graphene devices is discussed and compared to other doping mechanisms, including chiral midgap states for monovalent adsorbates. Screening effects for adsorbate induced dipole moments are considered with the example of water molecules.

TT 37.24 Thu 14:00 Poster A

Bistability and oscillatory motion of natural nano-membranes appearing within monolayer graphene on silicon dioxide investigated by scanning tunneling microscopy — •Marco Pratzer, Torge Mashoff, Viktor Geringer, Marcus Liebmann, and Markus Morgenstern — II. Physikalisches Institut B and JARA-FIT, Otto-Blumenthal-Straße, RWTH Aachen, 52074 Aachen

The truly two-dimensional material graphene is an ideal candidate for nanoelectromechanics due to its large strength and mobility. Monolayer graphene flakes were prepared by mechanical exfoliation on a SiO_2 substrate. Using scanning tunneling microscopy at $T = 4.8\,\mathrm{K}$ we found natural nano-membranes within the intrinsic rippling of the graphene with a size down to 3 nm. The membranes could be lifted either reversibly or hysteretically by the tip of the scanning tunneling microscope depending on the interacting forces of substrate, graphene and tip. Atomically resolved STM images show different atomic arrangements in compressed and relaxed graphene areas. The clamped-membrane model including van-der-Waals and dielectric forces explains the results quantitatively. By applying an AC bias voltage we could oscillate the nano-membranes, which might lead to a completely novel approach to controlled quantized oscillations or single atom mass detection.

TT 37.25 Thu 14:00 Poster A

Valley degeneracy of graphene nanoribbons — •Franziska Maier and Guido Burkard — Universität Konstanz, D-78457 Konstanz, Germany

Graphene quantum dots are fabricated by cutting the desired shape out of graphene sheets. Their electronic properties are highly influenced by the shape of lattice termination and effects due to local electric fields and strained bonds.

To allow the design of quantum dots showing specific electronic properties, we investigated the dispersion relation and valley degeneracy of graphene nanoribbons cut in arbitrary directions regarding the lattice. Therefore boundary conditions in form of a local linear restriction on the spinor wave function [1] were used.

[1] A. Akhmerov and C.W.J. Beenakker, Phys. Rev. B **77**, 085423 (2008).

TT 37.26 Thu 14:00 Poster A

Low Energy Effective Theory for Nanotubes with Spin Orbit coupling — •Stephan Weiss[1], Frederik Treue[1], Emmanuel Rashba[2,3], and Karsten Flensberg[1] — [1]Niels Bohr Institute & Nano-Science Center, University of Copenhagen — [2]Department of

Physics, Harvard University, Cambridge, Massachusetts 02138, USA — [3]Center for Nanoscale Systems, Harvard University, Cambridge, Massachusetts 02138, USA

Spin orbit coupling in nanotubes has motivated experimental and theoretical research activities recently. Due to the interplay between curvature and atomic SO coupling, the single particle spectrum exhibits a finite gap at zero magnetic field between the two Kramers doublets. We present different approaches in order to derive the low energy effective Hamiltonian [1]. First based on symmetry arguments we derive the Hamiltonian. This settles the number of free coupling constants as well as the general form of the Hamiltonian. In a second approach, we employ a four band tight binding calculation for the π and σ bands of graphene and include curvature between the bonds and atomic spin orbit coupling in lowest order perturbation theory. We are able to give estimates for the coupling constants, based on the known tight binding parameters for plane graphene. A fully numerical approach, which involves a Hückel approximation on the overlap integrals between neighboring atoms is used to calculate the SO coupling parameter for different chiralities of nanotubes and the zero field gap for electrons and holes.

[1] S. Weiss, F. Treue, E.I. Rashba, and K. Flensberg, in preparation.

TT 37.27 Thu 14:00 Poster A

Quasi-continuous generation of structual defects in graphene — •Verena Martin, Michael Krieger, Johannes Jobst, Daniel Waldmann, and Heiko B. Weber — Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

High-quality epitaxal graphene at low temperatures has metallic conductivity. This regime can be destroyed by the generation of structual defects. In our experiment, we carry out resistance measurements at low temperatures ($T \sim 4$ K) and slowly increase the amount of disorder by ion bombardement *in situ*. The implantation dose can be limited down to ~ 100 per μm^2 ion impacts per implantation step. An increase of the resistance by several orders of magnitude with increasing implantation dose is found. The transition between the metallic and the insulating regime is discussed.

TT 37.28 Thu 14:00 Poster A

Wave-packet propagation in graphene — •Viktor Krückl[1] and Tobias Kramer[1,2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

The unique electronic structure of graphene generates remarkable phenomena like the anomalous quantum Hall effect or the zitterbewegung. Our main focus are time-dependent effects in semiconductors with a major emphasis on zero gap semiconductors like graphene. We investigate the time evolution of wave packets in a perpendicular magnetic field and report about the collapses and revivals of initially localized cyclotron wave packets[1]. For complex setups we present an algorithm which is capable of solving the time-dependent scattering problem in arbitrary shaped potentials and magnetic fields. With this we study the scattering of wave-packets on ripples and impurities.

[1] Viktor Krueckl and Tobias Kramer, New J. Phys. 11 093010 (2009)

TT 37.29 Thu 14:00 Poster A

Scanning tunneling spectroscopy of graphene islands on Ir(111) — •Dinesh Subramaniam[1], Viktor Geringer[1], Mike Pezzotta[1], Marcus Liebmann[1], Marco Pratzer[1], Carsten Busse[2], Thomas Michely[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen and JARA-FIT, 52074 Aachen — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln

Epitaxial graphene islands are produced by ethylene deposition at room Temperature and subsequent annealing to 1320 K [1]. dI/dU curves on Ir(111) and graphene islands look quite similar, while dI/dU images provide confined states within the islands in addition to standing waves around the islands. Edge states are observed at around +50 mV sample voltage and are additionally probed by magnetoresistance curves using a spin-polarized tip.

