Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture Rooms HSZ 03, HSZ 105, HSZ 201, HSZ 301, and HSZ 304; Poster Areas P1, P3, P4)

Invited Talks

TT 1.1	Mon	10:30–11:00	HSZ 03	**Spin-orbit coupling in graphene: single layer, bilayer, trilayer, and graphite** — •Jaroslav Fabian
TT 26.1	Tue	14:00–14:30	HSZ 301	**Quantum paradoxes in quantum transport** — •Wolfgang Belzig
TT 31.1	Wed	10:30–11:00	HSZ 301	**New insights into the spin Hall effect** — •Peter Schwab
TT 34.7	Wed	15:45–16:15	HSZ 03	**Coupled evolution and coherence of two-electron spin qubits** — •Hendrik Bluhm
TT 60.3	Fri	11:00–11:30	HSZ 301	**Engineering Atomic-Scale Spin Systems** — •Sebastian Loth

Invited and Topical Talks of the Focused Session "Frontiers in Classical and Quantum Spin Liquids"

TT 6.1	Mon	14:00–14:45	HSZ 03	**Magnetolyte Properties of Spin Ice** — •Steve Bramwell
TT 6.2	Mon	14:45–15:30	HSZ 03	**Kitaev-Heisenberg Model on a Honeycomb Lattice: Possible Exotic Phases in Iridium Oxides $A_2\mathbf{IrO}_3$** — •George Jackeli
TT 6.3	Mon	15:45–16:30	HSZ 03	**Disorder in a quantum spin liquid: flux binding and local moment formation** — •John Chalker
TT 6.4	Mon	16:30–17:15	HSZ 03	**Fractional spin textures in the frustrated magnet $\mathbf{SrCr}_{9p}\mathbf{Ga}_{12-9p}\mathbf{O}_{19}$** — •Kedar Damle
TT 6.5	Mon	17:15–18:00	HSZ 03	**Quantum Criticality and E8 symmetry in an Ising Chain** — •Alan Tennant

Invited Talks of the Focused Session "50 Years of Flux Quantization"

TT 20.1	Tue	10:30–11:00	HSZ 03	**The discovery of fluxoid quantization: 2e or not 2e** — •Dietrich Einzel
TT 20.2	Tue	11:00–11:30	HSZ 03	**Fluxoid Quantization and the Superconducting Quantum Interference Device** — •John Clarke
TT 20.3	Tue	11:40–12:10	HSZ 03	**Flux Quantization driving Fractional Flux Quantum Generation** — •Hans Hilgenkamp
TT 20.4	Tue	12:10–12:40	HSZ 03	**Quantum information with quantized fluxoids: flux qubits** — •Johan E. Mooij
TT 20.5	Tue	12:40–13:10	HSZ 03	**Flux quantization and the quantum Hall effect** — •Klaus von Klitzing

Invited and Topical Talks of the Focused Session "100 Years of Superconductivity"

TT 45.1	Thu	10:30–11:00	HSZ 03	**Pairing fermions with population imbalance** — •Peter Fulde
TT 45.2	Thu	11:00–11:30	HSZ 03	**Unconventional Superconductivity - Aspects of Symmetry and Topology** — •Manfred Sigrist

TT 45.3	Thu	11:40–12:10	HSZ 03	**Large Scale Applications of Superconductors and the Challenges that they have posed** — •David Larbalestier
TT 45.4	Thu	12:10–12:40	HSZ 03	**Weak Superconductivity and Superconductor Electronics** — •Konstantin Likharev

Invited Talks of the SKM-Symposium "Spincaloric Transport" (SKM-SYST)

SKM-SYST 1.1	Mon	14:30–15:00	TRE Ma	**On the theory of the spin wave Seebeck effect** — •Gerrit Bauer
SKM-SYST 1.2	Mon	15:00–15:30	TRE Ma	**Spin Seebeck effect in metals and insulators** — •Ken-ichi Uchida
SKM-SYST 1.3	Mon	15:30–16:00	TRE Ma	**Spin-Seebeck effect: Local nature of thermally induced spin currents in GaMnAs** — •Roberto Myers
SKM-SYST 1.4	Mon	16:00–16:30	TRE Ma	**Heat conduction of low-dimensional quantum magnets** — •Christian Hess
SKM-SYST 1.5	Mon	16:30–17:00	TRE Ma	**Evidence of spin polarized heat current acting on magnetization** — •Jean-Philippe Ansermet

Invited Talks of the SKM-Symposium "Topological Insulators" (SKM-SYTI)

SKM-SYTI 1.1	Wed	10:30–11:00	TRE Ma	**Topological insulators and topological superconductors** — •Shoucheng Zhang
SKM-SYTI 1.2	Wed	11:00–11:30	TRE Ma	**Dirac Fermions in HgTe Quantum Wells** — •Laurens Molenkamp
SKM-SYTI 1.3	Wed	11:30–12:00	TRE Ma	**Interaction, disorder, and quantum criticality in Z_2 topological insulators** — •Alexander Mirlin
SKM-SYTI 1.4	Wed	12:00–12:30	TRE Ma	**Disorder and Interactions in Topological Insulators** — •Allan H. MacDonald
SKM-SYTI 1.5	Wed	12:30–13:00	TRE Ma	**Tunable multifunctional topological insulators in ternary Heusler and related compounds** — •Claudia Felser

Invited Talks of the Intersectional Symposium "Hybrid Quantum Systems – Interfacing Atoms, Solids and Light" (SYHQ)

SYHQ 1.1	Thu	10:30–11:00	HSZ 01	**Circuit Quantum Electrodynamics with Electrons on Helium** — •David Schuster
SYHQ 1.2	Thu	11:00–11:30	HSZ 01	**Strong coupling of a spin ensemble to a superconducting resonator** — •Patrice Bertet
SYHQ 1.3	Thu	11:30–12:00	HSZ 01	**Interfacing ultracold atoms and micromechanical oscillators** — •Philipp Treutlein
SYHQ 1.4	Thu	12:00–12:30	HSZ 01	**Interfacing Optomechanics and Atoms** — •Klemens Hammerer
SYHQ 1.5	Thu	12:30–13:00	HSZ 01	**Ultracold Atoms near Carbon Nanotubes** — •Andreas Günther

Invited Talks of the Intersectional Symposium "Cavity meets Circuit Quantum Electrodynamics" (SYQE)

SYQE 1.1	Fri	10:30–11:00	HSZ 01	**The driven Jaynes-Cummings system: from atoms and cavities to circuits** — •Howard Carmichael
SYQE 1.2	Fri	11:00–11:30	HSZ 01	**Light shifts of ground-state quantum beats in Cavity QED, a consequence of quantum jumps.** — •Luis Orozco
SYQE 1.3	Fri	11:30–12:00	HSZ 01	**Tomography and Correlation Function Measurements of Propagating Microwave Photons** — •Andreas Wallraff
SYQE 1.4	Fri	12:00–12:30	HSZ 01	**Artificial atom in 1D open space** — •Yasunobu Nakamura
SYQE 1.5	Fri	12:30–13:00	HSZ 01	**Quantum dot based bright sources of quantum light.** — •Pascale Senellart

Sessions

TT 1.1–1.8	Mon	10:30–13:00	HSZ 03	**TR: Graphene 1 (jointly with MA, HL, and DY)**
TT 2.1–2.9	Mon	10:30–13:00	HSZ 301	**SC: Properties, Electronic Structure, Mechanisms 1**
TT 3.1–3.10	Mon	10:30–13:15	HSZ 304	**CE: Charge Density Wave & Peierls Instability**
TT 4.1–4.9	Mon	10:30–13:00	HSZ 201	**CE: Quantum-Critical Phenomena 1**
TT 5.1–5.10	Mon	10:30–13:00	HSZ 02	**Micro Mechanical Oscillator 1 (jointly with Q)**
TT 6.1–6.5	Mon	14:00–18:00	HSZ 03	**Focused Session: Frontiers in Classical and Quantum Spin Liquids**
TT 7.1–7.9	Mon	14:00–16:15	HSZ 301	**SC: Properties, Electronic Structure, Mechanisms 2**
TT 8.1–8.16	Mon	14:00–18:30	HSZ 304	**TR: Graphene 2 (jointly with MA, HL, and DY)**
TT 9.1–9.15	Mon	14:00–18:15	HSZ 201	**CE: (General) Theory 1**
TT 10.1–10.57	Mon	14:00–18:00	P4	**Poster Session: Superconductivity**
TT 11.1–11.22	Mon	14:00–18:00	P4	**Poster Session: Matter at Low Temperature**
TT 12.1–12.3	Mon	14:30–15:15	HSZ 02	**Micro Mechanical Oscillator 2 (jointly with Q)**
TT 13.1–13.8	Mon	14:45–17:00	HSZ 04	**Multiferroics I (jointly with DF, DS, KR, MA)**
TT 14.1–14.7	Mon	17:00–18:45	HSZ 04	**Multiferroics II (jointly with DF, DS, KR, MA)**
TT 15.1–15.6	Mon	16:30–18:00	HSZ 301	**SC: Fabrication and Characterization**
TT 16.1–16.6	Mon	18:15–19:45	HSZ 03	**TR: Nanoelectronics III - Molecular Electronics 1**
TT 17.1–17.7	Mon	18:15–20:00	HSZ 301	**SC: Fe-based Superconductors - 1111**
TT 18.1–18.6	Mon	18:30–20:00	HSZ 201	**CE: Low-dimensional Systems - Materials 1**
TT 19.1–19.4	Mon	18:45–19:45	HSZ 304	**CE: Quantum Impurities, Kondo Physics**
TT 20.1–20.5	Tue	10:30–13:10	HSZ 03	**Focused Session: 50 Years of Flux Quantization**
TT 21.1–21.9	Tue	10:30–13:00	HSZ 301	**TR: Nanoelectronics III - Molecular Electronics 2**
TT 22.1–22.9	Tue	10:30–13:00	HSZ 304	**CE: Low-dimensional Systems - Materials 2**
TT 23.1–23.9	Tue	10:30–13:00	HSZ 105	**CE: Quantum-Critical Phenomena 2**
TT 24.1–24.1	Tue	10:15–10:45	HSZ 04	**Multiferroics III (jointly with DF, DS, KR, MA)**
TT 25.1–25.6	Tue	10:45–12:15	HSZ 04	**Multiferroics IV (jointly with DF, DS, KR, MA)**
TT 26.1–26.5	Tue	14:00–15:30	HSZ 301	**TR: Fluctuations and Noise**
TT 27.1–27.6	Tue	14:00–15:30	HSZ 304	**SC: Fe-based Superconductors - LiFeAs**
TT 28.1–28.6	Tue	14:00–15:30	HSZ 105	**CE: (General) Theory 2**
TT 29.1–29.11	Tue	18:00–21:00	P1	**Poster Session: Quantum Information Systems, Quantum Coherence (jointly with SAMOP)**
TT 30.1–30.9	Wed	10:30–13:00	HSZ 03	**TR: Quantum Coherence and Quantum Information Systems 1 (jointly with MA and HL)**
TT 31.1–31.8	Wed	10:30–13:00	HSZ 301	**TR: Nanoelectronics II - Spintronics and Magnetotransport 1 (jointly with HL and MA)**
TT 32.1–32.9	Wed	10:30–13:00	HSZ 304	**SC: Fe-based Superconductors - Theory**
TT 33.1–33.9	Wed	10:30–13:00	HSZ 105	**CE: Metal-Insulator Transition 1**
TT 34.1–34.16	Wed	14:00–18:45	HSZ 03	**TR: Quantum Coherence and Quantum Information Systems 2 (jointly with MA and HL)**
TT 35.1–35.20	Wed	14:00–19:45	HSZ 301	**CE: Low-dimensional Systems - Materials 3**
TT 36.1–36.16	Wed	14:00–18:30	HSZ 304	**SC: Fe-based Superconductors - 122 - Properties, Electronic Structure, Mechanisms**
TT 37.1–37.14	Wed	14:00–18:00	HSZ 105	**MLT: Quantum Liquids, Bose-Einstein Condensates, Ultracold Atoms, ...**
TT 38.1–38.41	Wed	14:00–18:00	P3	**Poster Session Transport**
TT 39.1–39.5	Wed	14:00–16:30	HSZ 04	**Spin Structures/ Skyrmions (jointly with MA)**
TT 40.1–40.10	Wed	16:45–19:15	HSZ 04	**Topological Insulators (jointly with HL, MA)**
TT 41.1–41.5	Wed	18:15–19:30	HSZ 105	**CE: Spin Systems and Itinerant Magnets 1**
TT 42.1–42.5	Wed	18:45–20:00	HSZ 304	**SC: Fe-based Superconductors - Fe(Se,Te)**
TT 43.1–43.5	Wed	19:00–20:15	HSZ 03	**TR: Nanoelectronics II - Spintronics and Magnetotransport 2 (jointly with HL and MA)**
TT 44.1–44.89	Thu	10:00–13:00	P1	**Poster Session Correlated Electrons**
TT 45.1–45.4	Thu	10:30–12:40	HSZ 03	**Focused Session: 100 Years of Superconductivity**
TT 46.1–46.9	Thu	10:30–13:00	HSZ 301	**SC: Tunneling, Josephson Junctions, SQUIDs 1**
TT 47.1–47.9	Thu	10:30–13:00	HSZ 304	**TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1**
TT 48.1–48.9	Thu	10:30–13:00	HSZ 105	**CE: Metal-Insulator Transition 2**
TT 49.1–49.17	Thu	14:00–18:45	HSZ 03	**CE: Spin Systems and Itinerant Magnets 2**
TT 50.1–50.5	Thu	14:00–15:15	HSZ 301	**SC: Tunneling, Josephson Junctions, SQUIDs 2**

TT 51.1–51.6	Thu	14:00–15:30	HSZ 304	**TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2**
TT 52.1–52.8	Thu	14:00–16:15	HSZ 105	**CE: Low-dimensional Systems - Models 1**
TT 53.1–53.7	Thu	15:15–17:00	HSZ 401	**Graphene (jointly with DY, DS, HL, MA, O)**
TT 54.1–54.7	Thu	15:30–17:15	HSZ 301	**SC: Heterostructures, Andreev Scattering, Proximity Effect**
TT 55.1–55.4	Thu	16:00–17:00	HSZ 304	**TR: Topological Insulators 1 (jointly with HL and MA)**
TT 56.1–56.9	Thu	16:30–19:00	HSZ 105	**CE: Heavy Fermions**
TT 57.1–57.6	Thu	17:15–18:45	HSZ 304	**SC: Fe-based Superconductors - 122 - Thin Films**
TT 58.1–58.6	Thu	17:30–19:00	HSZ 301	**SC: Vortex Dynamics, Vortex Phases, Pinning**
TT 59.1–59.9	Fri	10:30–13:00	HSZ 03	**TR: Topological Insulators 2 (jointly with HL and MA)**
TT 60.1–60.9	Fri	10:30–13:15	HSZ 301	**SC & MLT: Cryodetectors**
TT 61.1–61.8	Fri	10:30–12:45	HSZ 304	**TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3**
TT 62.1–62.10	Fri	10:30–13:15	HSZ 105	**CE: Low-dimensional Systems - Models 2**

Annual General Meeting Low Temperature Physics Division

Thursday 19:00–20:30 HSZ 304

TT 1: TR: Graphene 1 (jointly with MA, HL, and DY)

Time: Monday 10:30–13:00 Location: HSZ 03

Invited Talk TT 1.1 Mon 10:30 HSZ 03

Spin-orbit coupling in graphene: single layer, bilayer, trilayer, and graphite — •Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

In graphene at the Fermi level the spin-orbit splitting is about 25 μeV. Our first-principles [1] and tight-binding [2] investigations show that the splitting originates from d orbitals that hybridize with the p_z ones and form the π band. In an external transverse electric field there is an additional splitting of the bands (the Bychkov-Rashba effect). This extrinsic splitting is solely due to the hybridization of the σ and π orbitals, and is about 10 μeV for typical fields of 1 V/nm. In bi- and trilayer graphene, and in graphite, the intrinsic splitting is also due to the d electrons. The extrinsic splitting at K points has the intrinsic value, of 25 μeV; somewhat away from K the splitting saturates to the Bychkov-Rashba value similar to the single layer graphene. This work is supported by the DFG SFB 689.

[1] M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, *Band-structure topologies in graphene: spin-orbit coupling effects from first principles,* Phys. Rev. B 80, 235431 (2009).
[2] S. Konschuh, M. Gmitra, and J. Fabian, *Tight-binding theory of the spin-orbit coupling in graphene,* Phys. Rev. B 82, 245412 (2010).
[3] C. Ertler, S. Konschuh, M. Gmitra, and J. Fabian, *Electron spin relaxation in graphene: the role of the substrate,* Phys. Rev. B(R) 80, 041405 (2009)

TT 1.2 Mon 11:00 HSZ 03

Electron transport and spins in graphene — •Jan Bundesmann[1], Michael Wimmer[2], and Klaus Richter[1] — [1]Institut für theoretische Physik, Universität Regensburg, Deutschland — [2]Instituut-Lorentz, TU Leiden, The Netherlands

The weak atomic spin-orbit interaction (SOI) in graphene leads to the assumption of large spin relaxation times. Simulations, taking into account spin-scattering from charged impurities in the substrate, yielded spin relaxation times [1] much larger than spin injection experiments in graphene [2,3].
Still assuming that the model of spins scattered at charged impurities is correct, we implemented a tight-binding model for graphene in the presence of SOI.
In our work the focus lies on the effects of SOI on electron transport (i.e. low energy excitations and the role of symmetry classes manifested, e.g., in weak localization) as well as its influence on spin transport in the diffusive regime.

[1] Ertler, Konschuh, Gmitra and Fabian, Phys. Rev. B **80**, 041405(R) (2009)
[2] Tombros, Josza, Popinciuc, Jonkman and van Wees, Nature **448**, 571 (2007)
[3] Han, Pi, McCreary, Li, Wong, Swartz and Kawakami, Phys. Rev. Lett. **105**, 167202 (2010)

TT 1.3 Mon 11:15 HSZ 03

Electric field control of spin rotation in bilayer graphene — •Paolo Michetti[1], Patrik Recher[1], and Giuseppe Iannaccone[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Dipartimento di Ingegneria dell'Informazione, Universita' di Pisa, Via G. Caruso 16 - 56122 - Pisa (Italy)

The manipulation of the electron spin degree of freedom is at the core of the spintronics paradigm, which offers the perspective of reduced power consumption, enabled by the decoupling of information processing from net charge transfer.

Graphene, with its potentially long spin-coherence length, is a promising material for spin-encoded information transport. However, the small spin-orbit interaction is also a limitation for the design of conventional devices based on the canonical Datta-Das spin field-effect transistors. An alternative solution can be found in magnetic doping of graphene or, as discussed in the present work, in exploiting the proximity effect between graphene and ferromagnetic oxides (FOs). Graphene in proximity to FO experiences an exchange proximity interaction, that acts as an effective Zeeman field for electrons in graphene, inducing a spin precession around the magnetization axis of the FO.

Here we show that in an appropriately designed double-gate field-effect transistor, with a bilayer graphene channel and FO used as a gate dielectric, spin-precession of carriers can be turned ON and OFF with the application of a differential voltage to the gates. This feature is directly probed in the spin-resolved conductance of the bilayer.

TT 1.4 Mon 11:30 HSZ 03

Graphene Superlattices Studied by Ab-Initio Methods — •Lars Matthes, Karsten Hannewald, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany

The peculiar electronic properties of graphene have stimulated extensive research towards graphene-based electronics. Hereby, of particular interest are quasi-1D structures such as graphene nanoribbons [1] or, more recently, graphene superlattices [2] which allow a systematic tuning of the band structure. An impressive example for such modifications has been predicted by recent Kronig-Penney-type calculations [2] for a single graphene layer subject to a 1D periodic potential where a rather counterintuitive anisotropic renormalization of the Fermi velocity due to the Klein paradox is expected. Here, we present first-principles DFT calculations of graphene superlattices using the VASP code. The influence of the periodic external potential on the charge-carrier redistribution and corresponding screening effects is investigated in detail. The resulting consequences for the ab-initio band structure including anisotropy effects are studied and compared with analytical calculations based on the Dirac Hamiltonian. Deviations due to self-consistent inclusion of screening effects and nonlinear dispersions are analyzed. Finally, consequences for the practical realization of graphene superlattices with 1D transport properties are discussed.

[1] See, e.g., U. Treske, F. Ortmann, B. Oetzel, K. Hannewald, F. Bechstedt, phys. stat. sol. (a) 207, 304 (2010)
[2] C-H. Park et al., Nature Phys. 4, 213 (2008)

15 min. break

TT 1.5 Mon 12:00 HSZ 03

Nanomachining a Tunneling Barrier in Graphene — •Patrick Barthold and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

Utilizing an atomic force microscope, graphene is nanomechanically structured. It is selectively folded in order to produce two dimensional systems that are only a few Angstrom apart. Aditionally, insulating lines are crafted within the sample without inducing any chemical contamination which, in contrast, is inevitable, when traditional structuring methods, e.g. etching procedures, are used. Such manufactured tunneling barriers are characterized by electrical transport measurements at low temperatures on an exemplary few-layer sample. In the conductivity through this barrier we find a gap around zero bias voltage. The conductivity shows a backgate dependent opening of a band gap in the sample. Due to the asymmetric design of the emitter and collector we find an asymmetry in the backgate dependent conductivity through the barrier.