[1] J. Coraux, A.T. N Diaye, M. Engler, C. Busse, D. Wall, N. Buckanie, F.M. Heringdorf, R. van Gastel, B. Poelsema and T. Michely, New Journal of Physics 11, 023006 (2009)

TT 37.30 Thu 14:00 Poster A

Ballistic transport and counting statistics on disordered graphene — •Alexander Schüssler[1], Mikhail Titov[2,3], Pavel M. Ostrovsky[1], Igor V. Gornyi[1,2], and Alexander D. Mirlin[1,2,4] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK — [4]Institut für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

The full counting statistics for the charge transport through an undoped graphene sheet in the presence of strong potential impurities is studied. We develop two analytical approaches based on the scattering theory and on the Green function formalism, respectively. Treating the scattering off the impurity in the s-wave approximation, we calculate the impurity correction to the cumulant generating function. This correction is universal provided the impurity strength is tuned to a resonant value. In particular, the conductance of the sample acquires a correction of $16e^2/2\pi h$ per resonant impurity. Our results are fully supported by numerical simulations. We further analyze the crossover to the diffusive behavior with increasing system length and calculate the counting statistics in the latter regime for the case of random potential that does not mix two graphene valleys.

[1] M. Titov et al arXiv: 0908.3793

TT 37.31 Thu 14:00 Poster A

Spectral properties of coupled cavity arrays in one dimension — •Michael Knap, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

The experimental progress in controlling quantum optical and atomic systems, which has been achieved over the last few years, prompted ideas for new realizations of strongly-correlated many body systems, such as light-matter systems [1]. These systems consist of photons confined in optical cavities, which interact strongly with atomic-like structures. Similarly to the Bose-Hubbard model the light-matter systems exhibit a quantum phase transition from Mott to superfluid. Yet the physics of the latter is far richer as two types of particles are present.

We use the variational cluster approach (VCA) [2] to study the physics of light-matter models. This method allows to treat systems of large size and at zero temperature. In particular we evaluate the spectral functions of both photons as well as atomic-excitations [3]. Based on this information we are able to introduce polariton quasiparticles as appropriate, wave vector and filling dependent linear combinations of photons and atomic-like particles. Spectral properties are evaluated for the polariton particles and the weights of their constituents are analyzed. In addition we discuss improvements of VCA, more specifically the Q-matrix formalism, to deal with bosonic excitations.

[1] M. Hartmann, et al., Laser & Photonics Review **2**, 527 (2008).
[2] M. Potthoff, et al., Phys. Rev. Lett. **91**, 206402 (2003).
[3] M. Knap, E. Arrigoni, and W. von der Linden, arXiv:0912.4459.

TT 38: CE: Quantum-Critical Phenomena 2

Time: Friday 10:15–12:45 Location: H18

TT 38.1 Fri 10:15 H18

Low field spin dynamics of a Cu(II) S=1/2 antiferromagnetic Heisenberg chain studied by ^{14}N-NMR spectroscopy — •Marco Günther[1], Hannes Kühne[1], Matthias Falkner[2], Hans-Henning Klauss[1], K. Doll[3], C.P. Landee[4], and M.M. Turnbull[4] — [1]Institut für Festkörperphysik, TU Dresden — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig — [3]Institut für Mathematische Physik, TU Braunschweig — [4]DPC, Clark University, Worcester, USA

By means of ^{14}N-NMR spectroscopy we study the low field NMR frequency shift and electronic spin dynamics in $Cu(C_4H_4N_2)(NO_3)_2$

(CuPzN), which is one of the best experimental realizations of the antiferromagnetic S=1/2 Heisenberg chain model.

The observed pattern of angular dependent NMR frequencies is disentangled into magnetic and quadrupolar contributions. The electric field gradient tensor is determined and compared to density functional calculations at the nitrogen site. A comparison of the magnetic part of the NMR shift to a local dipole model of the electronic moments allows to construct the full hyperfine coupling tensor.

The experimentally observed anisotropy of the nuclear spin-lattice relaxation rate T_1^{-1} can be modulated with purely magnetic fluctuations, i.e. an isotropic dynamic structure factor and the magnetic coupling tensor derived from the static properties. Our results are compared with previous ^{13}C-NMR data in the low field regime of CuPzN [1].

[1] Kühne et al., Phys. Rev. B 80, 045110 (2009)

TT 38.2 Fri 10:30 H18

The concept of effective temperature in current carrying quantum critical states — •Stefan Kirchner[1] and Qimiao Si[2] — [1]Max Planck Institut fuer Physik komplexer Systeme — [2]Physics & Astronomy, Rice University, Houston, Texas

At a quantum critical point, a scale-invariant fluctuation spectrum implies the absence of intrinsic energy scales. The system is therefore readily driven out of equilibrium. The resulting non-linear response regime violates the fluctuation-dissipation theorem. We study the out-of equilibrium phenomena in a single electron transistor with ferromagnetic leads, which can be tuned through a quantum phase transition[1]. We consider the breakdown of the fluctuation-dissipation theorem and study the universal behavior of the fluctuation dissipation relation of various correlators in the quantum critical regime[2]. In particular, we explore the concept of effective temperature as a means to extend the fluctuation-dissipation theorem into the non-linear regime[3]. Such effective temperatures were introduced in the context of steady states in chaotic systems, and successfully used for non-stationary states in glassy systems.

[1] S. Kirchner et al.,PNAS 102, 18824 (2005).
[2] S. Kirchner and Q. Si, PRL 103, 206401 (2009).
[3] S. Kirchner and Q. Si, arXiv:0909.3925 (2009).

TT 38.3 Fri 10:45 H18

Quantum aging in a sub-Ohmic heat bath — •Peter Nalbach and Michael Thorwart — FRIAS, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg i.Br.

We show that the low-frequency modes of a sub-Ohmic bosonic heat bath generate a dynamical asymmetry for an intrinsically symmetric quantum spin$-1/2$, which induces a slowly-decaying quasiequilibrium for the spin resembling a generic "aging" dynamics. The symmetry breaking is related to the dynamic crossover between coherent and overdamped relaxation of the spin polarization. For nonequilibrium initial conditions, we identify a so far unknown phase, characterized by damped coherent oscillations in the localized phase. A zero-temperature phase diagram is sketched.

Invited Talk TT 38.4 Fri 11:00 H18

Neutron Scattering Studies of Spin-Ladders — •Bella Lake[1,2], Alexei M. Tsvelik[3], Susanne Notbohm[1,4], D. Alan Tennant[1,2], Toby G. Perring[5,6], Manfred Reehuis[1], Chinnathambi Sekar[7,8], Gernot Krabbes[7], and Bernd Büchner[7] — [1]Helmholtz-Zentrum Berlin, Germany. — [2]Technische Universität Berlin, Germany. — [3]Brookhaven National Laboratory, U.S.A. — [4]University of St. Andrews, U.K. — [5]Rutherford Appleton Laboratory, U.K. — [6]University College London, U.K. — [7]IFW-Dresden, Germany. — [8]Periyar University, Salem, India.

This presentation will discuss magnetic excitations of two-leg spin-ladders with spin-1/2 moments and antiferromagnetic exchange interactions. Inelastic neutron scattering measurements will be presented for two ladders systems. $La_4Sr_{10}Cu_{24}O_{41}$ has a strong rung coupling and the excitations are found to consist of a gapped one-magnon mode and a two-magnon continuum. A large cyclic exchange is found which reduces the gap. In contrast $CaCu_2O_3$ has a weak rung interaction and a substantial cyclic exchange which drives the system gapless and quantum critical. At high energies the excitations are described well by the Bethe Ansatz and the field theory solution for a Luttinger liquid quantum critical point. At low energies a gap appears in the bonding susceptibility while the antibonding susceptibility remains gapless. The data is well described by a model where a gapped singlet bound-spinon mode is located at the bonding wavevector while a gapless triplet lies at the antibonding wavevctor. The antibonding susceptibility is critical and is at the Wess-Zumino-Novikov-Witten quantum critical point.

15 min. break

TT 38.5 Fri 11:45 H18

High-temperature signatures of quantum criticality in heavy-fermion compounds and the relation to two-impurity Kondo systems — •Johann Kroha[1], Laszlo Borda[1], Markus Klein[2], Friedrich Reinert[2], Pascal Simon[3], Oliver Stockert[4], and Hilbert von Löhneysen[5] — [1]Universität Bonn — [2]Universität Würzburg — [3]Université Joseph Fourier, Grenoble — [4]Max-Planck-Institut CPfS — [5]Karlsruhe Institute of Technology

We propose a new criterion for distinguishing the Hertz-Millis (HM) and local quantum critical (LQC) scenarios of magnetic quantum phase transitions (QPT) in heavy-fermion systems from their high-temperature behavior [1]. The criterion is based on our finding that the complete screening of a single Kondo spin can be suppressed by the RKKY coupling to the surrounding magnetic ions even without magnetic ordering. As a consequence, the signature of Kondo breakdown can be observed in spectroscopic measurements above the lattice coherence and magnetic ordering temperatures, where fluctuations of the Fermi surface and quantum critical fluctuations do not play a role. We show that the predicted dependence of the screening scale T_K on the RKKY coupling agrees in detail with recent scanning tunneling microscopy (STM) results on two-impurity Kondo systems. Applying the resulting high-temperature criterion to high-resolution photoemission measurements on $CeCu_{6-x}Au_x$ suggests that the QPT in this system is dominated by the LQC scenario.

[1] M. Klein *et al.*, Phys. Rev. Lett. **101**, 266404 (2008); Phys Rev. B **79**, 075111 (2009).

TT 38.6 Fri 12:00 H18

Multiscale Quantum Criticality: The Pomeranchuk Instability in Isotropic Metals — •Mario Zacharias[1], Peter Wölfle[2], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Institut für Theorie der kondensierten Materie, Universität Karlsruhe

As a paradigmatic example of quantum criticality with multiple scales, we study the Pomeranchuk instability of an isotropic metal in $d=2$ dimensions. The effective Ginzburg-Landau theory has two modes with different dynamics. There is a Landau-damped mode with a dynamical exponent $z_> = 3$ and a ballistic mode with $z_< = 2$. The two modes are coupled to each other and become critical at the very same point.

Since the effective dimension, $d+z_<$, of the ballistic mode equals the upper critical dimension, $d_+ = 4$, self-interactions lead to logarithmic singularities which we sum up by the renormalization group technique. We find that the ballistic mode governs the system at zero temperature, $T = 0$, although the $z_> = 3$ mode has the lower characteristic energy.

At finite T, the existence of two time scales results in a modified quantum-to-classical crossover, which extends over a parametrically large regime and leads to an intricate interplay of classical and quantum fluctuations. As a result, we find a universal T-dependence of the correlation length independent of the interaction amplitude.

The phase diagram and the critical thermodynamics also reflect the existence of multiple scales. In particular, there are two crossover lines between the low temperature and the quantum critical regime and the thermodynamic quantities differ in their sensitivity to them.

TT 38.7 Fri 12:15 H18

De-Haas van-Alphen oscillations in nonrelativistic U(1) gauge theories — •Lars Fritz[1] and Subir Sachdev[2] — [1]Universitaet zu Koeln, Institut fuer theoretische Physik, Zuelpicher Strasse 77, 50937 Koeln — [2]Harvard University, 17 Oxford Street, Cambridge, MA 02138, USA

We investigate magento-oscillations in the specific heat of non-relativistic fermions with a Fermi surface minimally coupled to a fluctuating U(1) gauge field. Our study is motivated by the recent observation of quantum oscillations in the underdoped cuprates, and by theoretical models of pocket Fermi surfaces realizing a non-Fermi liquid *algebraic charge liquid*. Our main result is the computation of the order 1/N correction to the Lifshitz-Kosevich expression for the oscillation amplitude in the dirty limit in a model with N species of fermions.