TT 1.6 Mon 12:15 HSZ 03

Evidence for Josephson-coupled superconducting regions at the interfaces of highly oriented pyrolytic graphite — •Ana Ballestar, Jose Barzola-Quiquia, and Pablo Esquinazi — Abteilung für Supraleitung und Magnetismus, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany

The first observation of superconductivity in doped graphite goes back to 1965 when it was observed in the potassium graphite intercalated compound C8K. A considerable amount of studies had reported this phenomenon in intercalated graphite compounds or doped graphite, however the superconducting properties of pure graphite are still under discussion. Indirect evidences for superconductivity at graphite interfaces have been recently published. In order to better understand these interfaces properties, we prepared micro structured samples (Lamellas) from pure highly oriented pyrolitic graphite. By reducing the dimension in the in plane configuration to $\sim$ 200 nm we can measure the electrical response of graphite interfaces. We obtained evidence for the existence of Josephson-coupled quasi two dimensional superconducting regions. Temperature dependence of the voltage, as well as

I(V) characteristic curves indicate that superconductivity exists even above 150 K. The results support the view that HOPG is a system with interfaces containing non-percolative superconducting domains immersed in a semiconducting graphene-based matrix.

TT 1.7 Mon 12:30 HSZ 03

Tuning the electronic structure of graphene through ac fields: dynamical gaps and polarization effects — •Hernan L. Calvo[1,2], Horacio M. Pastawski[1], Stephan Roche[3], and Luis E. F. Foa Torres[1] — [1]Instituto de Fisica Enrique Gaviola and FaMAF UNC, 5000 Cordoba, Argentina — [2]Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany — [3]CIN2, CSIC-ICN, Campus UAB, E-08193 Barcelona, Spain

Thanks to its outstanding electrical, mechanical and thermal properties, graphene research is one of the most rapidly advancing fronts ever. Moreover, applications are around the corner, from ballistic transistors to ultracapacitors everything seems possible. Fortunately, there are still many fascinating open problems like the interaction between a laser field and the electrons in graphene. In this work, we discuss this issue within the non-adiabatic regime in terms of both Dirac band and tight-binding models and contrast the obtained results. Notably, we find that the interaction with the field gives rise to back-scattering processes that open dynamical gaps in the electronic structure. The strong dependence of these phenomena on the polarization is emphasized. Our predictions show that these effects should be observable with present laser technology, thereby opening promising prospects for graphene-based opto-electronic devices.

TT 1.8 Mon 12:45 HSZ 03

Relaxation dynamics of graphene in magnetic fields close to the Dirac point — •Martin Mittendorff[1], Stephan Winnerl[1], Paulina Plochocka[2], Piotr Kossacki[2], Harald Schneider[1], Milan Orlita[2], Marek Potemski[2], Mike Sprinkle[3], Claire Berger[3], Walter A. de Heer[3], and Manfred Helm[1] — [1]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden Rossendorf, Germany — [2]Grenoble High Magnetic Field Laboratory, France — [3]Georgia Institute of Technology, Atlanta, USA

The relaxation dynamics in graphene is of key importance for understanding the basic material properties as well as for high-frequency electronic and opto-electronic device applications. In addition to single colour pump-probe experiments in the THz range (photon energy: 14-30 meV) without magnetic field, we performed experiments at a photon energy of 18 meV in magnetic fields up to 1.34 T. For photon energies larger than twice the Fermi energy (approx. 10 meV) positive pump-probe signals were observed while for smaller photon energies pump-induced absorption occurred due to carrier heating. Relaxation times were around 30 ps. At magnetic fields around 0.23 T the pump-probe signal increases by a factor of 2.5. At this field the splitting of the zeroth to first Landau level is resonant with the photon energy.

TT 2: SC: Properties, Electronic Structure, Mechanisms 1

Time: Monday 10:30–13:00 Location: HSZ 301

TT 2.1 Mon 10:30 HSZ 301

Shubnikov-de Haas effect and angle-dependent magnetoresistance oscillations in the electron-doped cuprate superconductor $Nd_{2-x}Ce_xCuO_4$ — •Toni Helm[1], Carsten Putzke[2], Mark V. Kartsovnik[1], Nikolaj Bittner[1], Frederik Wolff-Fabris[2], Iliya Sheikin[3], Cyril Proust[3], Andreas Erb[1], Jochen Wosnitza[2], and Rudolf Gross[1] — [1]Walther-Meissner-Institute, Garching, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden-Rossendorf, Germany — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble/Toulouse, France

High-field magnetotransport has recently proved extremely efficient for elucidating the Fermi surface of cuprate superconductors. By applying sufficiently high magnetic fields superconductivity is suppressed and the normal-conducting state can be accessed for even lowest temperatures. We observed quantum oscillations of the magnetoresistance, the Shubnikov-de Haas (SdH) effect, in the electron-doped cuprate $Nd_{2-x}Ce_xCuO_4$. A dramatic change in the oscillation spectrum was found, revealing a transformation of the cyclotron orbit topology at a critical doping level. On the other hand, angle-dependent magnetoresistance oscillations (AMRO) did not show an appreciable change in the same doping range. In this talk we present new results on the AMRO and SdH oscillations obtained at higher magnetic fields for single crystals with x ranging from 0.145 to 0.17. Our data provides a compelling evidence for a translational symmetry breaking persisting in the material up to highest doping level.

TT 2.2 Mon 10:45 HSZ 301

Momentum-Resolved Ultrafast Electron Dynamics in Superconducting $Bi_2Sr_2CaCu_2O_{8+\delta}$ — •L. Rettig[1,2], R. Cortes[1,3], Y. Yoshida[4], H. Eisaki[4], M. Wolf[3], and U. Bovensiepen[2] — [1]Fachb. Physik, Freie Univ. Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fak. f. Physik, Univ. Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [3]Abt. Phys. Chemie, Fritz-Haber-Institut d. MPG, Faradayweg 4-6, 14195 Berlin, Germany — [4]Nat. Inst. of Adv. Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan

The processes responsible for the relaxation of hot quasiparticles (QPs) in high-T_c superconductors have been intensely studied by time-resolved optical and THz spectroscopy. These studies conclude on highly momentum dependent dynamics, which however cannot be resolved directly by these momentum integrating techniques.

Here, we report on the non-equilibrium state of the high-T_c superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ and its ultrafast dynamics investigated by femtosecond time- and angle-resolved photoemission spectroscopy. This technique allows direct investigation of excited QPs and the dynamics of the superconducting state with both momentum and energy resolution. Thus, we are able to investigate optically excited QPs at different electron momenta along the Fermi surface and detect metastable QPs near the antinode. Their decay through e-e scattering is blocked by a scattering phase space restricted to the nodal region. We find a single exponential relaxation of the excited QPs with momentum independent decay rates, in agreement with relaxation dominated by Cooper pair recombination in a boson bottleneck limit.

TT 2.3 Mon 11:00 HSZ 301

The energy scale in the cuprates: a Raman study — •B. Muschler[1], N. Munnikes[1], F. Venturini[1], L. Tassini[1], W. Prestel[1], Shimpei Ono[2], Yoichi Ando[3], A. Damascelli[4], D. Peets[4], W.N. Hardy[4,5], R. Liang[4,5], D. Bonn[4,5], H. Eisaki[6], M. Greven[7], A. Erb[1], and R. Hackl[1] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]CRIEPI, Komae, Tokyo 201-8511, Japan — [3]Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan — [4]Department of Physics & Astronomy, University of British Columbia, Vancouver, BC V6T 1Z4, Canada — [5]Canadian Institute for Advanced Research, Toronto M5G 1Z8, Canada — [6]Nanoelectronic Research Institute, AIST, Tsukuba 305-8568, Japan — [7]Department of Applied Physics and Photon Science, Stanford University, Stanford, CA 94305, USA

We present results of electronic Raman scattering experiments in single crystals of YBCO, Bi2212 and Tl2201 in the superconducting state. In B_{2g} symmetry we find universal, material independent spectra with the pair breaking peak $\Omega_{\rm peak}^{B2g}$ scaling as $6\,k_BT_c$. $\Omega_{\rm peak}^{B1g}$ depends on the individual samples and may change by up to 30% for samples with the same T_c. On the average $\Omega_{\rm peak}^{B1g}$ decreases from $9\,k_BT_c$ to $4.5\,k_BT_c$ with the doping level increasing from $p = 0.15$ to $p = 0.23$. While the spectral weights of the B_{2g} peaks are doping independent those in B_{1g} increase by almost a factor of 10 from optimal to overdoped samples.

This work is supported by the DFG via FOR538 and SPP1458.

TT 2.4 Mon 11:15 HSZ 301

Low-energy kink in the nodal dispersion of copper-oxide superconductors: Insights from Dynamical Mean Field Theory — •Johannes Bauer[1] and Giorgio Sangiovanni[2] — [1]Max-Planck Institute for Solid State Research, Heisenbergstr.1, 70569 Stuttgart — [2]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

Motivated by the observation in copper-oxide high-temperature superconductors, we investigate the appearance of kinks in the electronic dis-

persion due to coupling to phonons for a system with strong electronic repulsion. We study a Hubbard model supplemented by an electron-phonon coupling of Holstein type within Dynamical Mean Field Theory (DMFT) utilizing Numerical Renormalization Group as impurity solver. Paramagnetic DMFT solutions in the presence of large repulsion show a kink only for large values of the electron-phonon coupling λ or large doping and, contrary to the conventional electron-phonon theory, the position of such a kink can be shifted to energies larger than the renormalized phonon frequency ω_0^r. When including antiferromagnetic correlations we find a stronger effect of the electron-phonon interaction on the electronic dispersion due to a cooperative effect and a visible kink at ω_0^r, even for smaller λ [1]. Our results provide a scenario of a kink position increasing with doping, which can be related to recent photoemission experiments on Bi-based cuprates.
[1] J. Bauer and G. Sangiovanni, Phys. Rev. B. 82, 184535 (2010).

TT 2.5 Mon 11:30 HSZ 301

Pairing theory of striped superconductivity — •Florian Loder, Arno P. Kampf, Thilo Kopp, and Siegfried Graser — Center for Electronic Correlations and Magnetism, Institute of Physics, D-86135 Augsburg, Germany

Striped high-T_c superconductors such as $La_{7/8}Ba_{1/8}CuO_4$ show a fascinating competition between spin and charge order on the one hand and superconductivity on the other. A theory for these systems therefore has to capture both the spin correlations in an antiferromagnet and the pair-correlation of a superconductor. For this purpose we have developed an effective Hartree-Fock theory by merging electron pairing with finite center-of-mass momentum and antiferromagnetism. We show that this theory reproduces the key experimental features such as the formation of the antiferromagnetic stripe patterns at 7/8 band filling or the quasi one-dimensional electronic structure observed by photoemission spectroscopy.

15 min. break

TT 2.6 Mon 12:00 HSZ 301

Charge stripe order near the surface of 12-percent doped $La_{2-x}Sr_xCuO_4$ — •M. Buchholz[1], H.-H. Wu[1,2], C. Trabant[1,4], C.-F. Chang[1], A. Komarek[1], F. Heigl[3], E. Schierle[4], M. v. Zimmermann[5], M. Cwik[1], F. Nakamura[6], L. H. Tjeng[7], M. Braden[1], and C. Schüssler-Langeheine[1,4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]NSRRC, Hsinchu, Taiwan — [3]ALBA, Barcelona, Spain — [4]Helmholtz-Zentrum Berlin — [5]DESY, Hamburg — [6]ADSM, Hiroshima University, Japan — [7]MPI CPfS, Dresden

Stripe-like spin and charge order has been observed in many layered cuprate, nickelate and cobaltate systems by neutron or x-ray diffraction. For the prototypical high-temperature superconductor $La_{2-x}Sr_xCuO_4$ (LSCO) no charge-stripe signal has been found so far, but there are several indications for a proximity to the formation of charge stripes. We found a pronounced charge-stripe signal in the near surface region of 12-percent doped LSCO, but no such signal from the bulk. We conclude that this compound is so close to the formation of charge stripes that small perturbations near the surface can stabilize this order. Our finding of different phases in the bulk and near the surface of LSCO has to be taken into account for the interpretation of data from surface-sensitive probes like photoelectron spectroscopy or scanning tunnelling spectroscopy.

TT 2.7 Mon 12:15 HSZ 301

Electronic structure of striped phase of $Ca_{1.875}Na_{0.125}CuO_2Cl_2$ — •Charles Patterson — Trinity College Dublin, Ireland

We present hybrid DFT calculations on stripe formation in hole doped $Ca_2CuO_2Cl_2$ (CCOC) [1]. Stripes have been extensively studied by STM in sodium-doped CCOC with hole concentrations, x, in the range x = 0.05 to x = 0.15 per Cu ion [2]. Around x = 0.125, 1-D stripes are observed with a spacing of four lattice constants. STM imaging in topographic mode allows positions of Cl ions and Cu ions directly beneath to be observed. Stripes imaged in conductance mode are centred on O ions in rows running perpendicular to the stripe direction, i.e. they are bond centred stripes on O ions.

O ions between transition metal ions with a magnetic moment induce anti-ferromagnetic coupling between the metal ion magnetic moments via super-exchange. However, when a hole is localized on the O ion between two transition metal magnetic moments, it induces ferromagnetic coupling between the metal ion magnetic moments by double-exchange. We propose a magnetic order for Cu ion spins and hole localisation on O ions in the CuO_2 layers of CCOC with x = 0.125. Holes are localised in rows on O ions, separated by four lattice constants; each pair of Cu magnetic moments on either side of an O ion with a localized hole are parallel and each pair of Cu magnetic moments on either side of an ordinary O ion are anti-parallel, satisfying the rules for super- and double-exchange.
[1] C. H. Patterson, Phys. Rev. B 77, 094523 (2008).
[2] Y. Kohsaka et al, Science 315, 1380 (2007).

TT 2.8 Mon 12:30 HSZ 301

Effects of High Pressure on $YBa_2Cu_4O_8$ probed by ^{17}O NMR — •Thomas Meissner[1], Swee K. Goh[2,3], Jürgen Haase[1], and Grant V. M. Williams[4] — [1]Faculty of Physics and Earth Science, University of Leipzig, Germany — [2]Department of Physics, Cavendish Laboratory, University of Cambridge, United Kingdom — [3]Trinity College, Cambridge, United Kingdom — [4]The MacDiarmid Institute and Industrial Research Limited, New Zealand

The application of gigapascal pressure is a useful tool to tune the physical properties of high temperature superconductors but its effects have been scarcely studied by nuclear magnetic resonance (NMR) due a limited signal to noise ratio. Recently, some of us showed that this problem could be overcome with a new anvil cell probe design. Here we report on measurements of the ^{17}O Knight shifts in the normal state of the stoichiometric compound $YBa_2Cu_4O_8$ at pressures up to 6.3 GPa. Our data implies a significant pressure induced change of the spin susceptibility at the planar oxygen sites. The results are compared with doping effects observed in other cuprates.

TT 2.9 Mon 12:45 HSZ 301

Change of critical temperature by electric fields — •Klaus Morawetz[1,2], Pavel Lipavský[3], Jan Kolaček[4], and Ernst Helmut Brandt[5] — [1]University of Applied Science Münster, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Universidade Federal do Rio grande do Norte - UFRN, 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]Max Planck Institute for Metals Research, D-70506 Stuttgart, Germany

Electrostatic charging changes the critical temperature of superconducting thin layers. To understand the basic mechanism, it is possible to use the Ginzburg-Landau theory with the boundary condition derived by de Gennes from the BCS theory. Here we show that a similar boundary condition can be obtained from the principle of minimum free energy. We compare the two boundary conditions and use the Budd-Vannimenus theorem as a test of approximations. Resulting consequences on measurable surface potentials and surface deformations are discussed and a new effect of discontinuity of the magnetocapacitance near H_{c3} is presented.

[Phys. Rev. B 73 (2006) 052505-1-5, Phys. Rev. B 78 (2008) 174516-1-7, Phys. Rev. B 79 (2009) 174510-1-6, New J. Phys. 11 (2009) 023032-1-8]

TT 3: CE: Charge Density Wave & Peierls Instability

Time: Monday 10:30–13:15 Location: HSZ 304

TT 3.1 Mon 10:30 HSZ 304

Infrared study of the blue bronze $K_{0.3}MoO_3$ — •Rebecca Beyer, Neven Barišić, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

The blue bronzes $A_{0.3}MoO_3$ (A = Rb, K, Tl) are well known quasi-one-dimensional materials. They exhibit a Peierls-type metal-insulator phase transition around 180 K which is connected to the formation of a charge density wave (CDW) in the conducting direction. While temperature dependent dc-resistivity indicates the CDW in all three directions, so far most measurements concentrated on the conducting *b*-

and a^*-direction and no thorough investigations of the physical properties of the insulating c^*-direction have been carried out.
We report first optical conductivity measurements on the potassium blue bronze $K_{0.3}MoO_3$ along the b- and the c^*-direction in order to evaluate the influence of the long range order of the CDW on the perpendicular direction. Measurements were performed with polarized light in a wide frequency range from 30 cm^{-1} up to 11000 cm^{-1} for several selected temperatures between 300 K and 50 K. At high frequencies we have carefully analyzed the changes in the strong interband transition related to the gap opening. In addition two phonon lines are observed around 900 cm^{-1} and attributed to stretching vibrations of terminal O- with Mo-atoms. Degenerated at high temperatures, those lines split and shift in frequency once the CDW develops.

TT 3.2 Mon 10:45 HSZ 304

A band structure study of $BaNi_2P_4$ - Dimorphism from a Peierls instability? — •Eugen Wolf, Andreas Leithe-Jasper, Christoph Geibel, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The recent discovery of high temperature superconductivity in iron pnictide compounds stimulated a rebirth of interest in transition metal pnictides in general. In particular, a focus of attention is devoted to compounds that exhibit structural phase transitions caused by the interplay of electronic and lattice degrees of freedom. Here, we present a density functional based (LDA and GGA) computational study of the compound $BaNi_2P_4$ that shows a tetragonal to orthorhombic phase transition at about 370 K. In our calculations, we can reproduce the orthorhombic ground state which is non magnetic since the electronic density of states at the Fermi level is rather low in both phases with a sizably reduced value for the orthorhombic structure. However, the calculated energy difference between the tetragonal and the orthorhombic lattice is far to small to account for the high transition temperature. Possible scenarios for the transition are discussed, especially in the light of a Peierls instability that has been debated controversially in the literature [1,2].
[1] Keimes V, Johrendt D, Mewis A, ZAAC **621**, 925, (1995).
[2] Palacios AA, Alemany P, Alvarez S, et al. Annales de quimica - international edition **93**, 385-393, (1997).

TT 3.3 Mon 11:00 HSZ 304

Dynamic Charge Correlations Near the Peierls Transition — •Martin Hohenadler[1], Holger Fehske[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, GER — [2]Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17489 Greifswald, GER

The quantum phase transition between a repulsive Luttinger liquid and an insulating Peierls state is studied in the framework of the one-dimensional spinless Holstein model. We focus on the adiabatic regime but include the full quantum dynamics of the phonons. Using continuous-time quantum Monte Carlo simulations, we track in particular the dynamic charge structure factor and the single-particle spectrum across the transition. With increasing electron-phonon coupling, the dynamic charge structure factor reveals the emergence of a charge gap, and a clear signature of phonon softening at the zone boundary. The single-particle spectral function evolves continuously across the transition. Hybridization of the charge and phonon modes of the Luttinger liquid description leads to two modes, one of which corresponds to the coherent polaron band. This band acquires a gap upon entering the Peierls phase, whereas the other mode constitutes the incoherent, high-energy spectrum with backfolded shadow bands. Coherent polaronic motion is a direct consequence of quantum lattice fluctuations. In the strong-coupling regime, the spectrum is described by the static, mean-field limit. Importantly, whereas finite electron density in general leads to screening of polaron effects, the latter reappear at half filling due to charge ordering and lattice dimerization.

TT 3.4 Mon 11:15 HSZ 304

The role of charge order in the layered superconducter $NbSe_2$ — •Dirk Rahn[1], Stefan Hellmann[1], Christian Sohrt[1], Matthias Kalläne[1], Timur Kim[2], Bernd Büchner[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Germany — [2]IFW Dresden, Germany

The layered compound $2H$-$NbSe_2$ has emerged from a prototype BCS like superconductor to a material with a coexistence of charge-density waves (CDW) and superconductivity (SC) at low temperatures. These two phenomena have led to strong controversity about the symmetry of the gap function [1] and the nature of the interplay between them. Due to the analogy with the high-T_c cuprates, recent ARPES studies of the near-E_F electronic structure [2,3] tried to unveil the gap symmetry as well as the role of the CDW in SC. These studies end up with a contradiction between CDW enhanced and CDW weakened SC and with an uncertainty in the gap symmetry because the measurements were done at $T > T_c/2$. We present a comprehensive ARPES study of the momentum-resolved near-E_F electronic sturcture at $T \approx 1$ K. This allows us to determine the parts of the Fermi surface that stabilize the CDW as well as those parts that are gapped by SC. Furthermore, we see clear fingerprints of different phonon modes in the spectra, which enables us to reveal the correlation between SC, CDW, and the different parts of the phonon spectrum.
[1] Huang *et al.*, Phys. Rev. B **76**, 212504 (2007)
[2] Kiss *et al.*, Nat. Phys. **3**, 720 (2007)
[3] Borisenko *et al.*, Phys. Rev. Lett. **102**, 166402 (2009).

15 min. break

TT 3.5 Mon 11:45 HSZ 304

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

We investigated the phonon softening in the charge density wave compound $NbSe_2$ using the high-resolution hard inelastic x-ray scattering beamline 30-ID-C at the Advanced Photon Source, Argonne National Laboratory. The acoustic Σ_1 phonon branch was measured from the zone center Γ to the M point at temperatures between 250 K and 8 K across the CDW transition at $T_{CDW} = 33$ K. Density functional theory calculations for the lattice dynamical properties which predict an extended phonon breakdown are used to analyze the detailed nature of the softening phonon branch. Work supported by US DOE BES-DMS DE-AC02-06CH11357.

TT 3.6 Mon 12:00 HSZ 304

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

We investigated the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$ both theoretically in Density Functional Theory (DFT) based on ab-initio phonon calculations and experimentally by means of high resolution Inelastic X-ray Scattering (IXS). For both materials, the theoretical predictions for the phonon softening using the experimental lattice parameters coincide with the experimentally observed CDW instability behaviour. While $TiSe_2$ shows a rather sharp phonon anomaly at T = 190 K, the anomaly in $NbSe_2$ at T = 33 K is much broader than expected for a Fermi surface nesting driven CDW instability. For $NbSe_2$, we exclude Fermi surface nesting as main origin of the phonon softening. For $TiSe_2$, there is no need to go beyond DFT in order to describe the phonon softening.