TT 38.8 Fri 12:30 H18

Real space renormalization group approach to the two-dimensional antiferromagnetic Heisenberg model with plaquette deformations — Andreas Fledderjohann, K.-H. Mütter, and •Andreas Klümper — Universität Wuppertal

The low energy behaviour of the $2d$ antiferromagnetic Heisenberg model is studied in the sector with total spins $S = 0$, 1, 2 by means of a renormalization group procedure, which generates a recursion formula for the interaction matrix of 4 neighbouring 'n clusters' of size $2^n \times 2^n$ from the corresponding quantities of the 'n clusters'. Conservation of total spin S is implemented. An inhomogeneous Heisenberg model with plaquette distortion is investigated. Depending on the plaquette-plaquette coupling J, we find two regimes: 'confinement' $J_c < J \leq 1$, where the singlet ground state forms an infinite ('confined') cluster in the thermodynamical limit. Here the singlet-triplet gap vanishes, which is the signature for long range spin-spin correlators. We find 'deconfinement' $0 \leq J < J_c$, where the singlet ground state 'deconfines' – i.e. factorizes – into finite n-clusters of size $2^n \times 2^n$, with $n \leq n_c(J)$. Here the singlet-triplet gap is finite and the gap exponent is determined. The critical value turns out to be $J_c = 0.4822...$ in the chosen truncation scheme.

TT 39: SC: Iron-Based Superconductors - 1111

Time: Friday 10:15–12:45 Location: H19

TT 39.1 Fri 10:15 H19

Insight, puzzles, and problems into the physics of Fe-pnictides from optics — •S.-L. Drechsler[1], H. Rosner[2], R. Schuster[1], F. Roth[1], M. Grobosch[1], M. Rotter[3], K. Koepernik[1], D. Singh[4], L. Zhang[4], D. Jorendt[3], N. Wizent[2], G. Behr[1], J. van den Brink[1], N.L. Wang[5], B. Buechner[1], and M. Knupfer[1] — [1]Inst. f. Festkörper- & Werkstoffforsch., Dresden — [2]Max-Planck-Inst. f. Chem. Physik fester Stoffe, Dresden — [3]Department Chemie & Biochemie, Ludwig-Maximillians Universität München, München — [4]Oak Ridge Nat. Lab., Oak Ridge, Tennessee, USA — [5]Beijing Nat. Lab., f. Cond. Mat. Phys. Inst. of Phys., Chin. Acad. of Sci., Beijing, China

We report Drude plasma frequencies (PF) for 12 Fe-pnictides from density functional theory (DFT) based calculations and compare them with experimental PF from reflectivity. The observed renormalization points to moderate many-body effects beyond the DFT like in ordinary transition metals. From large empirical background dielectric constants $\varepsilon_\infty \sim 10$, we estimate strong As and P polarizabilities which significantly reduce the Hubbard U_d from about 4 eV as suggested by significantly correlated [1] "bad metal" scenarios to below 2 eV pointing to rather strong polaronic effects [2]. We compare the dielectric and loss functions calculated within the RPA employing the DFT band structure for the parent compounds LaOFeAs and LaOFeP with single crystal derived data [1] and determine the frequency region with the strongest many-body effects beyond the RPA.

[1] M.M. Qazilbash *et al. Nature Phys.* **5**, (2009) 647.
[2] G. Sawatzky *et al. Europhys. Lett.* **86** (2009) 17006.

TT 39.2 Fri 10:30 H19

Nature of Magnetism in Iron Pnictides: an *ab initio* study — •Yu-Zhong Zhang, Ingo Opahle, Harald Jeschke, and Roser Valenti — Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

While it is commonly believed that magnetic-mediate pairing is the source of superconductivity in the iron-based superconductors, the nature of magnetism is still under debate. We apply *ab initio* molecular dynamics to investigate physical properties of LaOFePn, $BaFe_2Pn_2$ and LiFePn (Pn = As, Sb), so-called 1111, 122 and 111 compounds, respectively. We find that, with substitution of As by Sb, the stripe-type antiferromagnetic orderings are always enhanced. By calculating Pauli susceptibility, we attribute the enhancement of magnetization to the increase of instability at (π, π) when As is substituted by Sb. Furthermore, we study the magnetic and lattice properties of LaOFePn (Pn=P, As, Sb, Bi) as well as ScOFeP, ScOFeAs and YOFeP and argue that LaOFeSb would be a candidate for a superconductor with highest transition temperature among the investigated compounds. We further suggest that the absence of antiferromagnetic phase in LaOFeP and the presence in LaOFeAs are due to the competition of instability in Pauli susceptibility between (π, π) and $(0, 0)$ and therefore argue that superconductivity can only occur through doping in LaOFeSb.

TT 39.3 Fri 10:45 H19

Effect of doping and pressure on the high-T_c superconductor YOFeAs – comparison with LaOFeAs — •Ingo Opahle[1], Yu-Zhong Zhang[1], Hem C. Kandpal[2], Harald O. Jeschke[1], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt/Main, Germany — [2]IFW Dresden, P.O.B. 270016, D-01171 Dresden, Germany

The electronic structure of the high-T_c superconductor YOFeAs is calculated in the framework of density functional theory. Undoped YOFeAs is found to show the same spin density wave (SDW) instability as previously reported for LaOFeAs. The calculated Fe moment at ambient pressure is slightly smaller in YOFeAs than in LaOFeAs, but remains nonzero up to higher pressures compared to LaOFeAs. The Fermi surface shows similar strong nesting features like the one of LaOFeAs, stabilizing the spin density wave state. The effect of doping on the SDW state and implications for the superconductivity will be discussed.

TT 39.4 Fri 11:00 H19

High field ESR spectroscopy on (Gd,La)OFeAs superconductors — •A. Alfonsov[1], F. Murányi[2], V. Kataev[1], N. Leps[1], R. Klingeler[1], A. Kondrat[1], C. Hess[1], S. Wurmehl[1], J. Werner[1], G. Behr[1], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Universität Zürich, CH-8057 Zürich, Schweiz

In the present work we have studied polycrystalline samples of the $(Gd,La)O_{1-x}F_xFeAs$ superconductor with different levels of fluorine and gadolinium doping by means of high field/high frequency electron spin resonance (HF-ESR) spectroscopy. The Gd ESR signal is found to be sensitive to the magnetic phase transition from the paramagnetic to the spin density wave (SDW) state occurring in the parent (Gd,La)OFeAs compounds at temperatures $T_{SDW} \sim 130 - 150$K. In addition, in case of $LaO_{1-x}F_xFeAs$ with 5% Gd doping there is a clear indication of the suppression of the magnetic order in the samples with the superconducting ground state. The GdOFeAs samples reveal an antiferromagnetic coupling between Gd and Fe planes which reflects in the splitting and shift of Gd ESR line below $T_{SDW} \sim 130$K. Surprisingly, the 15% and 17% fluorine doped GdOFeAs samples, with T_c=20K and T_c=45K respectively, show the low-T ESR response similar to the undoped sample which indicates that the SDW is not completely suppressed in the SC samples. We compare HF-ESR data with results of transport measurements on these samples and discuss a possible contribution of magnetic rare-earths to the interplay between magnetism of the FeAs planes and superconductivity which evolves upon the fluorine doping.