TT 3.7 Mon 12:15 HSZ 304

The influence of conduction band population on the charge density wave phase of $TiSe_2$ — •Matthias M. May[1,2], Isaak Unger[1], Christoph Janowitz[1], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The origin of the charge density wave (CDW) phase transition of the transition-metal dichalcogenide $TiSe_2$ has been subject of research for more than 30 years now with a recent tendency towards an excitonic model [1]. This view was probed by investigating the influence of an additional population of the Ti $3d$ conduction band. The population was realised by means of band bending due to H_2O adsorption [2] and band gap engineering via ternary compounds, monitored with ARPES at BESSY as well as conductivity measurements. Results indicate the existence of an optimal size for the band gap.
[1] C. Monney, C. Battaglia, E.F. Schwier, C. Didiot, M.G. Garnier, H. Beck, P. Aebi and H. Berger, Physica B 404, 3172 (2009)
[2] J. Rasch, T. Stemmler, B. Mueller, L. Dudy and R. Manzke, Phys. Rev. Letters 101, 237602 (2008)

TT 3.8 Mon 12:30 HSZ 304

Electron Energy-Loss Spectroscopy on the Transition-Metal Dichalchogenide $2H$-$TaSe_2$ — •Andreas König[1], Roman Schuster[2], Helmuth Berger[3], Martin Knupfer[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P. O. Box 270116, D-01171 Dresden, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]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 behavior of a common metal. Furthermore, the slope of the plasmon dispersion is doping dependent. We performed Electron Energy-Loss Spectroscopy in transmission on thin films of $2H$-$TaSe_2$ for different potassium contents as well as for different temperatures above and below the CDW transition temperature to investigate the connection of the CDW phase transition to the plasmon dispersion.

TT 3.9 Mon 12:45 HSZ 304

Raman study of the charge density wave system $ErTe_3$ — •Hans-Martin Eiter[1], Michela Lavagnini[1], Reinhard Rossner[1], Jiun-Haw Chu[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther-Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, CA 94304, USA

We present results of Raman scattering experiments on $ErTe_3$ as a function of temperature and photon polarization. At high energy, electron-hole excitations across the charge density wave (CDW) gap are observed. Below $100\,cm^{-1}$ strongly temperature dependent collective excitations dominate the spectra. With both light polarizations along the c-axis of the single domain crystal a large gap $2\Delta_0$ in the range of $0.4\,eV$ opens below the first CDW transition at $265\,K$. The gap of the second transition at $155\,K$ is only present for aa polarizations. The related amplitude modes do not exactly mirror the anisotropy of the electronic gaps but rather show components of the the higher tetragonal symmetry highlighting the intimate coupling of the electrons to the quasi-tetragonal lattice. The high gap ratios $2\Delta_0/k_BT_c$ in the range above 10 compare well to results of photoemission experiments and indicate that fluctuations substantially suppress the mean-field transition temperature.
This work is supported by the DFG under Grant No. Ha2071/5.

TT 3.10 Mon 13:00 HSZ 304

Collective excitations and low temperature transport properties of bismuth — •Piotr Chudzinski and Thierry Giamarchi — DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland

We examine the influence of collective excitations on several transport coefficients (conductivitiy, magneto-optical conductivity, Nernst effect) for semimetal, bismuth. A longstanding problem of the transport coefficients in this material is the fact that their amplitude and temperature dependences do not obey naive Fermi liquid expectations. For the conductivity, we show that at high temperatures Baber scattering is able to explain quantitatively the DC resistivity experiments, while at low temperatures many-body effects need to be introduced to explain qualitative deviations from the standard T^2 behavior. An atypical feature in magneto-optical conductivity is predicted. The Nernst effect in bismuth was recently the subject of several contradictory theoretical studies. We show that a plasmon physics allows to get a coherent picture and leads to very large values of the Nernst signal. We use two complementary methods- Feynmann diagrams and field theory (Hubbard-Stratonovich transformation). These methods, which go beyond the standard RPA study, allow to set a limit to the validity of our model and to make contact with the other family of semimetals, $1T-TiSe_2$, also subject of recent experimental interest. To complete the discussion of semimetals, we also study the case of graphite.

TT 4: CE: Quantum-Critical Phenomena 1

Time: Monday 10:30–13:00 Location: HSZ 201

TT 4.1 Mon 10:30 HSZ 201

Larmor diffraction studies on the ferromagnetic superconductor UGe_2 — •Robert Ritz[1], Dmitry Sokolov[2], Thomas Keller[3], Andrew D. 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 diffraction (LD) is a novel technique based on the Larmor precession of polarized neutrons that surpasses the resolution of conventional scattering methods by two orders of magnitude [1,2,3]. For a long time it was thought that it is not possible to measure LD on systems with depolarizing properties, such as ferromagnets. We present thermal expansion measurements under pressure by means of Larmor diffraction (LD) on the superconducting Ising ferromagnet UGe_2. LD allowed us to measure magnetization and thermal expansion under pressure in the same setup and hence to directly compare transition temperatures. We found that the thermal expansion near T_X, the transition between two ferromagnetic phases which is believed to drive superconductivity, shows a clear transition in the b- and c-axis under pressure at a temperature a few K higher than for the a-axis and the ferromagnetic Bragg peak. We are considering different mechanisms how this may be connected with the superconductivity in UGe_2.
[1] M.T. Rekveldt et al., Eur. Phys. Lett. **54**, 342 (2001)
[2] T. Keller et al., Appl. Phys. **A 74** , S332 (2002)
[3] C. Pfleiderer et al., Science **316**, 1871 (2007)

TT 4.2 Mon 10:45 HSZ 201

Quantum Phase Transitions in $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ — •Andreas Bauer[1], Tim Adams[1], Christian Franz[1], Andreas Neubauer[1], Maximilian Hirschberger[1], Christopher Krey[1], Robert Georgii[1,2], Peter Böni[1,2], Markus Garst[1,3], and Christian Pfleiderer[1] — [1]Physik Department E21/T30, Technische Universität München, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, Germany — [3]Institute for Theoretical Physics, Universität zu Köln, Germany

The helimagnetic order in MnSi may be suppressed by substitutional doping of Fe or Co on the Mn site. We report a comprehensive study of the magnetization, susceptibility, specific heat and small angle neutron scattering of single-crystal $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ at low temperatures [1]. In contrast to the pressure dependence of pure MnSi the spin polarized state in applied magnetic fields is characteristic of a putative ferromagnetic quantum critical point at a critical concentration x_c. The magnetic phase diagram as a function of composition up to $x \approx 0.5\,x_c$ is thereby essentially unchanged, exhibiting the well known phases (helical order, conical order, and skyrmion lattice phase [2]). When further increasing x the regime of the skyrmion lattice and

the cross-over between the paramagnetic and the helimagnetic state, which may be related to complex spin textures, extend over an increasing temperature and field range. This points at an important role of complex spin textures in the vicinity of x_c.
[1] A. Bauer et al., PRB **82**, 064404 (2010)
[2] S. Mühlbauer et al., Science **323**, 915 (2009)

TT 4.3 Mon 11:00 HSZ 201

Neutron spin echo measurements of magnetic fluctuations in helical $Mn_{1-x}Fe_xSi$ — •Alexander Tischendorf[1], Wolfgang Häussler[1,2], Andreas Bauer[1], Peter Böni[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik Department E21, 85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), 85748 Garching, Germany

Manganese silicide (MnSi) is a 3d intermetallic compound that crystallizes in the cubic B20 structure. In the absence of an applied magnetic field and for temperatures below $T_c = 29.5$ K MnSi displays a long-period helimagnetic state with a wavelength of approximately 180 Å. Under substitutional doping with Fe, the helimagnetic transition temperature decreases and terminates in a set of complex quantum phase transitions (QPT) [1]. We have studied the line width of the spin fluctuations in $Mn_{1-x}Fe_xSi$ by means of neutron spin echo measurements. The high energy resolution and the small angle scattering set up of the spin echo instrument RESEDA at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) thereby offered an ideal parameter range, that is not accessable in conventional triple-axes measurements. Our results will be discussed, in the context of the spin-fluctuation theory of weakly magnetic itinerant-electron compounds, which allows the identification of anomalous behavior at QPTs.
[1] A. Bauer et al., Phys. Rev. B **82**, 064404 (2010)

TT 4.4 Mon 11:15 HSZ 201

Incipient quantum criticality in single-crystal Fe_2TiSn — A. Neubauer[1], •M. Wagner[1], M. Schulz[1,2], A. Senyshyn[2], K. Hradil[2,3], R. Korntner[1], A. Bauer[1], S. Gottlieb-Schönmeyer[1], R. Jungwirth[2], G. Behr[4], J. Kübler[5], C. Felser[6], and C. Pfleiderer[1] — [1]Physik-Department, TU München, 85748 Garching — [2]FRM II, TU München, 85748 Garching — [3]Institut für physikalische Chemie, U Göttingen, 37077 Göttingen — [4]IFW Dresden, 01171 Dresden — [5]Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt — [6]Institut für Anorganische und Analytische Chemie, U Mainz, 55099 Mainz

We have grown single-crystals of the Heusler compound Fe_2TiSn by optical float-zoning. Two parasitic effects, notably the formation of an impurity phase and surface segregations, account for the ferromagnetic (FM) properties of polycrystals of Fe_2TiSn previously attributed to atomic site interchanges. A detailed structural characterization establishes that our single crystals are phase-pure with a typical abundance of twinning domains and a trend to split site disorder of the Fe and Ti atoms. In phase-pure single crystals the temperature dependence of the susceptibility and specific heat suggest incipient FM quantum criticality, masked below a few K by a weak spin-glass transition. With decreasing temperature the resistivity increases characteristic of a small charge gap. The Hall effect corresponds to a charge carrier concentration $n_H \approx 10^{22}\,\mathrm{cm}^{-3}$ with an additional anomalous magnetic field dependence. Compared to conventional scenarios of FM quantum criticality the properties of Fe_2TiSn differ in a number of surprising ways.

TT 4.5 Mon 11:30 HSZ 201

Single-crystal growth and low temperature properties of the non-centrosymmetric heavy-fermion comound $CeAuAl_3$ — •Christian Franz, Andreas Bauer, Kilian Mittermüller, Alfonso Chacon, Marco Halder, and Christian Pfleiderer — Physik Department E21, Technische Universität München, München, Germany

Non-centrosymmetric heavy fermion compounds attract great interest as a platform for unconventional superconductivity and complex forms of magnetic order. We report the first successful single-crystal growth of $CeAuAl_3$ – an isostructural relative with space group I4mm of the heavy-fermion superconductors $CeRhSi_3$ and $CeIrSi_3$. Our single crystals were prepared from high-purity starting elements (> 5N) using a bespoke all-metal sealed rod casting furnace and a bespoke image furnace. High crystal quality was established by Laue x-ray scattering, x-ray powder diffraction and EDX microprobe analysis. The low temperature properties, notably magnetisation, heat capacity and electrical resistivity, identify $CeAuAl_3$ as an antiferromagnetic heavy fermion compound with a low Neel temperature.

15 min. break

TT 4.6 Mon 12:00 HSZ 201

Low-temperarture x-ray powder diffraction in the itinerant antiferromagnet YMn_2 — •Kilian Mittermüller, Saskia Gottlieb-Schönemeyer, Andreas Bauer, and Christian Pfleiderer — Physik Department E21, TU München

The cubic C15 Laves compound YMn_2 displays itinerant antiferromagnetism below a Neel temperature $T_N = 100$ K that is accompanied by a large magnetoelastic expansion of order 5 %. We have set up a Siemens D5000 x-ray powder diffractometer with a pulse tube cryo-cooler for measurements at temperatures down to ~ 8 K. We report a detailed investigation of the structural modifications associated with the Neel transition in YMn_2 as inferred from the x-ray powder diffraction. In agreement with previous work the Neel transition is dominated by large changes of the lattice constants. In addition the transition is highly hysteretic possibly related to the presence of local strains in the powder. We will discuss putative evidence for a tetragonal lattice distortion in the antiferromagnetic state and its consequences for competing electronic instabilities such as charge density wave order in YMn_2.

TT 4.7 Mon 12:15 HSZ 201

Neutron depolarization imaging at milli-Kelvin temperatures of the Kondo-cluster-glass formation in $CePd_{1-x}Rh_x$ — •Philipp Schmakat[1], Michael Schulz[1,2], Christian Pfleiderer[1], Peter Böni[1], Elbio Calzada[1,2], Sergey Masalovich[2], Manuel Brando[3], Christoph Geibel[3], and Micha Deppe[3] — [1]Physik-Department E21, Technische Universität München — [2]Forschungs-Neutronenquelle FRM-II, München — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

In the f-electron compound $CePd_{1-x}Rh_x$ a new groundstate entitled as Kondo-Cluster-Glass has been proposed for $x > 0.65$ [1]. The origin of this cluster formation is assumed to be an interplay of metallurgical inhomogeneities and the effect of two competing interactions, namely the Kondo-screening and the long-range RKKY-interaction.

We have investigated the magnetic phase diagram of the Kondo-lattice $CePd_{1-x}Rh_x$ in the concentration range $0.40 \leq x \leq 0.80$ by means of neutron depolarisation imaging (NDI) down to 75 mK. The NDI technique allowed us to map out inhomogeneities of the transition temperature and the spontaneous magnetization over the sample, as well as the average domain size. Our data are consistent with previous studies and support the picture of the cluster formation where long-range order vanishes with increasing Rh content and short-range interactions become crucial.
[1] J.G. Sereni, Phys. Rev. B 75, 024432 (2007); T. Westerkamp, Phys. Rev. Lett. 102, 206404 (2009).

TT 4.8 Mon 12:30 HSZ 201

Violation of the Wiedemann-Franz law at the Quantum Critical Point of $YbRh_2Si_2$ — •Stefanie Hartmann[1], Cornelius Krellner[1], Stefan Kirchner[2], Ulrike Stockert[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden — [2]MPI PKS, Nöthnitzer Str. 38, 01187 Dresden

The prototype heavy-fermion system $YbRh_2Si_2$ appears to be situated extremely close to an antiferromagnetic (AF) quantum critical point (QCP). Besides the disappearance of the AF ordering ($T_N = 70$ mK) at a tiny critical magnetic field, $B_c \approx 60$ mT, applied perpendicular to the tetragonal c axis, the breakdown of the Kondo scale accompanied by an abrupt Fermi surface reconstruction is assumed to take place at the very same field. Beyond B_c a heavy Landau Fermi-liquid (FL) phase emerges.

We have studied the thermal conductivity $\kappa(T, B)$ as well as the electrical resistivity $\rho(T, B)$ in a wide temperature and field range ($T \geq 30$ mK, $B \leq 1$ T) using the same $YbRh_2Si_2$ single crystalline sample for both measurements. The comparison of both quantities evidences that, in the limit $T = 0$, the Wiedemann-Franz law, $\kappa\rho = L_0T$, is fulfilled deep inside the AF phase as well as in the FL regime of $YbRh_2Si_2$. The universal relation between heat and charge conduction is, however, distinctly violated upon approaching the field-induced QCP from either side, caused by the emergence of a novel type of inelastic small-angle scattering processes.

TT 4.9 Mon 12:45 HSZ 201

Anomalous effect of hole-doping on $YbRh_2Si_2$ — •Yoshi Tokiwa, Hirale S. Jeevan, Maik Schubert, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen,

Friedrich-Hund Platz 1, 37077 Göttingen, Germany

Substituting Fe at the Rh site in $YbRh_2Si_2$ causes both chemical pressure and hole doping. We have investigated single crystals of $Yb(Rh_{1-x}Fe_x)_2Si_2$ with x=0.05 by specific heat, magnetization, resistivity and magnetocaloric effect measurements down to ∼20 mK. The observed shift of the broad maximum in $\rho(T)$ from 140 to 115 K and the reduction of the Kondo temperature from 25 to 15 K could be ascribed to the effect of an effective chemical pressure of ∼0.8 GPa. Without charge carrier doping, such pressure enhances T_N from 0.07 to about 0.3 K. However, no magnetic order is found in $Yb(Rh_{0.95}Fe_{0.05})_2Si_2$ which might be due to the hole-doping effect. The energy scale $T^\star(H)$ that for undoped $YbRh_2Si_2$ collapses at a critical field of 0.05 T is moderately shifted and terminates at a slightly smaller field $H^\star(T \to 0) = 0.03$ T. Divergent behavior of the Sommerfeld coefficient, $\gamma \propto (H - H_c)^{G_r}$, and the magnetic Grüneisen ratio, $\Gamma_H = -G_r/(H - H_c)$ with $G_r = -0.18$ and $H_c = 0.03$ T, is found in the field-induced Landau Fermi liquid state at $H > H_c$ and suggests a quantum critical point in the absence of antiferromagnetic ordering in this system. Work supported by the DFG through research unit 960 (Quantum phase transitions).

TT 5: Micro Mechanical Oscillator 1 (jointly with Q)

Time: Monday 10:30–13:00 Location: HSZ 02

TT 5.1 Mon 10:30 HSZ 02

Listening to the Quantum Drum: Mechanics in its Ground State — •Tobias Donner[1,2], John Teufel[3], Ray Simmonds[3], and Konrad Lehnert[2] — [1]Institute for Quantum Electronics, ETH Zurich, CH-8093 Zurich, Switzerland — [2]JILA, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309, USA — [3]National Institute of Standards and Technology, Boulder, CO 80305, USA

A mechanical resonator is a physicist's most tangible example of a harmonic oscillator. If cooled to sufficiently low temperatures a mechanical oscillator is expected to behave differently to our classical perception of reality. Examples include entanglement and superposition states where a macroscopic, human made object can be in two places at once. Observing the quantum behavior of a mechanical oscillator is challenging because it is difficult both to prepare the oscillator in a pure quantum state of motion and to detect those states. I will present experiments in which we couple the motion of a micro-fabricated oscillator to the microwave field in a superconducting high-Q resonant circuit. The displacement of the oscillator imprints a phase modulation on the microwave field which we detect with a nearly shot-noise limited interferometer. We employ the radiation pressure force of the microwave photons to cool the mechanical oscillator to its motional ground state.

TT 5.2 Mon 10:45 HSZ 02

Optomechanical Coupling of Ultracold Atoms and a Membrane Oscillator — •Maria Korppi[1,2,3], Andreas Jöckel[1], Stephan Camerer[2,3], David Hunger[2,3], Theodor W. Hänsch[2,3], and Philipp Treutlein[1,2,3] — [1]Universität Basel, Switzerland — [2]Ludwig-Maximilians-Universität, München, Germany — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

We report the recent results of our experiment, where we couple a single mode of a high-Q membrane-oscillator to the motion of laser-cooled atoms in an optical lattice. The optical lattice is formed by retroreflection of a laserbeam from the membrane surface. The coupling is mediated by power modulation of the lattice beam due to the vibrations of the atoms in the lattice. If the trap frequency of the atoms in the lattice is matched to the eigenfrequency of the membrane, we observe resonant energy transfer between the two systems.

In the long term, such coupling mechanism could be exploited to develop hybrid quantum systems between atoms and solid-state devices. As another intriguing perspective, a new generation of optical lattice experiment is in sight, where the mirrors creating the laser standing waves are micromechanical oscillators interacting with the atoms on a quantum level.

TT 5.3 Mon 11:00 HSZ 02

Tuning the quality factor of a miromechanical membrane oscillator — •Andreas Jöckel[1], Maria Korppi[1,2,3], Stephan Camerer[2,3], Matthias Mader[2], David Hunger[2,3], Theodor W. Hänsch[2,3], and Philipp Treutlein[1,2,3] — [1]Departement Physik, Universität Basel, Switzerland — [2]Ludwig-Maximilians-Universität, München, Germany — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

We report on the characterization and tuning of the mechanical modes of high-Q SiN-membrane oscillators. Such membranes are used in many optomechanical experiments and have Q-factors up to 10^7 with frequencies in the hundreds of kHz regime and masses of a few ng, resulting in rather large ground state and thermal amplitudes.

We show that the membrane eigenfrequencies can be tuned by locally heating the membranes with laser light, resulting in a release of intrinsic stress. The frequencies of several modes were measured with a Michelson interferometer. We observe that the Q-factor changes dramatically while tuning and reveals resonances in the mechanical dissipation, which allows us to tune the Q-factor over two orders of magnitude. With this technique we achieve an improvement over the bare membrane Q-factor.
Another way of improving the properties of these membranes lies in structuring them with a focused ion beam (FIB) in order to reduce their mass, or applying mirrors to increase the reflectivity.

TT 5.4 Mon 11:15 HSZ 02

A closed-cycle dilution refrigerator with free-space and fiber optical access for quantum optomechanics experiments at 20mK — •Witlef Wieczorek[1], Simon Gröblacher[1], Matthias Bühler[2], Peter Christ[2], Jens Höhne[2], Doreen Wernicke[2,3], and Markus Aspelmeyer[1] — [1]University of Vienna, Faculty of Physics, A-1090 Vienna, Austria — [2]VeriCold Technologies GmbH, Bahnhofstr. 21, D-85737 Ismaning, Germany — [3]Entropy GmbH, Gmundner Str. 37a, D-81379 Munich, Germany

We report on the operation of a closed-cycle dilution refrigerator for quantum optomechanics experiments at 20mK. The sample chamber of the dilution fridge is optically accessible both via optical windows as well as optical fibers, allowing us to perform a variety of optical experiments at low temperatures. It is designed to vibrationally isolate the sample chamber allowing for stable operation of a high-finesse optical cavity. This enables us to perform cavity-optomechanics experiments at ultra-low temperatures.

TT 5.5 Mon 11:30 HSZ 02

Optomechanical cooling close to the ground state — •Rémi Rivière[1], Stefan Weis[1,2], Samuel Deléglise[1,2], Emanuel Gavartin[2], Olivier Arcizet[3], Albert Schliesser[1,2], and Tobias Kippenberg[1,2] — [1]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — [2]Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland — [3]Institut Néel, 38042 Grenoble, France

Optomechanical cooling of a mechanical oscillator mediated by the radiation pressure of the light enables preparing a macroscopic system in its quantum ground state. In our experiment, the vehicle used is a silica microtoroid resonator, hosting both optical and mechanical degrees of freedom within the same device. Combining both cryogenic and optomechanical cooling, we demonstrate an occupancy as low as 9±1 phonons, for which limitations to further phonon occupation reduction are only technical. The forthcoming ground state will then enable the study of quantum effects in a macro-object.

TT 5.6 Mon 11:45 HSZ 02

Cavity optomechanics with nonlinear mechanical resonators in the quantum regime — •Simon Rips, Martin Kiffner, Ignacio Wilson-Rae, and Michael Hartmann — Technische Universität München, Germany

The coupling of light and a mechanical resonator within an optomechanical setup can have significant effects on both the light field inside the cavity and the motion of the mechanical resonator. A prominent example is the cavity assisted side-band cooling of the mechanical motion, leading to low phonon occupation and thereby inducing the quantum regime.

Here, we consider the physics of a nonlinear mechanical resonator, coupled to different cavity modes that are each driven by a detuned laser. We show that the mechanical nonlinearity can be used to prepare a *nonclassical steady state* of mechanical motion. The nonclassicality criterion we use is the appearance of a negative Wigner function.

The open coupled quantum system is treated analytically with the projection operator technique. By tracing out the cavity modes, a master equation for the mechanical motion is derived. The structure of that master equation allows to understand the underlying physics and thereby to identify parameters (especially for detuning) that will produce the nonclassical steady state. The results are verified in a numerical treatment of the full coupled optomechanical system.

TT 5.7 Mon 12:00 HSZ 02

Stochastically activated opto-mechanical coupling — •Andrea Mari and Jens Eisert — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

We study the effect of stochastic noise on the standard opto-mechanical setup: an optical cavity with a vibrating mirror. We show how to engineer an effective bath for the mechanical resonator by using only incoherent thermal light. Thanks to the non-linear interaction Hamiltonian, optical stochastic noise can activate the coupling between a mechanical mode of the mirror and an optical mode of the cavity. This interaction can generate several non-trivial effects, e.g. the counter-intuitive process of cooling with thermal noise. This is another instance - different from stochastic resonance - where somewhat counterintuitively, incoherent noise helps to generate coherent quantum effects.

TT 5.8 Mon 12:15 HSZ 02

Optomechanically Induced Transparency — •Stefan Weis[1,2], Rémi Rivière[2], Samuel Deléglise[1,2], Emanuel Gavartin[1], Olivier Arcizet[3], Albert Schliesser[1,2], and Tobias Kippenberg[1,2] — [1]Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland — [2]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — [3]Institut Néel, 38042 Grenoble, France

Electromagnetically induced transparency is a quantum interference effect observed in atoms and molecules, in which the optical response of an atomic medium is controlled by an electromagnetic field. We demonstrate a form of induced transparency enabled by radiation-pressure coupling of an optical and a mechanical mode. A control optical beam tuned to a sideband transition of a micro-optomechanical system leads to destructive interference for the excitation of an intracavity probe field, inducing a tunable transparency window for the probe beam. Optomechanically induced transparency may be used for slowing and on-chip storage of light pulses via microfabricated optomechanical arrays.

TT 5.9 Mon 12:30 HSZ 02

Quantum dynamics in optomechanical arrays — •Florian Marquardt[1,2], Max Ludwig[1], Georg Heinrich[1], Andreas Kronwald[1], Michael Schmidt[1], Jiang Qian[3], and Björn Kubala[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg — [2]Max-Planck Institut für die Physik des Lichts — [3]Arnold Sommerfeld Center, Center for NanoScience, Department Physik, LMU München

Optomechanical arrays consist of a number of localized vibrational and optical modes coupled to each other via radiation forces. First versions of such structures have been realized recently based on photonic crystal designs. Future setups are projected to enter the quantum regime. We present our theoretical analysis of the linear and nonlinear quantum dynamics of interacting photons and phonons in such arrays.

TT 5.10 Mon 12:45 HSZ 02

Shot noise limited displacement measurement of a high Q micromechanical oscillator below the peak value of the SQL — •Henning Kaufer, Daniel Friedrich, Andreas Sawadsky, Tobias Westphal, Kazuhiro Yamamoto, and Roman Schnabel — Albert-Einstein-Institut, MPI für Gravitationsphysik, QUEST, Leibniz Universität Hannover

The standard quantum limit (SQL) is a classical limit for measurement precision of a test mass position. Using a SiN membrane with a Q-factor of 10^6 and a mass of 100 ng we achieved a displacement sensitivity of $3 \cdot 10^{-16}$ m/$\sqrt{\text{Hz}}$ in a Michelson-Sagnac interferometer and thereby beat the peak value of the SQL at resonance. The interferometer topology allows implementation of advanced interferometer techniques such as power- or signal recycling. The latter can enhance the displacement sensitivity by a factor of 10 in the first step and reveal thermal noise of the oscillator over a broad frequency range.

TT 6: Focused Session: Frontiers in Classical and Quantum Spin Liquids

Time: Monday 14:00–18:00 Location: HSZ 03

Invited Talk TT 6.1 Mon 14:00 HSZ 03

Magnetolyte Properties of Spin Ice — •Steve Bramwell — University College London UK

The discovery of emergent magnetic monopoles in spin ice opens the question as to what extent spin ice behaves like a "magnetolyte" or magnetic electrolyte: a magnetic Coulomb gas with diffusive monopole dynamics.

In this talk I shall illustrate how spin ice realises an almost ideal magnetolyte. In particular I will discuss experimental evidence for the Wien effect (the field -induced dissociation of charges) and the zero field application of the classical Debye-Hückel-Bjerrum theory. I will also discuss recent work that explores the Coulomb gas phase diagram to include regions of strong charge correlations.

I shall draw comparison with the analogous electrical system - an electrolyte containing a 'generation-dissociation' equilibrium, and identify universal aspect of the problem that transcend physical, chemical and biological systems.

Topical Talk TT 6.2 Mon 14:45 HSZ 03

Kitaev-Heisenberg Model on a Honeycomb Lattice: Possible Exotic Phases in Iridium Oxides $A_2\mathbf{IrO}_3$ — •George Jackeli[1], Jiri Chaloupka[1,2], and Giniyat Khaliullin[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Condensed Matter Physics, Masaryk University, Brno, Czech Republic

We discuss a spin one-half Hamiltonian on a honeycomb lattice describing the exchange interactions between Ir^{4+} ions in a family of layered iridates A_2IrO_3 (A=Li,Na). Depending on the microscopic parameters, the Hamiltonian interpolates between the Heisenberg and exactly solvable Kitaev models [1,2]. Exact diagonalization and a complementary spin-wave analysis [2] reveal the presence of an extended spin-liquid phase near the Kitaev limit and a conventional Néel state close to the Heisenberg limit. The two phases are separated by an unusual stripy antiferromagnetic state, which is the exact ground state of the model at the midpoint between two limits.

[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009).
[2] J. Chaloupka, G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **105**, 027204 (2010).

15 min. break

Invited Talk TT 6.3 Mon 15:45 HSZ 03

Disorder in a quantum spin liquid: flux binding and local moment formation — Adam Willans[1], •John Chalker[1], and Roderich Moessner[2] — [1]Theoretical Physics, Oxford University, UK — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden

We study the consequences of disorder in the Kitaev honeycomb model, using this exactly solvable spin liquid as a laboratory for the exploration of impurity effects in strongly fluctuating quantum magnets. The clean system has fermionic excitations and Z_2 fluxes as its degrees of freedom, and this remains the case with disorder. As a function of model parameters, it displays gapless and gapped phases.

We examine the effects of site dilution and exchange randomness in both phases. We show that a single vacancy binds a flux and induces a local moment. This moment is polarised by an applied field h: in the gapless phase, for small h the local susceptibility diverges as $\chi(h) \sim \ln(1/h)$; for a pair of nearby vacancies on the same sublattice, this even increases to $\chi(h) \sim 1/(h[\ln(1/h)]3/2)$. By contrast, weak ex-

change randomness does not qualitatively alter the susceptibility but has its signature in the heat capacity, which in the gapless phase is power law in temperature with an exponent dependent on disorder strength.

Topical Talk TT 6.4 Mon 16:30 HSZ 03

Fractional spin textures in the frustrated magnet $SrCr_{9p}Ga_{12-9p}O_{19}$ — •Kedar Damle[1], Roderich Moessner[2], and Arnab Sen[1,3] — [1]Tata Institute of Fundamental Research, Mumbai, India — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [3]Boston University, Boston, USA

Quantum mechanics constrains the total electronic spin S of magnetic ions to integer or half-integer values. For an isolated ion with only spin angular momentum and Lande g-factor $g_L = 2$, this results in a magnetic moment of $\mu = 2\mu_B S$, and a susceptibility $(2\mu_B)^2 S(S+1)/3T$, which is approximated by $(2\mu_B)^2 S^2/3T$ when spins are treated as classical length-S vectors. Here, we demonstrate that certain vacancy configurations, in a class of corner-sharing networks made up of such spin-S ions coupled antiferromagnetically, give rise to an extended spin texture with classical susceptibility $(2\mu_B)^2(S/2)^2/3T$.

This corresponds to a *fractional moment* of $\mu/2$ and represents an instance of fractionalisation yielding a fractional "effective spin" $S/2$ in a classical setting. This fractional-spin texture leaves an unmistakable imprint on the measured ^{71}Ga nuclear magnetic resonance lineshapes in the archetypal frustrated magnet SCGO, which we compute using Monte-Carlo simulations and compare with experimental data.

Topical Talk TT 6.5 Mon 17:15 HSZ 03

Quantum Criticality and E8 symmetry in an Ising Chain — •Alan Tennant — Helmholtz Zentrum Berlin

Quantum phase transitions take place between distinct phases of matter at zero temperature. Near the transition point, exotic quantum symmetries can emerge that govern the excitation spectrum of the system. A symmetry described by the E-8 Lie group with a spectrum of eight particles was long predicted to appear near the critical point of an Ising chain. We realize this system experimentally by using strong transverse magnetic fields to tune the quasi-one-dimensional Ising ferromagnet CoNb$_2$O$_6$ (cobalt niobate) through its critical point. Spin excitations are observed to change character from pairs of kinks in the ordered phase to spin-flips in the paramagnetic phase. Just below the critical field, the spin dynamics shows a fine structure with two sharp modes at low energies, in a ratio that approaches the golden mean predicted for the first two meson particles of the E-8 spectrum. Our results demonstrate the power of symmetry to describe complex quantum behaviors. \newline Science 327, 177 (2010)

TT 7: SC: Properties, Electronic Structure, Mechanisms 2

Time: Monday 14:00–16:15 Location: HSZ 301

TT 7.1 Mon 14:00 HSZ 301

Importance of spin-orbit coupling for the electron-phonon interaction of the strong-coupling superconductor Pb — •Rolf Heid[1], Klaus-Peter Bohnen[1], Irina Sklyadneva[2,1], and Evgeni Chulkov[2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik — [2]Donostia International Physics Center, San Sebastian, Spain

Electron-phonon coupling (EPC) properties can nowadays be calculated routinely from first principles within a DFT-based linear-response approach. All previous studies, however, have been carried out in a semi-relativistic framework, which does not take into account the effects of spin-orbit coupling (SOC). Based on a recent implementation of the SOC for linear response calculations within a mixed-basis pseudopotential approach [1], we analyze the effect of SOC on the EPC for the prototype strong-coupling superconductor Pb. We find that SOC increases the coupling constant λ by 44%, solving the longstanding puzzle of too small λ values obtained consistently in previous first principles calculations. The origin of the SOC-induced enhancement of λ lies both in a softening of the phonon spectrum and in an increase of the EPC matrix elements, which significantly improves the agreement with tunneling experiments. We also find a large influence of SOC on phonon-induced electronic self-energies and lifetimes. Finally, consequences for EPC properties of thin Pb films will be discussed.
[1] R. Heid, K.-P. Bohnen, I. Yu. Sklyadneva, E. V. Chulkov, Phys. Rev. B **81**, 174527 (2010)

TT 7.2 Mon 14:15 HSZ 301

First principles study of the spin-orbit coupling effect on the Tl-Pb-Bi superconducting alloys — •Omar De la Peña-Seaman, Rolf Heid, and Klaus-Peter Bohnen — Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Germany

We have studied the influence of spin-orbit coupling (SOC) on the phonon properties, the electron-phonon (e-ph) coupling and on the superconducting properties for the Pb-Bi and Pb-Tl alloys in the stable fcc-phase doping regimes. These systems have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloys. The Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated with and without SOC. The observed effects of SOC in the full phonon dispersion and $\alpha^2F(\omega)$ consist in a softening of the phonon frequencies and an increase of the e-ph coupling matrix elements, which become weaker on the Tl-rich side. SOC enhances λ by as much as 48% in some cases and improves its overall behavior as a function of the concentrations for the alloy systems, leading to a very nice agreement with experimental data from tunneling measurements.

TT 7.3 Mon 14:30 HSZ 301

Effects of the Born-Oppenheimer approximation in the electronic band structure of MgB_2 and ZrB_2. — •Vivien Petzold and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Electronic band structure calculations are routinely applied to many problems in chemistry and physics. The methods rely on a number of approximations, where the treatment of exchange and correlation is a very prominent issue, probably the most prominent in the development of new density functionals in the framework of density functional theory (DFT). The present work highlights effects that arise from the more fundamental Born-Oppenheimer approximation. Based on this approximation, the original problem - the quantum-mechanical description of matter consisting of nuclei and electrons - is decomposed into a nuclear and an electronic problem, the latter of which is treated by electronic band structure methods. Utilizing the most common density functionals, the local density approximation (LDA) and the generalized gradient approximation (GGA), we observe deviations between experimental and theoretical de Haas van Alphen (dHvA) frequencies for MgB_2 and ZrB_2 that can be consistently understood by electron-phonon coupling effects, which the theory is lacking. The explanation is based on a highly accurate computation of dHvA frequencies indicating an electron-phonon coupling-induced shift of the electronic bands.

TT 7.4 Mon 14:45 HSZ 301

Vibrational and thermal properties of ternary semiconductors and their isotopic dependence: chalcopyrite $CuGaS_2$ — •Reinhard K. Kremer[1], Manuel Cardona[1], Rudolf Lauck[1], Aldo H. Romero[2], and Alfonso Munoz[3] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]CINVESTAV, Unidad Queretaro, Queretaro, Mexico — [3]MALTA Consolider Team, Dep. de Fisica, Universidad de La Laguna, La Laguna , Tenerife, Spain

The availability of ab initio electronic calculations and the concomitant techniques for deriving the corresponding lattice dynamics have been profusely used in the past decade for calculating thermodynamic and vibrational properties of semiconductors, as well as their dependence on isotopic masses. The latter have been compared with experimental data for elemental and binary semiconductors with different isotopic compositions[1]. Here we present experimental and theoretical data for several vibronic and thermodynamic properties of a canonical ternary semiconductor of the chalcopyrite family: $CuGaS_2$[2]. Among these properties are the lattice parameters, the phonon dispersion relations and densities of states (projected on the Cu, Ga, and S constituents), the specific heat and the volume expansion coefficient. The calculations were performed with the ABINIT and VASP codes within the

LDA approximation for exchange and correlation.
[1] M. Cardona, et al., PRB 81, 075202 (2010).
[2] Gibin et al., Solid State Commun 133, 569 (2005); Sanati et al. Solid State Commun. 131 229 (2004).

TT 7.5 Mon 15:00 HSZ 301

Fermi-surface topology of the $Ce_{1-x}Yb_xCoIn_5$ — •A. Polyakov[1], O. Ignatchik[1], A. D. Bianchi[2], B. Prevost[2], G. Seyfarth[2], Z. Fisk[3], D. Hurt[3], R. G. Goodrich[4], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, Germany — [2]Department of Physics, University of Montreal, Canada — [3]Department of Physics and Astronomy, University of California, USA — [4]Department of Physics, George Washington University, USA

The heavy-fermion (HF) metals are very susceptible to chemical substitution. In these compounds the Kondo coupling between a lattice of local moments and the conduction band creates quasiparticle excitations with large effective masses and the dopants disrupt the coherent Kondo coupling. We study the effect of Yb doping on the Pauli-limited, HF superconductor, $CeCoIn_5$ via de Haas-van Alphen (dHvA) measurements. Yb acts as a non-magnetic divalent substitution for Ce, equivalent to hole doping on the rare-earth site. Our main goal consists in the systematic investigation of the dHvA oscillations on $Ce_{1-x}Yb_xCoIn_5$ in order to elucidate the evolution of the Fermi surface as a function of Yb. The dHvA data were obtained on high-quality single crystals with different concentrations of Yb atoms. The experiment was performed in a top-loading dilution refrigerator by use of a capacitive torque cantilever technique at temperatures down to 20 mK in magnetic fields up to 18 T.

Work supported in part by EuroMagNET, EU contract No. 228043.

TT 7.6 Mon 15:15 HSZ 301

Order parameter in $CeCu_2Si_2$ — •Hugo A. Vieyra[1], Manuel Brando[1], Niels Oeschler[1], Silvia Seiro[1], Hirale S. Jeevan[2], Christoph Geibel[1], David Parker[3], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [2]I. Physik. Institut, Georg-August-Universität Göttingen, Göttingen 37077, Germany — [3]US Naval Research Laboratory. Washington, DC 20375, USA

Understanding the interplay between magnetism and unconventional superconductivity remains a key challenge in solid-state physics. A clear example is the archetypical heavy-fermion compound $CeCu_2Si_2$ which exhibits superconductivity (T_c=600 mK) in the vicinity of a magnetic quantum critical point. It is believed that magnetic fluctuations mediate superconductivity and its order parameter possesses d-wave symmetry, both ideas still under debate. In this work, a high-quality single crystal with a purely superconducting ground state (S type) has been chosen to investigate the low-temperature thermal- and electric-transport characteristics of the superconducting state. Non-vanishing contributions of low-energy quasiparticle excitations to the thermal transport ($\kappa_0/T > 0$) suggest the presence of nodal structure in $CeCu_2Si_2$. In turn, angle-dependent resistivity measurements of the upper critical field H_{c2} point towards unconventional superconductivity with d-wave symmetry of the order parameter. Theoretical calculations reveal the strong influence of Pauli paramagnetic effects and a d_{xy} symmetry of the gap function.

TT 7.7 Mon 15:30 HSZ 301

Spin fluctuation mediated Cooper-pairing in non-centrosymmetric $CePt_3Si$ — •Ludwig Klam[1] and Dirk Manske[2] — [1]Institut für Theoretische Physik, Wolfgang-Pauli-Str. 27, CH-8093 Zürich — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

Non-centrosymmetric superconductors, and in particular $CePt_3Si$, attract special interest, since the antisymmetric spin-orbit coupling provides the unique opportunity to consider a microscopic mixture of a spin singlet and triplet superconducting order parameter. An efficient numerical method is introduced in order to calculate the dynamical spin and charge response of $CePt_3Si$, using an itinerant description for the electrons. With a realistic parametrization of the band structure, the nesting function is calculated for a selected band in the normal non-magnetic state. From the spin and charge susceptibility, a superconducting pairing interaction is constructed for the weak-coupling gap equation. A sign analysis of the decoupled gap equation supports the experimental evidence of a strong triplet contribution to the order parameter in $CePt_3Si$. In particular for this compound, it can be shown that an increasing Rashba-type of spin-orbit coupling strengthens the triplet contribution.

TT 7.8 Mon 15:45 HSZ 301

Electronic properties of molecular picene — •M. Grobosch[1], F. Roth[1], B. Mahns[1], M. Gatti[2], P. Cudazzo[2], B. Büchner[1], A. Rubio[2], and M. Knupfer[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Nano-Bio Spectrocopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales Universidad del País Vasco, Av. Tolosa, E-20018 San Sebastían, Spian

We have studied the electronic properties of molecular picene by a combination of accurate experimental (photoemission spectroscopy, absorption spectroscopy) and theoretical spectroscopy to get a deeper insight into the occupied and unoccupied electronic states of this recently discovered organic semiconductor. By means of combined photoelectron spectroscopy (XPS, UPS) we have determined the ionization potential of solid picene to be 6.4 eV and a work function of 4.4 eV, i.e. picene is rather stable against oxidation. The first occupied electronic levels of picene are quite close in energy and the onset of the electronic DOS is at about 2 eV below the chemical potential indicating a quite large band gap of solid picene. The C1s excitation data of solid picene measured using EELS compared to the unoccupied electronic DOS calculated in the GW approximation are in very good agreement if GW corrections are taken into account.

TT 7.9 Mon 16:00 HSZ 301

Dynamic response and anomalous plasmon dispersion of potassium doped picene — •Friedrich Roth[1], Benjamin Mahns[1], Mandy Grobosch[1], Matteo Gatti[2], Pierluigi Cudazzo[2], Bernd Büchner[1], Angel Rubio[2], and Martin Knupfer[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastián, Spain

We performed electron energy-loss spectroscopy studies in order to get a deeper insight into the electronic structure of the potassium intercalated picene and the peculiar physical properties of this recently discovered superconductor. A comparison of the loss function of the undoped and doped compound shows the appearance of a new peak in the optical gap, which we attributed to a charge carrier plasmon. We find a remarkable negative plasmon dispersion and a dramatic increase for the value of the background dielectric constant ϵ_∞ upon doping.