15 min. break

TT 39.5 Fri 11:30 H19

Structural transition and magnetic ordering in $(Sm,Ce)FeAsO_{(1-x)}F_x$ — •Jorge E. Hamann-Borrero[1], Agnieszka Kondrat[1], Hemke Maeter[2], Ralf Feyerherm[3], Hans-Henning Klauss[2], Ruediger Klingeler[1], Christian Hess[1], Guenther Behr[1], Dimitri Argyriou[3], and Bernd Buechner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Institut fuer Festkoerperphysik, TU Dresden, D-01069 Dresden, Germany — [3]Helmholtz Zentrum Berlin. Albert Einstein Str.15 12489 Berlin

The tetragonal to orthorhombic transition of the layered compounds $(Sm, Ce)FeAsO_{(1-x)}F_x$ is studied by means of synchrotron x-ray diffraction, μSR and resistivity. We particularly focus on the onset of the SDW and superconducting states by monitoring the structural transition temperature T_s the magnetic ordering temperature T_N and the critical temperature T_c. In the case of $SmFeAsO_{(1-x)}F_x$ the SDW state is only gradually suppressed upon doping until it is entirely suppressed in favour of the superconducting state. This is in contrast to $CeFeAsO_{(1-x)}F_x$ where the SDW state is suppressed much more effi-

ciently and where superconductivity coexists with magnetism. Moreover, in further contrast to the findings by Zhao et al [1], we do not observe any orthorhombic distortion in superconducting samples.

[1] Zhao et al. Nature Materials, 2008, 7, 953-959.

TT 39.6 Fri 11:45 H19

Interplay of rare earth and FeAs magnetism in the iron pnictides GdOFeAs and CeOFeAs studied by muon spin relaxation and ^{57}Fe moessbauer spectroscopy — •N. Yèche[1], H.-H. Klauss[1], T. Dellmann[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], R. Klingeler[3], B. Büchner[3], and G. Behr[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

*R*OFeAs with R = La, Ce, Pr, Sm, Gd are the magnetic mother compounds of the iron pnictide superconductors. We have investigated the magnetic properties and the interplay of iron and rare earth magnetic order in GdOFeAs by means of muon spin relaxation (μ^+SR) and ^{57}Fe moessbauer spectroscopy and compare these to other undoped *R*OFeAs. We find that the Gd mother compound shows magnetic interaction between the rare earth and the FeAs layers similar to the Ce compound as allready reported in [1]. This results indicate that the rare-earth-FeAs electronic interaction is not crutial for the enhanced T_C in these systems.

[1] H. Maeter et al., Phys.Rev.B 80, 094524 (2009)

TT 39.7 Fri 12:00 H19

Anomalous Nernst Effect and spin fluctuations in $LaFeAsO_{1-x}F_x$ — •Christian Hess, Agnieszka Kondrat, Günter Behr, Rüdiger Klingeler, and Bernd Büchner — Institute for Solid State Research, IFW Dresden, Helmoltzstrasse 20, 01069 Dresden

We present Nernst-effect investigations on $LaFeAsO_{1-x}F_x$. In the parent compound the formation of a SDW state leads to a huge enhancement of the Nernst coefficient at $T < T_N$. Despite the absence of SDW order at underdoped superconducting doping levels, a similar anomalous behavior is also observed (with smaller magnitude), which is suggestive of a spin-fluctuation enhanced Nernst-effect. Interestingly, at optimal doping level the Nernst coefficient is only weakly temperature dependent and appears more conventional.

TT 39.8 Fri 12:15 H19

Unusual disorder effects in $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$ as revealed by NMR spectroscopy — •Franziska Hammerath[1], Stefan-Ludwig Drechsler[1], Hans-Joachim Grafe[1], Guillaume Lang[1], Günter Fuchs[1], Günter Behr[1], Ilya Eremin[2], Maxim Korshunov[2,3], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- & Werkstoffforschung, Dresden, Germany — [2]MPI für Physik komplexer Systeme, Dresden — [3]L.V. Kirensky Inst. of Physics, Sib. Branch of Russ. Acad. Scs., Krasnoyarsk, Russia

We report ^{75}As NMR measurements of the spin-lattice relaxation in the superconducting state of $LaFeAsO_{0.9}F_{0.1}$ and As-deficient samples, $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$ with a drastic change of the $1/T_1$ temperature dependence below T_c from a T^3-law for $LaFeAsO_{0.9}F_{0.1}$ to a T^β-law ($\beta = 5-6$) for $LaFeAs_{1-\delta}O_{0.9}F_{0.1}$. T_c and the slope of the upper critical field near T_c increase unexpectedly in the As-deficient samples. Our results are discussed in terms of non-universal SC gaps in Fe-pnictides and the effect of As deficiency as an exotic case when non-magnetic 'smart' impurities even stabilize an $s_\pm$−wave superconductor as well as within a scenario of a disorder driven change to conventional s_{++} superconductivity.

[1] H.-J. Grafe *et al.*, Phys. Rev. Lett. **101**, 047003 (2008).