TT 8: TR: Graphene 2 (jointly with MA, HL, and DY)

Time: Monday 14:00–18:30 Location: HSZ 304

TT 8.1 Mon 14:00 HSZ 304

Radiation-induced quantum interference in graphene based n-p junctions — •Mikhail Fistul[1], Sergey Syzranov[1], Anatoly Kadigrobov[1,2], and Konstantin Efetov[1] — [1]Ruhr-Universität, Bochum, Germany — [2]University of Gothenburg, Göteborg, Sweden

We predict and analyze *radiation-induced quantum interference effect* in low-dimensional graphene based n-p junctions.

In the presence of radiation the ballistic transport of electrons is determined by two processes, namely, by the resonant absorption of photons near the "resonant points", and by the strong reflection from the junction interface, occurring at the "reflection points". There are two paths corresponding to the propagation of electrons through the junction, and the interference between these two paths manifests itself by *large oscillations of the ballistic photocurrent* as a function of the gate voltage or the frequency of the radiation. This coherent quantum phenomenon resembles Ramsey quantum beating and Stueckelberg oscillations well-known in atomic physics.

A suitable radiation frequency may be in the THz or in the infrared optical region. The effect can be observed best in one- and two-dimensional n-p junctions based on carbon nanotubes, monolayer

or bilayer graphene nanoribbons.

TT 8.2 Mon 14:15 HSZ 304

Resonant Scattering by Realistic Impurities in Graphene — •Tim Wehling[1], Shengjun Yuan[2], Alexander Lichtenstein[1], Andre Geim[3], and Mikhail Katsnelson[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Radboud University of Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom

We develop a first-principles theory of resonant impurities in graphene and show that a broad range of typical realistic impurities leads to the characteristic sublinear dependence of the conductivity on the carrier concentration. By means of density functional calculations various organic groups as well as adatoms such as H absorbed to graphene are shown to create midgap states within $\pm 0.03\,\mathrm{eV}$ around the neutrality point. A low energy tight-binding description is mapped out. Boltzmann transport theory as well as a numerically exact Kubo formula approach yield the conductivity of graphene contaminated with these realistic impurities in accordance with recent experiments. Consequences for spin-flip scattering are discussed.

TT 8.3 Mon 14:30 HSZ 304

Effect of Coulomb interaction on the gap in monolayer and bilayer graphene — Andreas Sinner and •Klaus Ziegler — Institut für Physik, Universität Augsburg

We study effects of a repulsive Coulomb interaction on the spectral gap in monolayer and bilayer graphene in the vicinity of the charge neutrality point by employing the functional renormalization-group technique. In both cases Coulomb interaction supports the gap once it is open. For monolayer graphene we correctly reproduce results obtained previously by several authors, e.g., an apparent logarithmic divergence of the Fermi velocity and the gap as well as a fixed point corresponding to a quantum phase transition at infinitely large Coulomb interaction. On the other hand, we show that the gap introduces an additional length scale at which renormalization flow of diverging quantities saturates. An analogous analysis is also performed for bilayer graphene with similar results. We find an additional fixed point in the gapless regime with linear spectrum corresponding to the vanishing electronic band mass. This fixed point is unstable with respect to gap fluctuations and can not be reached as soon as the gap is opened. This preserves the quadratic scaling of the spectrum and finite electronic band mass. Ref.:Phys. Rev. B, 82, 165453 (2010).

TT 8.4 Mon 14:45 HSZ 304

Dirac electrons in a spin-orbit periodic potential — •Lucia Lenz[1,2] and Dario Bercioux[1,2] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universitat, D-79104 Freiburg, Germany

In this talk we present a study of the the band structure of Dirac electrons in graphene in the presence of one-dimensional, periodically modulated spin-orbit interactions. It has been shown that the transmissions of the spin up and spin down channels are strongly dependent on the length of the barrier compared to the spin-precession length [1]. Based on the knowledge of the transfer matrix, we obtain an analytic equation for the band condition using the transfer matrix method [2]. We investigate how the band structure changes compared to potentials with no spin-orbit interactions [3], and give further interpretations to the additional eigenmodes of the transfer matrix.

[1] D. Bercioux, and A. De Martino, Phy. Rev. B **81**, 165410 (2010).
[2] B.H.J. McKellar, G.J. Stepheson, Phy. Rev. C, **35**, 2262 (1987).
[3] M. Barbier, F.M. Peeters, P. Vasilopoulos, J.M. Pereira, Phy.Rev. B **77**, 115446 (2008).

TT 8.5 Mon 15:00 HSZ 304

Transmission through electrostatic and magnetic barriers in the $\mathcal{T}_3$-lattice — •Daniel F. Urban[1], Dario Bercioux[1,2], and Wolfgang Häusler[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [3]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

Albeit the $\mathcal{T}_3$-lattice exhibits a reciprocal lattice similar to graphene with two inequivalent Dirac-points at six corners of the hexagonal first Brillouin zone, where relativistic electron-hole symmetric bands touch, $\mathcal{T}_3$ differs and considerably generalizes graphene. A peculiarity of $\mathcal{T}_3$ is the occurance of an additional dispersionless energy band at energy $E = 0$ and an enlarged pseudo-spin $S = 1$ [1] instead of $S = \frac{1}{2}$ as for graphene. As a result, we find enhanced Klein tunneling through rectangular electrostatic barriers, compared to the case of graphene. Moreover, at the particular energy of half the barrier height we find even complete transparency, $T = 1$, irrespective of barrier thickness and of incidence angle. We also investigate rectangular magnetic barriers and in this case identify regimes of zero barrier transparency, qualitatively similar to the case of graphene [2].

[1] D. Bercioux, D. F. Urban, H. Grabert, and W. Häusler, Phys. Rev. A **80**, 063603 (2009).
[2] A. De Martino, L. Dell'Anna, and R. Egger, Phys. Rev. Lett. **98**, 066802 (2007).

TT 8.6 Mon 15:15 HSZ 304

Weak Localization versus Weak Antilocalization in Graphene — •Frank Ortmann[1], Alessandro Cresti[2], Gilles Montambaux[3], and Stephan Roche[4] — [1]INAC/SPRAM, CEA Grenoble, France — [2]IMEP-LAHC, Minatec, Grenoble, France — [3]Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France — [4]Institut Català de Nanotecnologia and CIN2, Universitat Autònoma de Barcelona, Barcelona, Spain

The understanding of quantum transport phenomena in graphene-based materials is the current subject of great excitation. In the presence of disorder, one of the predicted signatures of pseudospin is the change in sign of the quantum correction to the semiclassical Drude conductivity. This phenomenon, referred to as weak antilocalization (WAL), results from complex quantum-interferences of charge carriers in a disordered potential landscape and has been recently observed experimentally with weak-field magnetotransport measurements.

In this talk we present a numerical weak-field magnetotransport study of huge graphene samples and the influence of a realistic (long-range) disorder potential describing charges trapped in the gate oxide. Our simulations give clearly different magnetoconductance responses in different regimes which are fingerprint of either weak localization or WAL. Depending on the strength of the perturbing potential, the magnetoconductance can be tuned from positive to negative. The gate potential provides a second handle to modify these characteristics. Our results therefore shed new light on experiments and unveil the possible origin of crossovers from positive to negative magnetoconductance.

15 min. break

TT 8.7 Mon 15:45 HSZ 304

Graphene-based electronic spin lenses — •Ali G. Moghaddam[1] and Malek Zareyan[2] — [1]Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institute for Advanced Studies in Basic Sciences (IASBS), P.O. Box 45195-1159, Zanjan, Iran

We have proposed a solid state electronic spin lens based on a ferromagnetic graphene which has an exchange potential higher than its Fermi energy. The key property is that an interface between such a spin-chiral ferromagnetic (FM) and a nomal (N) graphene region exhibits a negative electronic refractive index which has different signs for electrons with different spin-directions. We have shown that in a corresponding N-FM-N structure, an unpolarized electronic beam can be collimated with a finite spin-polarization producing a point spin accumulation with associated Friedel-like oscillations of spin-dependent local density of states. In this respect, our study reveals that magnetic graphene has the potential to be the electronic counterpart of the recently discovered photonic chiral metamaterials which exhibit a negative refractive index for only one direction of the circular polarization of the electromagnetic wave.

[1] A. G. Moghaddam and M. Zareyan, Phys. Rev. Lett. **105**, 146803 (2010).

TT 8.8 Mon 16:00 HSZ 304

Thermal fluctuations of free standing graphene — •Nils Hasselmann[1,3] and Fabio Braghin[2,3] — [1]MPIFKF Stuttgart — [2]Univ. Fed. de Goias, Goiania, GO, Brazil — [3]IIP, UFRN, Natal, RN, Brazil

We use non-perturbative renormalization group techniques to calculate the momentum dependence of thermal fluctuations of graphene, based on a self-consistent calculation of the momentum dependent elastic constants of a tethered membrane. We find a sharp crossover from

the perturbative to the anomalous regime, in excellent agreement with Monte Carlo results for the the out-of-plane fluctuations of graphene, and give an accurate value for the crossover scale. Our work strongly supports the notion that graphene is well described as a tethered membrane. Ripples emerge naturally from our analysis.

TT 8.9 Mon 16:15 HSZ 304

Transport through a quantum-spin-Hall-insulator/normal junction in graphene ribbons — •Georgo Metalidis[1] and Elsa Prada[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid, Spain

We have investigated a junction between a quantum-spin-Hall insulator and a metallic contact obtained by selectively doping a single graphene ribbon. In the absence of disorder, the transmission of the topological edge states through the junction is perfect due to the orthogonality of left- and right-movers. This is proven analytically by deriving exact wavefunctions for the topological edge states in armchair and zigzag ribbons. The wavefunction character depends fundamentally on the ribbon termination: the edge state width is only dependent on the spin-orbit coupling strength for armchair ribbons, whereas it is only weakly dependent of this parameter for zigzag edge states where the width becomes energy dependent instead. These observations are confirmed in numerical plots of the current density in the sample. When disorder is present, the orthogonality between left- and right-movers is destroyed and backscattering sets in. Nevertheless, the perfect transmission can be restored by increasing the ribbon width.

TT 8.10 Mon 16:30 HSZ 304

Edge magnetism in nanoribbons of graphene — •Hélène Feldner[1,2], Zi Yang Meng[3], Thomas C. Lang[4], Fakher Assaad[4], Stefan Wessel[3], Andreas Honecker[2], and Daniel Cabra[1] — [1]IPCMS, Strasbourg, France — [2]Institut für Theoretische Physik, Göttingen, Germany — [3]Institut für Theoretische Physik III, Stuttgart, Germany — [4]Institut für Theoretische Physik und Astrophysik, Würzburg Am Hubland, Germany

A simple tight-binding model is sufficient to describe most of graphene's properties, but a Hubbard model is needed to account for its magnetic properties. To be able to compute quantities in direct space and for big systems of realistic size with chosen geometry, we use a mean field approximation solved in a self-consistent way in the direct space. In agreement with known results, we find a Mott-Hubbard transition, and a magnetization of the zig-zag edge of finite samples. We have studied the accuracy of the approximation by a comparison of our results with those obtained by exact diagonalization and quantum Monte-Carlo simulations [1]. The main point of our current work consists of a study of the graphene zig-zag ribbons by mean field and quantum Monte-Carlo simulations. First we have looked at the static magnetism of the zig-zag edges and in a second part the local spectral function. These quantities allow us to study the influence of static magnetism on dynamical properties and the local density of states which is a quantity accessible experimentally by STM and shows different behavior on the edge with and without magnetic properties.
[1] Phys. Rev. B 81, 115416 (2010).

TT 8.11 Mon 16:45 HSZ 304

Screening of external electrical fields for different graphene nanoribbons — •Tobias Burnus[1], Gustav Bihlmayer[1], Daniel Wortmann[1], Yuriy Mokrousov[1], Stefan Blügel[1], and Klaus Michael Indlekofer[2] — [1]Peter Grünberg Institut & 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. In this talk the effect of the screening of an in-plane oriented external electric field due to the electrons in graphene nanoribbons is studied in the framework of density functional theory calculations based on the full potential linearized augmented planewave method. These calculations offer a direct link to the static dielectric constant in the ribbon. We compare armchair ribbons of different width to see the effect of the bandgap on the electric response, as well an orientation with zig-zag edges, which show a metallic edge state. The formation of QDs in structures with both types of edges in an external field is considered. The presence of metallic states, e.g. from a substrate, significantly modifies the behavior of QD states in the external field. The work is supported by the DFG Research Unit 912 "Coherence and Relaxation Properties of Electron Spins".

TT 8.12 Mon 17:00 HSZ 304

Color-dependent conductance of graphene with adatoms — •Jörg Schelter[1], Pavel Ostrovsky[2,3], Igor Gornyi[2,4], Björn Trauzettel[1], and Mikhail Titov[2,5] — [1]Institut für Theoretische Physik und Astrophysik, University of Würzburg, 97074 Würzburg, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [4]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [5]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK

We study ballistic transport properties of graphene with a low concentration of vacancies or adatoms. The conductance of graphene doped to the Dirac point is found to depend on the relative distribution of impurities among different sites of the honeycomb lattice labeled in general by six colors. The conductivity is shown to be sensitive to the crystal orientation if adatom sites have a preferred color. Our theory is confirmed by numerical simulations using recursive Green's functions with no adjustable parameters.

15 min. break

TT 8.13 Mon 17:30 HSZ 304

Edge effects on correlations in quasiparticle spectra of graphene billiards — •Jürgen Wurm[1], 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 study the energy spectrum of quasiparticles in chaotic billiards realized in nanostructured graphene. In particular, we focus on the different types of edges and show how they effect correlations in the spectrum. Previously we have investigated 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. Here we describe the quasiparticle dynamics in graphene analytically using the effective 2D Dirac Hamiltonian and imposing appropriate boundary conditions that depend on the specific structure of the graphene edges. Starting from the multiple reflection expansion for the exact Green function, we develop a semiclassical theory for graphene and derive a trace formula for the oscillating part of the density of states. We then focus on correlations in the spectrum investigating the spectral form factor and its dependence on the edge structure of the graphene billiard.
[1] J.Wurm, A.Rycerz, I.Adagideli, M.Wimmer, K.Richter and H.U.Baranger. Phys. Rev. Lett. 102, 056806 (2009)
[2] J.Wurm, M.Wimmer, I.Adagideli, K.Richter and H.U.Baranger. New J. Phys. 11, 095022 (2009)

TT 8.14 Mon 17:45 HSZ 304

Transport in Rough Quasi-One-Dimensional Systems — •Otto Dietz[1], Ulrich Kuhl[1,2], Hans-Jürgen Stöckmann[1], Felix M Izrailev[3], and Nykolay M Makarov[3] — [1]Universität Marburg, Germany — [2]Université de Nice, France — [3]Universidad de Puebla, Mexico

Scattering at rough disordered boundaries strongly influence the conductance of nanowires. For rough silicon nanowires a much higher ratio of electric conductivity to thermal conductivity has been reported than expected from the Wiedemann-Franz law [1]. These findings have not been explained yet.

In the case of bulk disorder it is well known that correlations can drastically change conductance properties [2]. Similar effects have been predicted for rough nanowires [3] but drew little attention before their applicability to conductivity in silicon nanowires became evident.

We present a first experimental test of this theory in microwave waveguides with rough walls. Because of the strict analogy between the 2d Schrödinger equation and the Helmholtz equation, the results can be directly applied to electron transport in nano structures. Microwave techniques can be helpful in this respect, since in contrast to real nanowires the surface roughness is both known and controllable. We could confirm that certain rough boundaries can block or enhance wave transport in given frequency windows. \newline [1] A.

I. Hochbaum, et. al., Nature 451, 163 (2008). \newline [2] U. Kuhl, et.al., Appl. Phys. Lett. 77, 633 (2000). \newline [3] M. Rendón, et.al., Phys. Rev. B 75, 205404 (2007).

TT 8.15 Mon 18:00 HSZ 304

Strong suppression of thermal conductivity in defected graphene nanoribbons: Order-N methodology and thermoelectric properties — •Hâldun Sevinçli[1], Wu Li[1,2], Stephan Roche[1,3,4], and Gianaurelio Cuniberti[1] — [1]1Institute for Materials Science and Max Bergmann Center of Biomaterials, TU-Dresden, 01062 Dresden, Germany — [2]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [3]Institut Català de Nanotecnologia (ICN) and CIN2, Campus UAB, 08193 Bellaterra, Barcelona, Spain — [4]Institució Catalana de Recerca Avançats (ICREA), 08010, Barcelona, Spain

We investigate electron and phonon transport through defected graphene nanoribbons (GNRs). For phonon transport, we develop an efficient linear scaling method which is based on the Chebyshev polynomial expansion of the time evolution operator and the Lanczos tridiagonalization scheme, and also use molecular dynamics simulations. We show that edge-defects reduce phonon thermal transport dramatically in both armchair and zigzag GNRs, while in zigzag GNRs edge-defects are only weakly detrimental to electronic conduction. On the other hand, bulk defects suppress both charge and thermal transport for relatively high density of defects. The behavior of the electronic and phononic elastic mean free paths of zigzag GNRs with edge-defects points to the possibility of realizing an electron-crystal coexisting with a phonon-glass.

TT 8.16 Mon 18:15 HSZ 304

Orbital magnetism in ballistic graphene quantum dots — •Lisa Hesse[1], Jürgen Wurm[1], Inanç Adagideli[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 — [2]Faculty of Engineering and Natural Sciences, Sabancı University, Orhanlı - Tuzla, 34956, Turkey

We study the magnetic response of quasiparticles in graphene quantum dots. To this end we derive the density of states (DOS) of graphene nanostructures including the effect of a small magnetic field, starting from an exact expansion for the Green function of a graphene flake with arbitrary types of edges. We then consider systems much larger than the Fermi wavelength, for which we can evaluate this expansion in the semiclassical limit and obtain the DOS. For graphene, the structure of the boundary has significant effects on both the average DOS and the DOS oscillations. We then calculate the orbital magnetic susceptibility that is closely related to the DOS and discuss the pecularities that arise due to the different types of edges and the pseudospin degrees of freedom of charge carriers in graphene.

TT 9: CE: (General) Theory 1

Time: Monday 14:00–18:15 Location: HSZ 201

TT 9.1 Mon 14:00 HSZ 201

Non-equilibrium self-energy-functional theory — •Matthias Balzer and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Hamburg

Using standard perturbation theory to all orders, the grand potential of a system of strongly correlated electrons can be expressed as a functional of the self-energy such that the physical self-energy is a stationary point. Non-perturbative approximations can be constructed by restricting the domain of the self-energy functional $\Omega[\Sigma]$ to a subspace of trial self-energies spanned by an exactly solvable reference system [1]. This comprises approximations, such as the dynamical mean-field theory (DMFT) and the variational cluster approximation (VCA).

Here we show that this concept can be extended straightforwardly to the non-equilibrium case. Green's functions and self-energies have to be defined on the three-branch Keldysh-Matsubara contour in the complex time plane [2], and Ω must be reinterpreted accordingly. The resulting variational scheme is extremely general and provides a rederivation of non-equilibrium DMFT [3], for example.

To discuss practical issues relevant for a numerical implementation of a non-equilibrium VCA, we consider in a first step a coupling of Hubbard-type reference systems consisting of two sites only. Different initial states will be considered, e.g. an uncorrelated Neel state or a correlated singlet state, to study the time evolution of spin correlations.

[1] M. Potthoff, Eur. Phys. J. B 32, 429 (2003).
[2] M. Wagner, Phys. Rev. B 44, 6104 (1991).
[3] J. Freericks et al., Phys. Rev. Lett. 97, 266408 (2006).

TT 9.2 Mon 14:15 HSZ 201

Efficient Legendre representation of Many-Particle Green's functions — •Lewin Boehnke[1], Frank Lechermann[1], Michel Ferrero[2], and Olivier Parcollet[3] — [1]1. ITP, Universität Hamburg, D-20355 Hamburg, Germany — [2]CPhT, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]IPhT, CEA/DSM/IPhT-CNRS/URA 2306 CEA-Saclay, F-91191 Gif-Sur-Yvette, France

Even though a way of obtaining frequency and wave-vector-dependent lattice susceptibilities within the dynamical mean-field theory (DMFT) is known for some years [1], only very few calculations were actually performed. A reason therefore is the numerically expensive handling of the two-particle Green's function with respect to three slowly decaying frequency variables. Within quantum Monte-Carlo (QMC) methods, the latter fact renders the accumulation lengthly and leads to numerical instabilities in the further use of the obtained many-particle objects.

We propose tailored representation of the one- and two-particle Green's function for an accurate QMC accumulation within the class of continuous-time impurity solvers [2,3] for the DMFT approximation, based on the expansion of fermionic degrees of freedom in Legendre polynomials. This leads to a substantial increase in performance, allowing for the efficient calculation of spin and charge susceptibilities for canonical models as well as realistic materials over wide ranges of temperature, doping and interaction strength.

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[2] A.N. Rubtsov and A.I. Lichtenstein, JEPT Lett. **80**, 61 (2004).
[3] P. Werner, A. Comanac, L. de' Medici, et al., PRL **97**, 76405 (2006).

TT 9.3 Mon 14:30 HSZ 201

Numerical correlation-energy functional for lattice density-functional theory: A systematic approach to the ground-state properties of strongly correlated systems — •Matthieu Saubanere and Gustavo Pastor — Institut für Theoretische Physik Heinrich-Plett-Str. 40 D-34132 Kassel

We present an accurate method to determine ground-state properties of strongly-correlated electrons described by lattice-model Hamiltonians. In lattice density-functional theory (LDFT) the basic variable is the one-particle density matrix γ. From the HK theorem, the ground state Energy $E_{gs}[\gamma_{gs}] = \min_\gamma E[\gamma]$ is obtained by minimizing the energy over all the representable γ. The energy functional can be divided into two contributions: the kinetic-energy functional, which linear dependence on γ is exactly known, and the correlation-energy functional $W[\gamma]$, which approximation constitutes the actual challenge. Within the framework of LDFT, we develop a numerical approach to $W[\gamma]$, which involves the exact diagonalization of an effective many-body Hamiltonian of a cluster surrounded by an effective field. This effective Hamiltonian depends on the density matrix γ. In this talk we discuss the formulation of the method and its application to the Hubbard and single-impurity Anderson models in one and two dimensions. The accuracy of the method is demonstrated by comparison with the Bethe-Ansatz solution (1D), density-matrix renormalization group calculations (1D), and quantum Monte Carlo simulations (2D).