TT 39.9 Fri 12:30 H19

Superconductivity and Ferromagnetism in $CeFeAs_{1-x}P_xO$ — •Anton Jesche, Cornelius Krellner, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The emergence of superconductivity in *R*FeAsO (R = rare earth) is connected with the suppression of the antiferromagnetic (AFM) ordering of Fe which can be achieved by the substitution of e.g. La by Sr, Fe by Co, As by P, and O by F. A special case here is $CeFeAs_{1-x}P_xO$, which shows AFM ordering of Fe at $T_N^{Fe} = 145\,K$ and AFM ordering of Ce at $T_N^{Ce} = 3.7\,K$ for pure CeFeAsO, whereas pure CeFePO is a paramagnetic heavy fermion metal. The substitution of As by P results in a decrease of T_N^{Fe} similar to F doping. An extrapolation suggests a complete suppression of the Fe ordering for $x \simeq 0.35$. However, instead of the 'expected' superconducitivity, the Ce ordering changes from AFM to FM at the disappearance of T_N^{Fe} and superconductivity emerges only in a small concentration range around $x = 0.3$. We report on measurements of electrical resistivity, specific heat, and magnetic susceptibility on single- and polycrystalline samples. Our results are supported by NMR, ESR, and μSR measurements and reveal a competition of superconductivity and ferromagnetic ordering of Ce.

TT 40: TR: Nanoelectronics III: Molecular Electronics 2

Time: Friday 10:15–13:45 Location: H20

Invited Talk TT 40.1 Fri 10:15 H20

Heating, Heat Conduction and Cooling in Molecular Junctions — •Abraham Nitzan[1], Michael Galperin[2], and Keiji Saito[3] — [1]School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel — [2]Department of Chemistry, University of California, La Jolla, CA, 92093, USA — [3]Graduate School of Science, University of Tokyo, 113-0033, Japan

Heating in molecular conduction junction depends on the balance between the rate of heat deposit by the electronic current and the efficiency of heat conduction away from the junction. I will review our recent work on such processes, then focus on models for current induced cooling in such systems.

TT 40.2 Fri 10:45 H20

Spin-polarized transport and thermoelectric properties of organometallic nanocontacts — •Steven Achilles[1], Volodymyr V. Maslyuk[1], Mads Brandbyge[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University, D-06120 Halle, Germany — [2]DTU Nanotech - Department of Micro- and Nanotechnology, Technical University of Denmark, DK-2800 Kongens Lynby, Denmark

Understanding the electronic and thermoelectric transport properties is the key issue in understanding new devices based on the principles of quantum mechanics. We present a theoretical study of the length dependence of both conductance and thermopower of organometallic vanadium-benzene molecules (V_nBz_{n+1}) sandwiched between magnetic Co(100) electrodes. We show that the molecules with $n \geq 3$ are efficient spin-filters. Namely, we find that the zero bias conductance of the majority electrons is small and decays exponentially with increasing length of the molecule and is in the tunneling regime while the minority electrons show metallic conductance. We show furthermore that the thermopower strongly depends on the length of the molecules and can even change sign as a function of length and temperature [1], and as a function of the relative orientation of the lead magnetizations [2].

[1] V. V. Maslyuk, S.Achilles, and I. Mertig, Solid State Communications, in press

[2] V. V. Maslyuk, S.Achilles, and I. Mertig, submitted

TT 40.3 Fri 11:15 H20

Single-Molecule Junctions: progress on gated mechanically controlled break junctions — •Stefan Ballmann, Stefan Wagner, Daniel Secker, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, D-91058 Erlangen, Germany

The mechanically controlled break junction (MCBJ) technique provides a powerful tool for immobilization of single molecules between two atomically sharp gold tips. However, three-terminal devices incorporating a gate electrode have not been realized on highly flexible substrates so far.

Here we report on promising methods to reproducibly structure an insulating layer in between two metal bridges within a three-step electron beam lithography process. The misalignment of both bridges has been successfully reduced below 25 nm. Moreover, the 15 nm insulat-

ing layer is highly stable upon bending the substrate while the leakage current remains below 1 nA at gate voltages of ± 4.5 V. The formation of atomically sharp gold contacts is not perturbed by the presence of the gate. We consider this as an important experimental step towards gated single-molecule contacts.

TT 40.4 Fri 11:45 H20

Electronic Transport Measurements on Si_4 Clusters — •Jochen Grebing[1,2], Rainer Dietsche[1], Gerd Ganteför[1], Thomas Kirchner[1], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, D-77457 Konstanz, Germany — [2]Forschungszentrum Dresden-Rossendorf, D-01328 Dresden, Germany

A still intriguing issue in the field of molecular electronics is the dependence of the transport properties of a molecule or cluster on the exact geometric realization of the contact at the atomic scale. Here, Si_4 clusters come in handy as they have a very well known rhombohedral geometry as well as a limited yet diverse number of possibilities of being contacted.

After soft-landing from the gas phase, using a mechanically controlled breakjunction technique, possibly single or few Si_4 clusters were contacted with atomically sharp tips and transport characteristics were measured. In addition to conductance histograms, current-voltage (IV) curves with and without clusters in the junction have been recorded. By comparison with the outcome of DFT calculations, the presence of the clusters could be identified in the histograms.

By fitting a resonant tunneling model to the IV curves, the coupling between the clusters and the leads as well as the energy difference of the molecular orbital contributing to the transport and the Fermi energy in the leads could be determined.

We thank F. Pauly for providing the DFT code and for introducing us to it's use, A. Erbe and J. C. Cuevas for the introduction to the resonant tunneling model and valuable discussions.

15 min. break

TT 40.5 Fri 12:30 H20

Density-functional study of transmission channel degeneracy in biphenyl-based single-molecule junctions — •M. Bürkle[1], F. Pauly[1], J.K. Viljas[1], and G. Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, KIT, 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, KIT, 76128 Karlsruhe, Germany

Using density functional theory, we investigate the charge transport for a series of biphenyl molecules [1]. The torsion angle between the two phenyl rings, and hence the degree of π conjugation is controlled by alkyl chains and methyl side groups. Considering different bonding geometries, we find that the conductance can vary by one order of magnitude for the same molecule [2]. We explain this by the different hybridisation of molecular states with those of the electrode. For all molecules, except for those with completely broken conjugation, we observe that the transmission is dominated by one channel, formed from the π electrons. For molecules with D_{2d} point group symmetry at 90°, two degenerate transmission channels should dominate the transport. However, in the molecular junction the electrodes reduce the symmerty and destroy the channel degeneracy. We show that for bonding geometries with a small degree of hybridisation between the electrode and the molecule, nevertheless, the channel degeneracy presists .