TT 9.4 Mon 14:45 HSZ 201

Effective models for gapped phases of strongly correlated quantum lattice models — Hong Yu Yang and •Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

We present a robust scheme to derive effective models non-perturbatively for quantum lattice models when at least one degree of freedom is gapped. A combination of graph theory and the method of continuous unitary transformations (gCUTs) is shown to efficiently capture all zero-temperature fluctuations in a controlled spatial range. The gCUT can be used either for effective quasi-particle descriptions

or for effective low-energy descriptions in case of infinitely degenerate subspaces. We illustrate the method for 1d and 2d lattice models yielding convincing results in the thermodynamic limit. Various extensions and perspectives of the gCUT are discussed.

TT 9.5 Mon 15:00 HSZ 201

Lower energy bounds for condensed matter systems — •Robert Hübener, Thomas Barthel, and Jens Eisert — Universität Potsdam

Greens function methods, known e.g. from quantum chemistry, allow to calculate lower energy bounds for bosonic and fermionic models in the thermodynamic limit. In the context of condensed matter physics, they can be used to complement variational methods, e.g. DMRG, which generally provide upper bounds. The tightness of the lower bounds depends on the level of compliance with so called N-representability conditions. In this talk we discuss technical aspects, like the formulation of the optimization problem as a semidefinite program, as well as the underlying issue of N-representability. Applications will be demonstrated.

15 min. break

TT 9.6 Mon 15:30 HSZ 201

Spectra and kinks in the electronic dispersion of charge-transfer systems — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

We investigate kinks in the effective dispersion of correlated multi-band systems, concentrating on the perovskite geometry. Previously it was shown that the one-band Hubbard model exhibits kinks due to an entirely electronic mechanism [1], which is different from conventional mechanisms such as the coupling between electrons and phonons or other bosonic modes. Here we demonstrate the applicability of this mechanism in the case of the Emery model (two/three-band Hubbard model) for hole-doped cuprate compounds. We solve these multi-band models within dynamical mean-field theory using the numerical renormalization group (NRG), which is ideally suited to resolve spectral features at comparably low energy, including kinks. We discuss in detail the construction of the effective impurity Hamiltonian and the corresponding Wilson chains within the NRG procedure for such multi-band models.

[1] K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke and D. Vollhardt, Nature Physics 3, 168 (2007).

TT 9.7 Mon 15:45 HSZ 201

Loschmidt echo and work distribution in isolated many-body systems after a global quench — •Marcus Kollar[1], Malte Lehmann[2], and Eric Lutz[2] — [1]Theoretical Physics III, University of Augsburg, 86135 Augsburg — [2]Department of Physics, University of Augsburg, 86135 Augsburg

For a sudden quench of the Hamiltonian of an isolated quantum system there is a relation between (i) the distribution of the performed work and (ii) the Loschmidt echo, which is a measure of the overlap of the initial and the time-evolved state, but which is notoriously difficult to measure. We derive an uncertainty relation for the widths of these two functions and argue that for global quenches in many-body systems both functions are typically Gaussians, thus fulfilling their uncertainty relation as an equality. This suggests that it may be possible to measure the Loschmidt echo via the experimentally more easily accessible work distribution.

TT 9.8 Mon 16:00 HSZ 201

Non-Fermi-liquid signatures in the Hubbard model due to van Hove singularities — •Sebastian Schmitt — Theoretische Physik II, Technische Universität Dortmund

We consider the Hubbard model within the single-site dynamical mean-field theory (DMFT) on lattices which exhibit a van Hove singularity in the vicinity of the Fermi level. Analytical treatment of the lattice summation reveals a non-analytic contribution of the van Hove singularity to the local effective medium (Weiss field). This leads to a non-Fermi liquid self-energy and transport properties within a full numerical solution of the DMFT on a two-dimensional square lattice with nearest- and next-nearest-neighbor hoppings. At temperatures on the order of the low-energy scale T_0 an unusual maximum emerges in the imaginary part of the self-energy which is renormalized toward the Fermi level for finite doping. At zero temperature this double-well structure is suppressed but an anomalous energy dependence of the self-energy remains. The asymptotic low-temperature behavior of the resistivity changes from Fermi liquid to non-Fermi liquid behavior as function of doping. The results are also discussed regarding their relevance for quantum cluster approximations and high-temperature cuprate superconductors.

TT 9.9 Mon 16:15 HSZ 201

Dimensional aspects of antiferromagnetism: dynamical mean-field theory versus direct quantum Monte Carlo — •Elena V. Gorelik[1], Theresa Paiva[2], Richard Scalettar[3], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil — [3]Department of Physics, UC Davis, USA

Although the dynamical mean-field theory (DMFT) is well established for strongly correlated fermions, it is clear that nonlocal correlations will modify all DMFT results. Thus, the recently revealed [1] antiferromagnetic (AF) signatures in the double occupancy D of fermions on a cubic lattice could shift to lower T or the DMFT scenario might even break down. The situation should be worse in 2 dimensions, for which the Mermin-Wagner theorem excludes AF order at $T > 0$.

However, our DMFT predictions for $D(T)$ in the square-lattice agree with direct quantum Monte Carlo (QMC) results [2] within 10%. In 3 dimensions, we find nearly exact agreement between DMFT and QMC both at large T and for $T \lesssim T_{\mathrm{N}}^{\mathrm{DMFT}}$. The primary effect of nonlocal correlations is a smoothing of the DMFT curves at $T \gtrsim T_{\mathrm{N}}^{\mathrm{DMFT}}$.

Somewhat surprisingly, $T_{\mathrm{N}}^{\mathrm{DMFT}}$ is much more relevant for the AF signatures in $D(T)$ than the true T_{N}. Thus, magnetism is more local in many respects than previously assumed, and real-space DMFT is well-suited for addressing inhomogeneous 3-dimensional systems.

[1] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).
[2] Th. Paiva, R. Scalettar, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **104**, 066406 (2010).

TT 9.10 Mon 16:30 HSZ 201

New routes to frustration and the suppression of antiferromagnetic signatures — •Nils Blümer and Elena Gorelik — Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

An established route for studying frustration effects in Hubbard-type models is the addition of frustrating bonds to a bipartite lattice. In particular, one can tune from the square towards the triangular lattice by adding hopping along one diagonal per plaquette with amplitude $t' \in [0, t]$ (for square-lattice hopping t). While this tuning exposes frustration effects, it also changes the coordination ($4 \leq Z \leq 6$), i.e., affects the energy scales and, thereby, all observables in all phases.

We complement the above model with an additional inter-plane hopping $t_z = \sqrt{t^2 - t'^2}$; then $t' \in [0, t]$ tunes between the cubic and the triangular lattice at constant $Z_{\mathrm{eff}} = 6$. Our quantum Monte Carlo based dynamical mean-field calculations at half filling ($n = 1$) show that the recently suggested signature [1] of antiferromagnetic (AF) correlations, an enhanced double occupancy at strong coupling, is suppressed (proportional to t'^2) even before the AF order breaks down; in contrast, nonmagnetic phases are unaffected. This confirms our strong-coupling picture [1] quantitatively and should be useful for cold-atom experiments.

[1] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).

15 min. break

TT 9.11 Mon 17:00 HSZ 201

Non-Abelian SU(N) symmetries applied to matrix product states — •Andreas Weichselbaum and Jan von Delft — Ludwig Maximilians University, Munich, Germany

We generalized our numerical framework of matrix product states (MPS) from arbitrary Abelian to non-abelian quantum symmetries. It is based on the simple observation that Clebsch Gordan coefficient spaces can be split off in a tensor product like fashion for all objects relevant within MPS, and is thus applicable to the numerical or density matrix renormalization group (NRG or DMRG, respectively). As an example, I will present results on a generalized SU(3) symmetric Anderson impurity model within the numerical renormalization group based on the explicit treatment of U(1)⊗SU(2)⊗SU(3) and $\mathrm{SU}(2)^{\otimes 4}$ symmetries. This model of a fully screened S=3/2 spin Anderson model was suggested recently as the effective microscopic Kondo model

for Fe impurities in gold or silver.

TT 9.12 Mon 17:15 HSZ 201

The Crooks relation in optical spectra - universality in work distributions for weak local quenches — •Markus Heyl and Stefan Kehrein — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany

We show that work distributions and non-equilibrium work fluctuation theorems can be measured in optical spectra for a wide class of quantum systems. We consider systems where the absorption or emission of a photon corresponds to the sudden switch on or off of a local perturbation. For the particular case of a weak local perturbation, the Crooks relation establishes a universal relation in absorption as well as in emission spectra. Due to a direct relation between the spectra and work distribution functions this is equivalent to universal relations in work distributions for weak local quenches. As two concrete examples we treat the X-ray edge problem and the Kondo exciton [1].
[1] M. Heyl and S. Kehrein, arXiv:1006.3522

TT 9.13 Mon 17:30 HSZ 201

Tunnelling matrix elements with Gutzwiller wave functions — •Andrea Di Ciolo, Luca F. Tocchio, and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt Am Main, Germany.

We use a generalized Gutzwiller approach [N. Fukushima, et al., Phys. Rev. B 72, 144505 (2005)], in order to study projected particle (hole) excitations for superconducting systems and systems with antiferromagnetic (AFM) order. As in the standard Gutzwiller scheme [M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963); F. C. Zhang, et al., Supercond. Sci. Tech. 1, 36 (1988)] the effects of the strong electronic correlations are given via the suppression of the site double occupancy; for our computations it is helpful to consider a lattice with a reservoir site unaffected by this suppression of the double occupancy.

In this approach we obtain the probabilities for the tunnelling of a particle (hole) into the projected state [A. Di Ciolo, et al., arXiv:1010.5055] . Our results are due only to the physical properties of the trial state and not to the choice of a specifical Hamiltonian: in this sense, they are model-independent but not universal, because they rely on the features of the chosen Gutzwiller wave function (projected Fermi Sea, BCS superconductor, AFM...)

The accuracy and the reliability of our analytical approximation is tested using the Variational Monte Carlo. Possible comparisons with tunnelling experiments will be discussed.

TT 9.14 Mon 17:45 HSZ 201

Simulations of excitons in coupled quantum dots — •Alexander Stark[1], Philipp Schneider[1], Sergey Grishkevich[1,2], and Alejandro Saenz[1] — [1]Humboldt-Universität, Berlin, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

We present the extension of our program code for two atoms in optical lattices to excitons in coupled quantum dots, i.e. quantum dot molecules. To obtain the eigenvalues and the corresponding wave functions we are using a full configuration-interaction approach based on an one particle B-Spline basis for the radial part and spherical harmonics for the angular part of the wave function. The double well confinement potential is treated in full dimensionality. This allows us to handle variably confined lateral and vertical coupled quantum dots. The separation of the dots can be adjusted from box-like unified dots to nearly full separated individual dots. The interaction between the electron and the hole can be also varied arbitrarily, including the repulsive electron-electron Coulomb potential and possible shielding effects. Further, to study quantum dot molecules in different materials the effective masses of the particles can be set to corresponding values. The next step is to include a time-dependent perturbation and to study the dynamics of the exciton. First results of the calculations are presented.

TT 9.15 Mon 18:00 HSZ 201

Competing chiral and multipolar electric phases in the extended Falicov-Kimball model — •Bernd Zenker[1], Holger Fehske[1], and Cristian Daniel Batista[2] — [1]Ernst-Moritz-Arndt Universität Greifswald, Greifswald, Germany — [2]Los Alamos National Laboratory, Los Alamos, USA

We study the effects of interband hybridization within the framework of an extended Falicov-Kimball model with itinerant c and f electrons. An explicit interband hybridization breaks the U(1) symmetry associated with the conservation of the difference between the total number of particles in each band. As a result, the degeneracy between multipolar electric and chiral orderings is lifted. We analyze the weak- and strong-coupling limits of the c-f electron Coulomb interaction at zero temperature, and derive the corresponding mean-field quantum phase diagrams at half-filling for a model defined on a square lattice.

TT 10: Poster Session: Superconductivity

Time: Monday 14:00–18:00 Location: P4

TT 10.1 Mon 14:00 P4

Growth of YBCO thin films and their interaction with gold nano clusters — •Christian Katzer[1], Ralf Erlebach[1], Daniel Kuhwald[1], Peter Michalowski[1], Frank Schmidl[1], Ingo Uschmann[2], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, 07743 Jena, Germany

Using Pulsed Laser Deposition (PLD) our team is able to fabricate and examine Yttrium-Barium-Copper-Oxide (YBCO) thin films of high quality. A particular point of investigation is the influence of an in situ pre-deposited gold film. While growing the superconducting film one can achieve a formation of gold nano clusters in an YBCO matrix through heating of the initial gold layer. We studied the temperature dependence of the resistance in respect to the YBCO film thickness for various gold layers. Furthermore the critical current density at 77 K and their temperature dependence will be compared with the one of non-modified YBCO thin film structures.

TT 10.2 Mon 14:00 P4

Characterization of $YBa_2Cu_3O_{7-x}$ -grain boundary contacts with Au-clusters — •Daniel Kuhwald, Christian Katzer, Ralf Erlebach, Matthias Schmidt, Veit Grosse, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

In the course of the work $YBa_2Cu_3O_{7-x}$ (YBCO) layers have been deposited epitaxially onto a bicrystalline strontium titanate substrate with an intermediate gold layer. During the deposition of YBCO the gold forms clusters, changing the crystallographic properties of the superconducting layer and especially the emerging grain boundary. In this way Josephson-junctions and simple DC-Superconducting Quantum Interference Devices (SQUIDs) have been produced both with and without gold nanoclusters and their electrical properties were investigated and compared among each other. We present the dependency of the critical current and the I_CR_N-product on the temperature. Furthermore the behaviour of the junctions in external magnetic fields and under microwave irradiation is shown. In all cases we discuss and compare the behaviour of junctions with and without gold nanoclusters.

TT 10.3 Mon 14:00 P4

Integration of predefined gas-phase condensed nanoparticles into $YBa_2Cu_3O_{7-\delta}$ thin film multilayers — •Maria Sparing, Tom Thersleff, Jens Hänisch, Ingolf Mönch, Ruben Hühne, Sebastian Fähler, Bernd Rellinghaus, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box: 270116, 01171 Dresden, Germany

The critical current density J_c in $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films, which limits their application in external magnetic fields, can be enhanced by the introduction of artificial pinning centers e.g. created by non-superconducting nanoparticles and surrounding defects and strain states. A controlled preparation of nanoparticles with adjustable properties is required in order to understand the correlation between the superconducting characteristics, the particles and the defect structure. Isolated particles with a predefined diameter in the range of 10 nm

and an independently chosen areal density can be prepared via dc-magnetron sputtering in an inert gas flow. Here we present the integration of such gas phase condensed Hafnium nanoparticles into PLD-grown YBCO thin film multilayers in a combined PLD-Sputtering system. These heterostructures were investigated by TEM on cross sectional FIB lamellae. The influence of the areal density and the particle volume content on the structural and superconducting properties of YBCO thin films is discussed. Furthermore, advantages and consequences of this new technique for the preparation of nanoparticle thin film heterostructures are evaluated.

TT 10.4 Mon 14:00 P4

Phase formation and critical current density in YBCO based quasimultilayers prepared by off-axis pulsed laser deposition — •Elke Reich[1,3], Thomas Thersleff[1,3], Ruben Hühne[1], Kazumasa Iida[1], Ludwig Schultz[1,2,3], and Bernhard Holzapfel[1,3] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]TU Dresden, Department of Physics, Institute for Physics of Solids, D-01062 Dresden, Germany — [3]TU Dresden, Department of Mechanical Engineering, Institute for Material Science, D-01062 Dresden, Germany

The use of coated conductors for power applications requires the improvement of the critical current densities in high magnetic fields. Significant research effort has been undertaken to investigate and enhance the flux pinning forces of high-temperature superconducting thin films. One possibility is the introduction of nano-sized defects into the superconductor thereby creating quasimultilayers of a complete superconducting layer and an incomplete dopant layer. In this work we present the phase formation and critical current density characteristics of YBCO based quasimultilayers doped with the double perovskite phase $Y_2Ba_4CuMO_y$ (Y2411) (M=Zr and Nb). We will show evidence for a reaction from the Y2411 phase to a simple Yttrium doped perovskite $Ba(M_{1-x}Y_x)O_3$ during film deposition. These second-phase inclusions clearly enhance J_c in high magnetic fields.

TT 10.5 Mon 14:00 P4

Low-temperature MFM based on piezoresistive cantilevers — Philip Meiser, •Michael R Koblischka, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany

We present the construction of a low-temperature magnetic force microscope (MFM) operating at temperatures down to 1.5 K and in fields up to 5 T. The MFM is based on commercial piezoresistive cantilevers, coated with 30 nm-thick layers of CoCr. In this contribution, we show details of the construction of the home-built MFM head and discuss the dependence of the piezoresistive signal, the resonance frequency, the obtained resonance curves and the quality facors on temperature. Furthermore, we present measurements on magnetite thin films and superconducting ring structures based on Pb thin films.

TT 10.6 Mon 14:00 P4

$NdBa_2Cu_3O_x$ nanowires grown in anodized alumina templates by microwave heating — •Michael R Koblischka, Anjela Koblischka-Veneva, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany

Nanowires of $NdBa_2Cu_3O_x$ (NdBCO) are grown employing commercial anodized alumina templates (pore diameters of 10 nm and 100 nm, overall thickness of 50 μm) and pre-prepared NdBCO powders. The heating was performed employing a kitchen-type microwave furnace at a power of 550 W for 5 min. This treatment is sufficient to melt the NdBCO powder on top of the alumina template. In contrast to previous experiments using a laboratory furnace at a temperature of 1050 °C, the temperature here is not surpassing 450 °C. As a result, the templates remain fully flat and the structure of the nanopores is not affected by the heat treatment. An additional 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 (SQUID, AC susceptibility). The resulting nanowires are analyzed in detail employing electron microscopy (SEM, TEM).

TT 10.7 Mon 14:00 P4

Mechanically alloyed in-situ MgB_2: Aspects of powder preparation towards an industrial scale wire preparation — •Marko Herrmann[1], Wolfgang Häßler[1], Christian Rodig[1], Margitta Schubert[1], Ania Kario[1], Konstantin Nenkov[1], Juliane Scheiter[1], Ludwig Schmolinga[2], André Aubele[3], Bernd Sailer[3], Klaus Schlenga[3], Bernhard Holzapfel[1], and Ludwig Schultz[1] — [1]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]Bruker HTS GmbH, Alzenau, Germany — [3]Bruker EAS GmbH, Hanau, Germany

During the powder-in-tube preparation using sheath materials, e.g. Monel or CuNi alloys, it is necessary to recover the metallic sheath in order to reduce work hardening and allow for further deformation. In combination with a mechanically alloyed in-situ precursor this intermediate heat treatment is a sensitive processing step. Due to the high reactivity of the nanocrystalline precursor an unintended MgB_2 formation starting at around 350°C is observed. With ongoing phase formation the hardness of the precursor is increasing and therefore limiting the deformability of the wire composite.

In order to allow for a reliable wire preparation this paper concentrates on the characterization of the reactivity of mechanically alloyed precursor powders using x-ray diffraction studies with subsequent Rietveld analysis. Experimental results of transport measurements and microstructural investigations on MgB_2 bulk samples, wires and tapes prepared with precursor powders of different processing, e.g. variation of milling energy and carbon addition, will be discussed.

TT 10.8 Mon 14:00 P4

Fabrication of superconducting MgB_2 thin films and characterization by THz-transmission spectroscopy — Savio Fabretti[1], •Martin Scheuch[2], Tobias Kampfrath[2], Christian Frischkorn[2], Martin Wolf[2], Patrick Thomas[1], and Andy Thomas[1] — [1]Thin films and physics of nanostructures, Bielefeld University — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Superconducting MgB_2 thin films were fabricated by magnetron rf and dc co-sputtering on heated silicon and diamond substrates. They were annealed ex-situ for one hour at 650 °C. The superconducting phase transition was characterized contactless by means of terahertz time-domain spectroscopy in the frequency range from 0.8 to 4 THz. For this purpose, amplitude- and phase-resolved transmission measurements of the MgB_2 films for temperatures between 5 and 50 K were performed to extract the complex conductivity. The data show that both samples are homogeneous on a length scale of millimeters and superconducting below a transition temperature of about 22 K. This paves the way to investigate charge-carrier dynamics in MgB_2 with time-resolved THz spectroscopy.

S.F. and A.T. are supported by the NRW MIWF.

TT 10.9 Mon 14:00 P4

Thermodynamic Investigations and Superconductivity in $A(Fe_{1-x}Co_x)_2As_2$ (A = Ba, Ca, K) Systems — •M. Abdel-Hafiez, L. Harnagea, S. Singh, S. Aswartham, C. Nacke, G. Friemel, M. Kumar, C. Hess, S. Wurmehl, R. Klingeler, A.U.B. Wolter, and B. Büchner — Leibniz Institut für Festkörper- und Werkstoffforschung IFW Dresden, 01069 Dresden, Germany

We report on thermodynamic properties of single crystals $A(Fe_{1-x}Co_x)_2As_2$ (A = Ba, Ca, K) combining magnetization, specific heat and resistivity investigations. In comparison to a similar phase diagram for Co-doped Ba122 and Ca122, which exhibits split quasi-continuous magnetic and structural transitions upon Co-doping, the parent compound KFe_2As_2 lacks such structural/magnetic transitions completely. Furthermore, its superconducting transition temperature has been determined to be around 3.8 K, while Ca122 and Ba122 systems only become superconducting upon doping. In addition to these doping-dependent studies, thorough investigations on the magnetic phase diagram have been performed on individual compounds of all three systems. The Werthamer-Helfand-Hohenberg model was used to determine the upper critical field for different directions $H||c$ and $H||(ab)$.