[1] A. Mishchenko, D. Vonlanthen, V. Meded, M. Bürkle, C. Li, I.V. Pobelov, A. Bagrets, J.K. Viljas, F. Pauly, F. Evers, M. Mayor, and T. Wandlowski, Nano Lett. (in press).

[2] M. Bürkle, F. Pauly, J.K. Viljas, V. Meded, A. Bagrets, and G. Schön (submitted).

TT 40.6 Fri 12:45 H20

Vibronic Cooling Mechanisms in Molecular Junctions — •Rainer Härtle[1], Michael Thoss[1], Roie Volkovich[2], and Uri Peskin[2] — [1]Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

We study vibrational nonequilibrium effects in charge transport through single-molecule junctions. Vibrational degrees of freedom of a molecular junction can be excited by inelastic electron transmission processes (local heating). Such processes are active even if the junction is in its vibrational ground state or thermal equilibrium, and manifest themselves in pronounced structures in the junction's transport characteristics. Cooling processes, however, can usually only occur if the junction is driven out of thermal equilibrium and require the junction to provide vibrational energy. We show that these processes may be as important as heating processes and that local cooling may induce transport phenomena, which are not present in thermal equilibrium. The methodology we have used to study these transport phenomena includes a nonequilibrium Green's function approach [1,2,3], and a master equation approach [3], which provide complementary schemes.

[1] M. Galperin, A. Nitzan, M. A. Ratner, Phys. Rev. B 73, 045314 (2006).

[2] R. Härtle, C. Benesch, M. Thoss, Phys. Rev. B 77, 205314 (2008).

[3] R. Härtle, C. Benesch, M. Thoss, Phys. Rev. Lett. 102, 146801 (2009).

TT 40.7 Fri 13:00 H20

Controlling the conductance of molecular wires by defect engineering: a *divide et impera* approach — •Daijiro Nozaki[1], Horacio M. Pastawski[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden, Germany — [2]Instituto de Física Enrique Gaviola (CONICET) and Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Córdoba, Argentina

Charge transport through 1D molecular systems connected between two contacts is influenced by several parameters such as the electronic structure of the molecule and the presence of disorder and defects. In this work, we have modeled 1D molecular wires connected between electrodes and systematically investigated the influence of both soliton formation and the presence of defects on properties such as the conductance and the density of states. Our numerical calculations have shown that the transport properties are highly sensitive to the position of both solitons and defects. Interestingly, the introduction of a single defect in the molecular wire which divides it into two fragments both consisting of an odd number of sites creates a new conduction channel in the center of the band gap resulting in higher zero-bias conductance than for defect free systems. This phenomenon suggests routes toward engineering molecular wires with enhanced conductance.

TT 40.8 Fri 13:15 H20

Electron transport through σ- and π-derived transmission channels — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Nanoscale electronic devices utilizing organic molecules, a possibility that was revealed in the 1970's, have been ceaselessly studied experimentally and theoretically. Nowadays, various organic molecules are recognized as potentially functional components for future molecular devices. In some molecules, the functionality may rely on the difference in electron transport properties between the σ and π states.

In this paper, we theoretically investigate the electron transport through σ- and π-derived transmission channels of organic molecules, and discuss the difference in transport properties between them. Transport calculations are carried out by means of the Lippmann-Schwinger equation and a real-space finite-difference method based on the density functional theory (DFT).

As a preliminary calculation, we have investigated the transport property of a benzene molecule sandwiched between a pair of planar metal electrodes, which involves both σ and π states. Although no electron transport through any of the two transmission channels are confirmed at the Fermi level, significant electron transmission through a π-derived channel can be seen at 0.7eV above the Fermi level. In the presentation, we are going to show electron transport properties of larger molecules followed by detailed discussions on the functionality.

TT 40.9 Fri 13:30 H20

Dynamical properties of charge transport in organic systems — •Pedro D Manrique[1,2], Rafael Gutierrez[1], Gotthard Seifert[2], and Gianaurelio Cuniberti[1] — [1]Institute Material Science and Max Bergmann Center of Biomaterials. Dresden University of Technology, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry. Dresden University of Technology, Dresden, Germany

We derive a non Markovian master equation for electronic transport including the interaction with external bosonic degrees of freedom. Within this formalism we calculate the time dependent current (TDC) at different temperatures. Results for the TDC are shown for different

values of the coupling to the bosonic environment and we found significant changes in the short-time dynamics. The electronic parameters of the model are calculated via a combination of molecular dynamics simulations with a density functional-based approach including dispersion energy corrections.

TT 41: CE: Low-dimensional Systems - Models 2

Time: Friday 10:15–12:30 Location: H21

TT 41.1 Fri 10:15 H21

Spatial Fluctuation effects on Orbital Selective Mott Transitions — •Hunpyo Lee[1], Yu-Zhong Zhang[1], Harald Jeschke[1], Roser Valenti[1], and Hartmut Monien[2] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Bethe Center for Theoretical Physics, Universität Bonn, 53115 Bonn, Germany

Orbital selective Mott transitions have been extensively studied on an anisotropic two-band Hubbard model in the framework of dynamical mean field theory with various impurity solvers. Effects of interband hybridization, spin flip and pair-hopping processes, anisotropy in the Hund's rule coupling and bandwidth, crystal field splitting, and inclusion of more bands have been already addressed in the past. In the present work we investigate the role of spatial fluctuations. By considering the dynamical cluster approximation and employing the continuous time quantum Monte Carlo method, we obtain a rich phase diagram of the anisotropic two-band Hubbard within a 4-site cluster. We analyze the cluster size dependence of the phase diagram by also performing 2-site cluster calculations and discuss possible Slater versus Mott physics.