TT 10.10 Mon 14:00 P4

A quasi-optical setup for sub-terahertz ESR spectroscopy: application to superconducting iron pnictides — •R. Zahn[1], A. Alfonsov[1], G. Lang[1], F. Lipps[1], V. Kataev[1], S. Aswartham[1], S. Wurmehl[1], J. S. Kim[2], J. Deisenhofer[3], H.-A. Krug von Nidda[3], A. Loidl[3], and B. Büchner[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Pohang University of Science and Technology, Pohang, Korea — [3]Center for Electronic Correlations and Magnetism, Augsburg University, D-86135 Augsburg, Germany

We present a high-sensitivity quasi-optical electron spin resonance

(ESR) setup working in a frequency range of 250 - 800 GHz. Combination of optical means of propagation with a low-loss corrugated waveguide enables full control of the polarisation of the microwaves, which is essential for the high-sensitivity ESR measurements. The detection is realised by Millimeterwave Vector Network Analyzer. The setup is operational with a magneto-cryostat with a magnetic field up to 17 T and in a temperature range of 2 - 300 K. It enables to measure weak ESR signals not only from the insulating samples transparent for microwaves but also from metallic samples where the penetration of the microwaves is restricted by the skin depth. As an example of the application of this setup we show the temperature- and frequency-dependent ESR measurements on small single crystals of $(Eu,Ba)(Fe,Co)_2As_2$ superconductor. We find that the Eu^{2+} ESR is sensitive to the structural and magnetic phase transitions occurring in this material. We discuss the interaction between the Eu- and Fe-subsystems and its relevance for the understanding of the properties of these novel superconductors.

TT 10.11 Mon 14:00 P4

Low temperature specific heat and thermal expansion measurements of $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals in high magnetic fields — •Philipp Burger[1,2], Frédéric Hardy[1], Devang Joshi[1], Peter Adelmann[1], Doris Ernst[1], Rainer Fromknecht[1], Peter Schweiss[1], Thomas Wolf[1], and Christoph Meingast[1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

Low temperature specific heat and thermal expansion measurements have been performed on underdoped (T_c=12.7 K), optimally doped (T_c=24.5 K) and overdoped (T_c=9.1 K) $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals in magnetic fields up to 14 T applied both parallel and perpendicular to the Fe layers. Whereas the specific heat anomalies in under- and over-doped crystals are significantly reduced in size by the magnetic field, the size of the thermal expansion anomalies are hardly affected by the field. The electronic Grüneisen parameters associated with the superconducting properties are calculated from the data and will be examined for signs of quantum criticality. Further, the anisotropy associated with the superconducting state, as well as the low temperature field dependence of the Sommerfeld coefficients will be discussed.

TT 10.12 Mon 14:00 P4

High resolution thermal expansion of isovalently doped $BaFe_2(As_{1-x}P_x)_2$ — •Anna Böhmer[1,2], Philipp Burger[1,2], Devang Joshi[1], Frédéric Hardy[1], Peter Schweiss[1], Christoph Meingast[1], Shigeru Kasahara[3], Takahito Terashima[3], Takasada Shibauchi[4], and Yuji Matsuda[4] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Fakultät für Physik, 76131 Karlsruhe, Germany — [3]Research Center for Low Temperature and Materials Sciences, Kyoto University, Kyoto 606-8501, Japan — [4]Department of Physics, Kyoto University, Kyoto 606-8502, Japan

In the intensively studied 122-family of iron-based superconductors, superconductivity can be induced not only by charge-doping but also by isoelectronic substitution in the FeAs-layer ("chemical pressure") and by hydrostatic pressure.

We have performed high-resolution thermal expansion measurements between 5 K - 300 K on under- and optimally doped $BaFe_2(As_{1-x}P_x)_2$ single crystals with a T_c up to 30 K. They allow us to study the uniaxial pressure derivatives of their spin-density wave (structural) and superconducting transition temperatures. Parallels to electron doped $Ba(Fe_{1-x}Co_x)_2As_2$ will be drawn. Structural parameters derived from four circle X-ray diffraction measurements contribute to our comparative study of physical pressure and P-doping in $BaFe_2As_2$.

TT 10.13 Mon 14:00 P4

Single-Crystal Growth of $Sr_{1-x}K_xFe_2As_2$ superconductors using Sn flux — •Devang Joshi, Anna Böhmer, Frederic Hardy, Peter Adelmann, Doris Ernst, Thomas Wolf, Rainer Fromknecht, Peter Schweiss, and Christoph Meingast — Institute für Festkörperphysik, Karlsruher Institute für Technologie, 76021 Karlsruhe, Germany

Single crystals of $Sr_{1-x}K_xFe_2As_2$ were grown by a high-temperature solution growth method using Sn flux. Stochiometric amounts of FeAs, Sr, K and Sn (1:20) were put in alumina crucibles, which were then sealed in iron crucibles under argon atmosphere. The iron crucibles were further sealed in evacuated quartz tubes. The total assembly was then heated to 900 °C followed by slow cooling to 450 °C in roughly 15 days. The single crystals were separated from the Sn flux using a centrifuge, and the K-contents of the single crystals were determined using EDAX. The spin-density-wave and superconducting transitions in these crystals were further characterized using magnetic SQUID, high-resolution thermal expansion and specific heat measurements.

TT 10.14 Mon 14:00 P4

Optical Investigations on the Effect of Phosphorous Substitution in $EuFe_2(As_{1-x}P_x)_2$ Single Crystals — •Sina Zapf[1], Geoffrey Chanda[1], Dan Wu[1], Hirale S. Jeevan[2], Philipp Gegenwart[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]I. Physikalisches Institut, Universität Göttingen, Germany

The ab-plane optical, magnetic and transport properties of $EuFe_2(As_{0.88}P_{0.12})_2$ single crystals have been investigated and were compared to those of $EuFe_2As_2$ (T_{SDW}=189 K) and the superconducting $EuFe_2(As_{0.82}P_{0.18})_2$ (T_c=28 K). We identify in the case of $x = 0.12$ a spin density wave (SDW) transition below 110 K.
Isovalent P substitution on the As site depresses the SDW in $EuFe_2As_2$. For $x = 0.18$, the SDW has already disappeared. The resistivity curve of our $x = 0.12$ sample shows an anomaly below 110 K with a different shape compared to the SDW feature of the parent compound. However, the Drude-Lorentz analysis on the optical conductivity spectra indicates a SDW gap formation similar to $EuFe_2As_2$. We observe a drop in reflectivity between 170 and 1200 cm^{-1} as well as the transfer of the spectral weight up to 3500 cm^{-1}. The latter effect can be understood as a many-body (interband) interaction in the multiband system. The magnetic ordering of the Eu^{2+} spins and thus the interplay between magnetism and superconductivity are examined by susceptibility measurements. We found a similar ordering as in the parent compound with a decrease of T_N down to 16.5 K.

TT 10.15 Mon 14:00 P4

^{75}As NMR study on $(Eu/Sr)(Fe/Co)_2As_2$ single crystal. — •Rajib Sarkar[1], Panchanana Khuntia[1], Michael Baenitz[1], Ramesh Nath[3], Hirale Jeevan[2], Philipp Gegenwart[2], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]I. Physik. Institut, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [3]IISER-TVM, Trivandrum-695016, India

The AFe_2As_2 (122)(A= Sr, Ba, Ca Eu) systems is the focus of research interest because of high temperature superconductivity (SC) with T_c's up to =38 K. The $EuFe_2As_2$ compound is special because of highest Fe SDW transition of T_{sdw}=190 K among the pnictides [1]. In addition at T_N=19 K antiferromagnetic order of Eu^{2+} shows up. Moreover Eu^{2+} is magnetic with S=7/2, while Ba^{2+}, Sr^{2+} and Ca^{2+} are nonmagnetic ions [2]. Interestingly, the Fe SDW is completely suppressed in $Eu_{0.5}K_{0.5}Fe_2As_2$ and SC is found below T_c=32 K. However unlike the other 122 system SC could not be achieved only by substitution of Co^{2+} at the Fe site, may be due to the Eu^{2+} AFM ordering. Nevertheless with the 80% Sr doping at the Eu^{2+} site and the optimal doping of Co at the Fe site, one can get the SC with T_c=20 K[3, 4]. Being a local probe, NMR is a very useful tool to study the microscopic properties of these Fe-pnictides. Here we report the ^{75}As field sweep NMR investigations superconducting $(Eu/Sr)(Fe/Co)_2As_2$ single crystals.
[1] Phys. Rev. B 78, 092406 (2008).
[2] Phys. Rev. B 82, 054525 (2010).
[3] J. Phys.: Condens. Matter 22 (2010) 235701.
[4] Sarkar et. al. to be published.

TT 10.16 Mon 14:00 P4

Superconductivity and local-moment magnetism in $Eu(Fe_{0.89}Co_{0.11})_2As_2$ — •Shuai Jiang[1,2], Philipp Gegenwart[1], and Guanghan Cao[2] — [1]I. Physikalisches Institut, The University of Goettingen, Goettingen, Deutschland — [2]Department of Physics, Zhejiang University, Hangzhou, China

Here we report the anisotropic measurements of resistivity and magnetization under magnetic fields on a $Eu(Fe_{0.89}Co_{0.11})_2As_2$ single crystal. We observed a resistivity drop at T_c=21 K, which suggests a superconducting transition. The low-field magnetic susceptibility data also show the evidence of superconductivity. Instead of expected zero-resistance below T_c, a resistivity reentrance appears at 17 K under zero field, coincident with the magnetic ordering of Eu^{2+} moments. According to the temperature and field dependences of anisotropic magnetization, we propose there exists a helical magnetic structure for the Eu^{2+} spins. The external magnetic fields easily changes the

helimagnetism into ferromagnetism with fully polarized Eu^{2+} spins, accompanying by disappearance of the resistivity reentrance. Therefore, superconductivity coexists with ferromagnetic state of Eu^{2+} spins under relatively low magnetic field. The magnetic and superconducting phase diagrams are finally finished for magnetic fields parallel and perpendicular to the basal plane.

TT 10.17 Mon 14:00 P4

Applicability of the vitual crystal approximation to the band structure of Fe pnictides — •Alexander Yaresko — Max Planck Institute for Solid State Research, Stuttgart, Germany

Band structure calculations were performed for supercells of $BaFe_2As_2$ with an Fe ion substituted by 3d (Mn, Co) or 4d (Ru) transition metal one. Comparison of the Fermi surfaces to those calculated for electron (hole) doped $BaFe_2As_2$ using the virtual crystal approximation shows that the variation of the size of the Fermi surfaces upon Co (Mn) substitution can be well reproduced by corresponding doping. Substitution of Fe by Ru does not affect the size of the Fermi surfaces but leads to an appreciable increase of the band width. The strength of intra- and inter-band impurity scattering is estimated.

TT 10.18 Mon 14:00 P4

Magnetic and orbital order in a spin-fermion model for pnictides — •Thomas Prestel and Maria Daghofer — Institute for Theoretical Solid State Physics, IFW Dresden, 01171 Dresden, Germany

We study a spin-fermion model for iron pnictides [1] that couples itinerant electrons in the xz and yz orbitals to a local spin degree of freedom, which is modelled as a classical spin.We use classical Monte Carlo simulation as well as Exact diagonalization technique to investigate this model. At half filling, corresponding to undoped compounds, we find Flux-phase magnetic ordering rather than the experimentally observe C-type ordering, while slight doping as well as a magnetic single-ion anisotropoy stabillize the observed magnetic phase. We study this phase competition. We also study the model supplemented by local impurities and find the impurities to have a small impact on the orbital occupation of surrounding sites.

[1] W.-G. Yin, C.-C. Lee, W. Ku, PRL **105**, 107004 (2010)

TT 10.19 Mon 14:00 P4

Theory of normal state incoherence in iron superconductors. — •Luis Craco and Stefano Leoni — Physical Chemistry - Technical University Dresden

The precise nature of unconventional superconductivity in Iron superconductors is presently a hotly debated issue. An issue for theory is (a) whether these materials are incoherent, bad metals in the normal state and (b) how close they are to Mottness?

In this poster, we will show our recent efforts to describe the correlated nature of Fe-based superconductors. We will highlight how a combination of first principles and many-body calculations allows us to interpret and/or predict experimental results. In particular, we will show our results for spectroscopic [1], electrical [2] and thermal transport [3] of tetragonal-FeSe superconductor, all found to be in good agreement with extant data. We will also present a comparative study of the electronic states of tetragonal- and hexagonal-FeSe [4], showing normal state incoherence in both structural phases and orbital-selective Mott localization in hexagonal FeSe.

[1] L. Craco, M.S. Laad, and S. Leoni, arXiv:0910.3828.
[2] L. Craco, M.S. Laad, and S. Leoni, Europhys. Lett. 91, 27001 (2010).
[3] L. Craco and M.S. Laad, arXiv:1001.3273.
[4] L. Craco and S. Leoni, submitted to Europhysics Letters.

TT 10.20 Mon 14:00 P4

Structural and magnetic properties of the FeAs-based superconductors — •Navid Qureshi[1], Johanna Brand[1], Yvo Drees[1], Jochen Werner[2], Sabine Wurmehl[2], Christian Hess[2], Rüdiger Klingeler[2], Bernd Büchner[2], María Teresa Fernández-Díaz[3], Paul Steffens[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Festkörper- und Werkstoffforschung, Dresden — [3]Institut Laue Langevin, Grenoble

The recently discovered family of oxypnictides superconductors has focused the interest of the scientific community as they represent the first non-copper-oxide based layered superconductors reaching a T_c of 55 K. We have combined high-flux and high-resolution neutron and x-ray powder diffraction experiments to study the magnetic and crystal structure of the $RE O_{1-x}F_xFeAs$ series. For RE=La we may unambiguously determine the magnetic symmetry of the undoped material. Upon cooling through the structural and magnetic transitions, the pure and slightly doped materials exhibit anomalies in bond distances and in bond angles which reflect the general magnetophonon coupling in FeAs compounds. Furthermore, we have performed an inelastic neutron scattering study with polarized neutrons and linear polarization analysis on a $BaFe_2As_2$ single crystal, which may distinguish between the different directional components of the spin fluctuations. Energy scans at the magnetic zone centers (1 0 l) with l being an odd number reveal clear evidence for an anisotropic spin wave excitation at the magnetic zone centers, where the out-of-plane spin fluctuation component surprisingly sets in at lower energy than the in-plane component.

TT 10.21 Mon 14:00 P4

A method to contact individual microcrystalline oxypnictide single crystals — •Andreas Teichgräber, Christian Hess, Sabine Wurmehl, and Bernd Büchner — IFW Dresden

Despite the rapid general progress in fabricating large high-quality single crystals of pnictide superconductors, the controlled synthesis of 1111-type iron pnictide sample remains up to now possible only in the form of polycrystalline samples or tiny single crystals. This work describes a method to prepare electronic contacts on individual micrometer sized pnictide single crystals (extracted from a polycrystalline pellet of 1111-type iron pnictide samples). The micro-crystals were embedded in epoxy resin and subsequently contacted electrically using electron beam lithography. First test measurements demonstrate the applicability of the method which thus opens a new route to systematically investigate the electronic transport of 1111-type iron pnictide superconductors on individual single crystals over a wide range of compositions and doping levels.

TT 10.22 Mon 14:00 P4

Magnetic properties of $CeFeAs_{1-x}P_xO$ iron pnictides studied by Moessbauer spectroscopy — •Ph. Materne[1], J. Spehling[1], H.-H. Klauss[1], T. Dellmann[1], H. Maeter[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], A. Jesche[3], C. Krellner[3], and C. Geibel[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Max-Planck-Institut für Chemische Physik fester Stoffe Dresden

The iron pnictide system $CeFeAs_{1-x}P_xO$ ($0 \leq x \leq 1$) exhibits a rich variety of electronic ground states ranging from coexisting long-range antiferromagnetic (AF) Fe-3d SDW order with AF Ce-4f order at low doping levels to short-range static Fe order with long-range FM Ce order for the midregime ($0.34 \leq x \leq 0.9$) to finally a non-magnetic ground state for high phosphorus concentrations, i.e. $x > 0.9$. By means of Moessbauer spectroscopy we determined the magnetic hyperfine field at the Fe site for representative phosphorus compositions. Our Moessbauer data are discussed in comparizon with results obtained from recent muon spin relaxation measurements.

TT 10.23 Mon 14:00 P4

^{75}As NMR Study of Iron Pnictides $RFeAsO_{1-x}F_x$ — •Marc Lux[1], Damian Rybicki[1], Thomas Meissner[1], Jürgen Haase[1], Grant Williams[2], and Chong Shen[2] — [1]Faculty of Physics and Earth Science, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany — [2]The MacDiarmid Institute, Industrial Research, P.O. Box 31310, Lower Hutt 5040, New Zealand

Since the recent discovery of superconductivity in iron pnictides they continuously attract an enormous amount of attention. Nuclear magnetic resonance (NMR) is a perfect tool to study their local properties through measurements of Knight shifts and relaxation rates. We present a ^{75}As NMR study of the $RFeAsO_{1-x}F_x$ family. We show temperature dependence of Knight shift, spin-spin and spin-lattice relaxation rates as a function of fluorine doping and orientation of the crystal structure with respect to the external magnetic field. The results are discussed and compared to other families of iron pnictides.

TT 10.24 Mon 14:00 P4

Ein Ferropniktid mit Phosphor: $Sr_{1-x}Na_xFe_2P_2$ — •Daniel Schmidt und Hans F. Braun — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth

In der Arbeit wird ein Syntheseverfahren für die Verbindungen $Sr_{1-x}Na_xFe_2P_2$ (x = 0.2, 0.4, 0.6, 0.8) über die Precursorphase FeP dargestellt. Dieser Precursor wird ebenfalls hergestellt und kristallo-

grafisch mittels Röntgenpulverdiffraktometrie untersucht. Alle Syntheseschritte werden unter Inertgasatmosphäre durchgeführt. Die gefundene Fremdphase Fe_2P wird über ein magnetisches Reinigungsverfahren weitestgehend aus der Precursorprobe eliminiert. In Anlehnung an die Syntheseverfahren und Überlegungen der Eisenarsenidverbindungen stellt eine mit Phosphor hergestellte Verbindung eine isoelektrische Variante dar. Durch das Natrium werden Löcher in den Kristall eingebracht. Über Röntgenpulverdiffraktometrie werden die Änderungen der Gitterkonstanten des tetragonalen Gitters mit $ThCr_2Si_2$ -Struktur in Abhängigkeit des nominellen Natrium-Anteils beobachtet. Eventuelle magnetische oder supraleitende Übergänge konnten mit Hilfe der magnetischen Wechselfeldsuszeptibilität in einem Temperaturbereich zwischen 5 K und 260 K untersucht werden. Um Fremdphaseneffekte des noch in gewissem Mengenanteil vorhandenen Fe_2P zu erkennen, wurde diese Verbindung gezielt hergestellt und der magnetische Übergang aufgezeichnet.
Es konnte gezeigt werden, dass sich die Verbindungen prinzipiell herstellen lassen. Im Rahmen dieser Arbeit konnten jedoch keine magnetischen oder supraleitenden Übergänge gefunden werden.

TT 10.25 Mon 14:00 P4

Electronic Transport Properties of LiFeAs and Co doped LiFeAs — •Anne Bachmann, Dirk Bombor, Saicharan Aswaratham, Luminita Harnagea, Sabine Wurmehl, Christian Hess, and Bernd Büchner — Leibnitz Institute for Solid State and Materials Research, IFW Dresden, Germany

Electronic transport properties of the new unconventional superconductor LiFeAs and Co doped LiFeAs have been studied. Unlike in other iron arsenide superconductors this undoped compound exhibits no spin density wave but superconducting properties. Resistivity measurements show this transition at $T = 17\,\mathrm{K}$. We have studied the magnetoresistance of LiFeAs and extracted the $H_{c2}(T)$ phase diagram. In contrast to other Fe-As based compounds we find that in $LiFe_{1-x}Co_xAs$ electron doping suppresses superconductivity.

TT 10.26 Mon 14:00 P4

Effect of spin state, ordered moment and lattice anharmonicity on phonons in FeTe — Vladimir Gnezdilov[1,2], •Peter Lemmens[2], Yurii Pashkevich[3], Alexander Gusev[3], Karina Lamonova[3], Oleksandr Afanasiev[1], Sergei Gnatchenko[1], Vladimir Tsurkan[4,5], Joachim Deisenhofer[5], and Alois Loidl[5] — [1]ILTPE NAS, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]DonFTI NAS, Ukraine — [4]IAP AS, Moldova — [5]EP V, Univ. Augsburg, Germany

Investigations of FeTe single crystals as function of temperature show a relation between the magnitude of the ordered magnetic moment and the A_{1g} phonon linewidth at low temperatures. Based on microscopic modeling using density-functional theory this effect is attributed to the Fe spin state and orbital degeneracy. Our observations show the importance of orbital degrees of freedom for the Fe-based superconductors with large ordered magnetic moments.

Work supported by DFG.

TT 10.27 Mon 14:00 P4

Magnetic properties and superconductivity in $FeSe_{1-x}$ — •Stephan Knöner, Mariano de Souza, Amir Haghighirad, Sebastian Köhler, Wolf Assmus, and Michael Lang — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), Germany

The discovery of superconductivity in Fe-pnictides has attracted enormous interest to this class of materials [1]. Among these, the binary alloy $FeSe_{1-x}$ with $T_c \approx 8.5$ K is particularly interesting due to its simple structure [2], which enables to explore the intrinsic properties of this class of superconductors. In this contribution, we report on synthesis, structural characterization, resistivity and magnetic measurements on the hitherto not explored δ'-phase of $FeSe_{1-x}$ [3]. In the case of samples with Fe excess as inclusions, we show that superconductivity survives despite the presence of a large saturated magnetic moment of up to $0.9\mu_B$/Fe. By an annealing process, the quality of the samples has been improved and the saturated magnetic moment is reduced dramatically to $0.1\mu_B$/Fe. Furthermore, the magnetization curves show clear presence of a hysteresis loop, typical for ferromagnets, also at temperatures below T_c. Our results indicate the robustness of superconductivity in $FeSe_{1-x}$ against ferromagnetic precipitations. Aspects relating to sample quality will also be discussed.
This work is part of the DFG priority program (SPP 1458).
[1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (08).
[2] F.C. Hsu *et al.*, Proc. Natl. Acad. Sci. U.S.A. **105**, 14262 (08).
[3] M. de Souza *et al.*, Eur. Phys. J. B **77**, 101 (10).