TT 41.2 Fri 10:30 H21

Nonequilibrium electron spectroscopy of Luttinger liquids — So Takei, •Mirco Milletari, and Bernd Rosenow — Max-Planck-Institut für Festkörperforschung, Stuttgart

We theoretically study a Luttinger liquid (LL) driven out of equilibrium by injection of high-energy electrons. The electrons enter the LL locally, far away from any contacts, and at a fixed energy. Their spectral properties are detected at another spatial point some distance away by evaluating the average tunneling current from the LL into a resonant level with tunable energy. For energies slightly below the injection energy, the dependence of the detected current on the difference between injection and detection energies is described by a power law whose exponent depends continuously on the Luttinger parameter. In contrast, for tunneling into the chiral LL edge of a fractional quantum Hall state from the Laughlin sequence, we find that the detected current grows linearly with the energy difference, independent of the LL parameter determined by the inverse filling fraction. We develop a diagrammatic approach for the standard (non-chiral) LL which provides an intuitive physical picture for how the electrons can relax inside the wire.

TT 41.3 Fri 10:45 H21

Frustrated local moment models for Fe-pnictide magnetism — •Burkhard Schmidt, Mohammad Siahatgar, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The low energy spin excitations of the Fe pnictide parent compounds have been determined by inelastic neutron scattering and interpreted within the local moment $J_{1a,b}$-J_2 Heisenberg model with orthorhombic symmetry. This has led to alternative exchange models that strongly differ in the size of anisotropy. Although the compounds are itinerant the localised spin model can explain basic features of the excitations. The inherent frustration of this model leads to quantum fluctuations and possible moment reduction. We investigate this question in detail using spin wave approximation and partly exact diagonalisation Lanczos calculations for finite clusters. We find that the orthorhombic anisotropy stabilizes the columnar AF phase and its moment. For the exchange models proposed from inelastic neutron scattering we can exclude a strong influcence of frustration on the moment size. We also investigate dependence of magnetisation and susceptibility on field and temperature.

TT 41.4 Fri 11:00 H21

Phase diagram of the kagomerized Kitaev model — •Michael Kamfor[1], Julien Vidal[2], Sébastien Dusuel[3], and Kai Phillip Schmidt[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, Germany — [2]Université Pierre et Marie Curie Paris 06, France — [3]Lycé Saint-Louis, 75006 Paris, France

One of the simplest spin models exhibiting topological order and Z2-anyonic Abelian as well as non-Abelian excitations is the Kitaev model on a trivalent 2D-lattice. The two kinds of anyons live in different phases of the system. The model can be transformed with Majorana fermionization onto free fermions in a static gauge field and is thus exactly solvable. The originally defined Kitaev model leads to an effective square lattice in the isolated dimer limit. We introduce a new kind of Kitaev model where the limit of isolated dimers yields an effective kagome lattice. We investigate the phase diagram for certain gauges depending on the three-spin coupling for both Kitaev models. Interestingly the phase diagram strongly depends on the gauge choice and shows a rich amount of distinct Abelian and non-Abelian phases.

15 min. break

TT 41.5 Fri 11:30 H21

Breakdown of the topologically-ordered Z(3) Toric Code — •Marc Daniel Schulz[1], Sébastien Dusuel[2], Julien Vidal[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]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 standard Toric Code invented by Kitaev is an exactly solvable two-dimensional spin 1/2 model which exhibits an topologically ordered ground state and is strongly debated in the context of topological quantum computation. The elementary excitations are Z(2) Abelian anyons which are completely local because they are protected by conservation laws. Here we investigate an extension of the Toric Code to Z(3) anyons which yields a higher degeneracy of the groundstate and is thus a more favorable candidate towards a realization of a topological quantum memory. Our major aim is to understand the breakdown of a topologically ordered state with Z(3) anyonic excitations. To this end we study the influence of an external 'magnetic field' which leads to dynamic and interacting Z(3) anyons. As a consequence, one expects a rich phase diagram with interesting phase transitions out of the topological phase. We use perturbative continous unitary transformations to derive an effective low-energy describtion for the relevant elementary excitations in order to study this question.

TT 41.6 Fri 11:45 H21

The effect of surface curvature on conductivity in 3D topological insulators — •Jan Dahlhaus, Chang-You Hou, Anton Akhmerov, and Carlo Beenakker — Instituut-Lorentz, Universiteit Leiden, The Netherlands

The surface spectrum of a three-dimensional (3D) topological insulator consists of massless Dirac fermions. Their movement on the surface has to follow a geodesic trajectory, akin to a photon in curved space. In this work, we study electron scattering due to surface roughness which is modeled as curvature of the surface. The resulting effect on conductivity is estimated using the Boltzmann Equation. This scattering mechanism leads to a distinguishable signature of the conductivity on the electron density.

TT 41.7 Fri 12:00 H21

Pseudospin Resonance in two Coaxial Tubes — •Benedikt Scharf, Jaroslav Fabian, and Alex Matos-Abiague — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Deutschland

In a 2DEG confined to two coaxial tubes the 'tube degree of freedom' can be described in terms of pseudospin-1/2 dynamics. The presence of tunneling between the two tubes leads to a collective oscillation

known as pseudospin resonance. We employ perturbation theory to examine the dependence of the frequency of this mode with respect to a coaxial magnetic field for the case of small intertube distances. Coulomb interaction leads to a shift of the resonance frequency and to a finite lifetime of the pseudospin excitations. Depending on the material the presence of the coaxial magnetic field can give rise to pronounced peaks in the shift of the resonance frequency. For very large magnetic fields this shift vanishes due to the effects of Zeeman splitting. Finally, an expression for the linewidth of the resonance is derived. Numerical analysis of this expression suggests that the linewidth strongly depends on the coaxial magnetic field, which leads to several peaks of the linewidth as well as regions where damping is almost completely suppressed. This work has been supported by the Deutsche Forschungsgemeinschaft via GRK 638 and GRK 1570.

TT 41.8 Fri 12:15 H21

Spectra of integrable Chalker-Coddington network models — •Michael Brockmann and Win Nuding — Bergische Universität Wuppertal, Germany

We study an integrable Chalker-Coddington model with $sl(2,1)$ supersymmetry. These systems can be represented as vertex models with staggering in both lattice directions. The objects of interest are the eigenvalues of the transfer matrices. For these objects a Bethe ansatz treatment was presented by Essler, Frahm and Saleur (2005).

So far the Bethe ansatz equations could only be solved numerically for large but finite lattices. Here we present an analytic treatment for arbitrary lattice sizes.