TT 10.28 Mon 14:00 P4

Systematic investigations of the ternary system Fe-Se-Te — •Michael Schulze, M. Yasin Hacisalihoglu, Christian G.F. Blum, Christian Hess, Manoj Kumar, Anja U.B. Wolter, Sabine Wurmehl, and Bernd Büchner — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Among iron based superconductors the iron chalcogenides gain special attention due to the discovery of superconductivity in the Fe-Se-system by Hsu et al. [1]. The highest critical temperature in the so called 11-systems was first observed by Sales et al. [2] in a $FeSe_{0.5}Te_{0.5}$-sample. This poster presents a systematic investigation of the the ternary system Fe-Se-Te by means of powder diffraction, magnetization and transport measurements.
[1] Hsu et al., Proc. Natl Acad. Sci. USA 105, 14262 (2008)
[2] Sales et al., Phys. Rev. B 79, 094521 (2009)

TT 10.29 Mon 14:00 P4

Electronic properties across the first-order phase transition in $Fe_{1.05}Te$ — •Sahana Rössler[1], Dona Cherian[2], Sasidharan Harikrishnan[2], Handadi L. Bhat[2], Suja Elizabeth[2], John A. Mydosh[3], Frank Steglich[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Department of Physics, Indian Institute of Science, Bangalore 560012, India — [3]Kamerlingh Onnes Laboratory, Leiden University, P. O. Box 9504, 2300 RA Leiden, The Netherlands

We present scanning tunneling microscopy and spectroscopic (STM/S) studies on $Fe_{1.05}Te$ single crystals. In this compound, the superconductivity appears upon Se doping and the physical properties are found to be extremely sensitive to non-stoichiometry and disorder [1]. In our FeTe crystals, a first-order phase transition is observed around 57 K in the resistivity, magnetization, and the specific heat measurements. This transition is associated with a structural transition from a tetragonal $P4/nmm$ to a monoclinic $P2_1/m$ space group. At this temperature, the compound becomes antiferromagnetically ordered and the temperature dependence of the resistivity changes from log $(-T)$ to T^2. This observation suggests that the material behaves as a Fermi-liquid metal at low temperatures. Metallic behavior is also confirmed by the $I-V$ characteristics of the STM measurements.
[1] S. Rößler *et al.*, Phys. Rev. B, 82 (2010) 144523.

TT 10.30 Mon 14:00 P4

Thermodynamic, magnetic and transport properties of $Rh_{17}S_{15}$ — •M. Uhlarz[1], O. Ignatchik[1], J. Wosnitza[1,2], A. Haase[1,2,3], M. Doerr[2], R. Daou[3], H. Rosner[3,4], H.R. Naren[5], A. Thamizhavel[5], and S. Ramakrishnan[5] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung, 01069 Dresden — [5]Tata Institute of Fundamental Research, Mumbai-400005, India

We determined thermodynamic (specific heat), magnetic (magnetization, magnetostriction and susceptibility) and transport (electrical resistivity) properties of the 4*d*-electron superconductor $Rh_{17}S_{15}$ ($T_c = 5.3\,\mathrm{K}$). The upper critical field is $19.2\,\mathrm{T}$ at $T = 0.07\,\mathrm{K}$. We investigated both a polycrystal and a single crystal. Specific heat gives $\gamma(B=0) = 107\,\mathrm{mJ/\,mol\,K^2}$, $m_{\mathrm{eff}} = 35\,m_0$, and a superconducting energy gap $\Delta_0 = 0.94\,\mathrm{meV}$. The magnetic properties are dominated by flux-line pinning; resistivity likely reveals an amplification of electron-phonon coupling by weak disorder. Additionally, band-structure calculations are presented and interpreted in the context of our own experiments and other recently published results. We interpret our findings in order to find the origin of the strong electronic correlations in $Rh_{17}S_{15}$ both in the superconducting and in the normal-conducting state.

Part of this work has been supported by EuroMagNET II under the EU contract no. 228043.

TT 10.31 Mon 14:00 P4

Coexistence of ferromagnetism and superconductivity in Bi_3Ni nanostructures — •Thomas Herrmannsdörfer[1], Richard Skrotzki[1], Rico Schönemann[1], Joachim Wosnitza[1], Daniel Köhler[2], Regine Boldt[3], and Michael Ruck[2] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), D-01328 Dresden, Germany — [2]Department of

Chemistry and Food Chemistry, TU Dresden, D-01062 Dresden, Germany — [3]Leibniz Institute of Polymer Research, D-01069 Dresden, Germany

Materials where superconductivity emerges in an already ferromagnetic orderd phase are explicitly rare. Here we demonstrate that Bi_3Ni nanostructures exhibit a coexistence of superconductivity and ferromagnetism by making use of novel chemical-reaction paths. Via magnetometry and electrical-transport measurements we have characterized their magnetic and superconducting properties. Other than in bulk geometry, submicron-sized particles and quasi one-dimensional nanoscaled strains of single-phase Bi_3Ni undergo ferromagnetic order and still become superconducting at lower temperatures. Furthermore superconductivity is also stable up to remarkably high magnetic fields. Uniquely, ferromagnetic hysteresis at zero resistance is observed in nanostructured Bi_3Ni. An extended study of electronically confined intermetallics may bear the chance to find much more systems which exhibit coexistence phenomena of fundamental ground states of condensed matter.

TT 10.32 Mon 14:00 P4

Enhanced T_c in a Dual-Layered Molecular Superconductor — •Mariano de Souza[1], Leonor Wiehl[2], John A. Schlueter[3], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt (M), Germany — [2]Institut für Geowissenschaften, J.W. Goethe-Universität, D-60438 Frankfurt (M), Germany — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We have revisited the structural and electronic properties of the filamentary organic superconductor $(BEDT\text{-}TTF)_2Ag(CF_3)_4(TCE)$, first synthesized in 1994 [1]. Detailed structural investigations reveal that the BEDT-TTF molecules are arranged in two distinctly different packing motifs, κ and α', which alternate from layer to layer [2]. This molecule-based superconductor with dual BEDT-TTF packing motifs has a T_c five times higher than that of its polymorph that contains only κ-type packing. Using the established empirical correlations between the bond lengths (C–S and C=S) and the oxidation state of the BEDT-TTF molecule, we have found that there is a uniform charge distribution in the κ-layers (corresponding to an oxidation state of +0.5 for all BEDT-TTF molecules), whereas in the α'-layer, half of the molecules are nearly fully oxidized to +1, while the other half are close to neutral, resulting in a charge-ordered neutral layer. These findings indicate that this material can be considered as a promising candidate for a distinctly two-dimensional superconductor.
[1] J. A. Schlueter *et al.*, Physica C **233**, 379 (1994).
[2] J. A. Schlueter *et al.*, J. Am. Chem. Soc. (2010)
doi: 10.1021/ja105854m.

TT 10.33 Mon 14:00 P4

Insights into the phase diagram of high-temperature superconductors obtained by terahertz spectroscopy — •Martin Scheuch[1,2], Luca Perfetti[3], Christian Frischkorn[1,2], Martin Wolf[2], and Tobias Kampfrath[2] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [3]Laboratoire des Solides Irradiés, Ecole polytechnique, 91128 Palaiseau cedex, France

High resolution data of the electrons scattering rate $\tau^{-1}(\omega, T)$ in the range of 10 to 35 THz and 30 to 320 K measured by THz-transmission spectroscopy on optimally doped and underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ samples show the doping dependence of the superconducting gap. In addition a second doping-dependent kink at temperatures above the critical temperature T_c is observed. This feature correlates to the pseudo-gap as its temperature fits to the phase diagram obtained with other techniques.

TT 10.34 Mon 14:00 P4

Two-component behaviour of high-temperature superconductor $HgBa_2CuO_{4+\delta}$ - a ^{199}Hg and ^{63}Cu NMR study — •Damian Rybicki[1], Jürgen Haase[1], Charles Slichter[2], Marc Lux[1], Martin Greven[3], Guichuan Yu[4], and Yuan Li[4] — [1]Faculty of Physics and Earth Science, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany — [2]Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801-3080,USA — [3]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — [4]Department of Physics, Stanford University Stanford, CA 94305, USA

One of the early, central questions of cuprate high-temperature superconductivity was whether a single-fluid description of the electronic spin susceptibility was appropriate in explaining nuclear magnetic resonance (NMR) experimental data. Recently, it has been shown that in the case of $La_{1.85}Sr_{0.1}CuO_4$ a single fluid picture is inappropriate and two components are necessary. Here, we present the results of ^{199}Hg and ^{63}Cu NMR study of two single crystals of hole doped high-temperature superconductor (HTS), $HgBa_2CuO_{4+\delta}$ an optimally doped and underdoped with T_c=97 K and T_c=74 K, respectively. Careful analysis of the temperature dependence of ^{199}Hg and ^{63}Cu shifts measured for two orientations of the crystal with respect to the external field shows that also in this system, which can be viewed as a model HTS, a single component scenario does not agree with experimental data.

TT 10.35 Mon 14:00 P4

Fluctuation of the hole density of a slightly under-doped $(Bi,Pb)_2$ $Sr_2CaCu_2O_{8+\delta}$ single crystal studied by X-ray absorption spectroscopy — •Ailakbar Ghafari, Ahmad Kamal Ariffin, Robin Weyrich, Christoph Janowitz, Helmut Dwelk, Rüdiger Mitdank, Alica Krapf, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

The effects of in-plane polarization change and temperature variation on the determination of the hole density for under-doped (Bi,Pb)-2212 single crystals by XAS have been studied. The XAS signal at the CuL_3 edge (925 eV-940 eV) and O-K edge (525 eV-539 eV) was recorded under continuous rotation of the CuO_2 plane by 180 degree with a minimum increment of 1.8 degree yielding experimentally an in-plane polarization dependence for the absorption signals at the respective thresholds and from that the in-plane angular dependence of the hole density ($n_H(\phi)$). Fermi's golden rule was then used for the evaluation of the in-plane polarization dependence showing unexpected polarization independence. Second, the polarisation geometry was kept fixed and spectra were taken from room temperature to 10 K with a decrement about 10 K. While the polarization dependence $n_H(\phi)$ differed for the respective thresholds the temperature dependence showed less variation. Our results point out to the role of out of plane orbitals which is supported by Anderson and Weber [1, 2].
[1] P. W. Anderson, Science, 235, 1196 (1987)
[2] C. Weber, et al. Phys. Rev. B 82, 125107 (2010)

TT 10.36 Mon 14:00 P4

Temperature dependence of itinerant holes of Bi(Pb)-2212 single crystals in the nearly optimally and under -doped regime by XAS — •Ailakbar Ghafari, Ahmad Kamal Ariffin, Christoph Janowitz, Helmut Dwelk, Rüdiger Mitdank, Alica Krapf, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

We have measured x-ray absorption spectra at the CuL_3 edge for nearly optimum and slightly under-doped single crystals of Bi(Pb)-2212 in a temperature range of 10 K to 300 K. Both fluorescence and total electron yield modes were used. Analysis of the XAS data obtained on the CuL_3 edge yields the change of hole density in the CuO_2 planes with temperature showing a pronounced minimum between 100 K and 200 K. The results are compared to studies on other HTc samples and existing ideas on its origin. Additional the Hall coefficient was determined experimentally by transport measurements at temperatures between 10 K and 300 K. Tentatively an empirical formula to calculate the temperature dependence of the hole density in form of a linear relation with three terms and a second empirical formula of the temperature dependence of the Hall coefficient is not strictly a derivation.

TT 10.37 Mon 14:00 P4

63 Cu and 17 O NMR of electron-doped cuprates — •Michael Jurkutat[1], Grant V. M. Williams[2], Damian Rybicki[1], and Jürgen Haase[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, 04103 Leipzig, Germany — [2]The MacDiarmid Institute, Industrial Research, P.O. Box 31310, Lower Hutt 5040, New Zealand

The electron-doped cuprates have scarcely been investigated particularly with nuclear magnetic resonance (NMR), but promise further insight into the still unresolved mechanism of high-temperature superconductivity. We present results of 63 Cu and 17 O NMR of electron-doped $Pr_{2-x}Ce_xCuO_4$ probing the electronic structure locally. Using double resonance methods we were able to separate signals from different sites, which allows a comparison to the electronic structure of hole-doped materials. Interestingly, despite some clear differences our findings suggest the presence of a two-component electronic fluid as is

increasingly accepted to be the case in the hole-doped cuprates and associated with their curious normal-state properties.

TT 10.38 Mon 14:00 P4

Optical conductivity of Pr_2CuO_4 in the terahertz range — •T. Fischer[1], A. V. Pronin[1], J. Wosnitza[1], A. Ikeda[2], and M. Naito[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]Tokyo University of Agriculture and Technology, Tokyo, Japan

Recently, it has been shown that nominally undoped Pr_2CuO_4 can become superconducting, being grown in form of thin films with T' structure [1]. We have measured the temperature and frequency-dependent complex transmission coefficient of these films at terahertz frequencies. From the measured spectra, we have directly calculated the complex optical conductivity. Both components of the conductivity demonstrate a behavior typical for the HTS cuprates. The stiffness of the superconducting condensate is, however, quite low, leading to a large value of the London penetration depth (1.8 μm). We discuss our results in comparison with literature data on terahertz properties of other HTS.

[1] O. Matsumoto, A. Utsuki, A. Tsukada, H. Yamamoto, T. Manabe, and M. Naito, Phys. Rev. B 79, 100508 (2009).

TT 10.39 Mon 14:00 P4

Surface and bulk electronic structure of Sr_2RuO_4 — •Volodymyr Zabolotnyy[1], Emanuela Carleschi[2], Timur Kim[1], Alexander Kordyuk[1], Jan Thöne[1], Johen Geck[1], Daniil Evtushinsky[1], Bryan Doyle[2], Rosalba Fittipaldi[3], Mario Cuoco[3], Antonio Vecchione[3], Bernd Büchner[1], and Sergey Borisenko[1] — [1]IFW - Dresden, Germany — [2]University of Johannesburg, South Africa — [3]CNR-INFM SuperMat Regional Laboratory, University of Salerno, Italy

Strontium ruthenates are famous for p-type superconductivity, metamagnetism, and notable spin-orbit coupling. Understanding all these phenomena requires a detailed knowledge of the electronic structure. Unfortunately recent ARPES on Sr_2RuO_4 was confronted with a problem of an acute 'surface state' (SS). Here we argue that, instead of the earlier proposed remedy of high temperature cleaving, one may rely on excitation energy dependence of matrix elements enhancing surface or bulk features, while circularly polarized light can be used to establish their origin. Owing to the minimized surface degradation we observe bulk α, β, γ bands and their surface counterparts along with additional δ feature. According to the dichroic pattern the new feature must be yet another surface counterpart of the β band. Also the narrower momentum width together with negligible k_z dispersion are distinct properties specific to a surface state. Since there are numerous examples where the surface state undergoes splitting due to spin-orbit interaction we suggest that full relativistic calculation might be needed to understand the origin of the new feature.

TT 10.40 Mon 14:00 P4

Nonlinear transport near the superconductor/insulator transition in thin TiN films — •D Kalok[1], A. Bilušić[1,2], T.I. Baturina[3,4], I. Schneider[1], V.M. Vinokur[4], and C. Strunk[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Department of Physics, Faculty of Science, University of Split, Croatia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia — [4]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, USA

We investigate experimentally the electric transport at the insulating side of the superconductor to insulator transition in thin TiN-films. At temperatures $T > 50\,\mathrm{mK}$ we observe an Arrhenius-type conductance, with an activation energy depending logarithmically on the sample size. At high bias the current voltage (I-V) characteristics display a large current jump into an electron heating dominated regime. For the largest samples, and below 50 mK we observe a low-bias power law $I \propto V^{\alpha}$ characteristics with an exponent $\alpha > 1$ rapidly growing with decreasing temperature, which is expected for a binding-unbinding crossover of the charge-Berezinskii-Kosterlitz-Thouless type.

TT 10.41 Mon 14:00 P4

Discontinuity of capacitance at the onset of surface superconductivity controlled by electric fields — •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 Institute of Physics (IIP), Universidade Federal do Rio grande do Norte - UFRN, 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

The effect of the electrostatic field is discussed on superconductivity near the surface exposed to magnetic fields. The Ginzburg-Landau equation is solved near the surface and the surface energy is calculated. The nucleation critical field is shown to be changed in dependence on the magnetic and electric field. The surface energy becomes strongly dependent on the width of the sample. 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.

[Phys. Rev. B 78 (2008) 054525; New J. Phys. 11 (2009) 023032-1-8; Lecture notes in Physics 733, Springer Verlag Berlin (2007); Springer Series NanoScience and Technology, Springer (2010)]

TT 10.42 Mon 14:00 P4

Static and dynamic properties of Abrikosov vortices in Nb thin films with superconducting pillar landscapes — •Benedikt Betz, Daniel Bothner, Matthias Kemmler, Markus Turad, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

The static and dynamic properties of Abrikosov vortices in artificially patterned potential landscapes were subject to many experimental and theoretical investigations since the 1960s. Up to now the potential landscapes were in most cases generated by a well-defined distribution of local potential minima, so called pinning sites, for Abrikosov vortices. In this work, we experimentally investigate the properties of vortices in potential landscapes, which are generated by a lattice of superconducting Nb pillars on the top of Nb thin films, used as highly controllable local anti-pinning centers, see [1]. The structures were fabricated by a combination of lithography and reactive ion etching. We produced several sets with variations in the pillar lattice constant, in the height of the pillars with respect to the film thickness and in the radius of the pillars from one half to a fifth of the lattice constant. By measuring I-V-characteristics for different values of temperature T and applied magnetic field B, we investigate the vortex-pillar interaction with respect to static commensurability effects. The superposition of dc and ac driving currents allows for the investigation of possible phase locking of the vortex motion to the ac drive.

[1] G.R. Berdiyorov *etal.*, Phys. Rev. B **77**, 024526 (2008)

TT 10.43 Mon 14:00 P4

Vortex imaging in YBCO grain boundary junction SQUIDs using low-temperature scanning electron microscopy — •Matthias Bailer, Christian Gürlich, Matthias Kemmler, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

We used low-temperature scanning electron microscopy (LTSEM)[1] for imaging of Abrikosov vortices in $YBa_2Cu_3O_7$ (YBCO) washer dc SQUIDs at 77 K, with a spatial resolution of about 1 μm. This imaging technique is based on the electron-beam-induced apparent displacement of vortices, which is detected as a flux change in the SQUID [2]. Vortex images obtained by LTSEM allow e.g. to estimate the distribution of pinning energies in YBCO films, or to image the sheet-current distribution in SQUID washers [3].

We report on recent progress in imaging of single vortices. Using new SQUID designs with bicrystal grain boundary junctions optimized for imaging and detection of the flux noise of a single vortex trapped in the SQUID washer, the investigation of single vortex properties by LTSEM will be presented.

[1] R. Gross and D. Koelle, Rep. Prog. Phys. 57, 651-741 (1994).
[2] D. Doenitz et al., Appl. Phys. Lett. 85, 5938-5940 (2004).
[3] D. Doenitz et al., Phys. Rev. B 73, 064508 (2006).

TT 10.44 Mon 14:00 P4

Vortex motion in granular MgB_2 thin films - Investigations with magneto-optical imaging — •Claudia Stahl[1], Sebastian Treiber[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Hochschule Aalen, Germany

In magnesium diboride (MgB_2) thin films there are different kinds of vortex motion. Flux flow and thermally activated flux creep form the current carrying state in an external magnetic field. At lower temperatures dynamically driven flux avalanches containing areas of vanishing supercurrents occur. Flux penetration as well as the critical current density can be determined locally and quantitatively via magneto-optical imaging based on the Faraday effect.

We use this method to measure properties of MgB_2 films with different granularity. In a particular production process we achieved to create areas of varying granularity on an individual substrate. This allows a direct analysis of the consequences of granularity.

It is shown that in granular films the dendritic state as well as the regular critical state both are modified: we find a reduced critical current density j_c, which decreases rapidly with increasing temperature. Additionally magnetic avalanches are favoured in the granular area, whereas generally they are triggered by high current densities. This requires a more detailed understanding of formation and propagation of magnetic avalanches in inhomogeneous media [1].

[1] S. Treiber and J. Albrecht, *New Journal of Physics* **12**, 093043 (2010).

TT 10.45 Mon 14:00 P4

Tunable double well potential for fractional Josephson two-vortex molecule — •Dennis M. Heim[1], Karl Vogel[1], Wolfgang P. Schleich[1], Edward Goldobin[2], Dieter Koelle[2], and Reinhold Kleiner[2] — [1]Institut für Quantenphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, D-72076 Tübingen, Germany

We study a fractional Josephson two-vortex molecule in a long Josephson 0-κ-2κ junction. The ground state is degenerate, corresponding to two configurations with topological charges $(\kappa, \kappa-2\pi)$ and $(\kappa-2\pi, \kappa)$ of fractional vortices. We propose to use such a system to study macroscopic quantum phenomena involving fractional vortices. Similar to the previous proposal based on a 0-π-0 junction [1], the two-vortex-molecule states can be mapped to a double well potential. However, by changing the value of κ during experiment we are able to tune the energy barrier separating the two classical ground states. We calculate characteristic properties (e.g. barrier height, eigenfrequency) and demonstrate that a controlled transition into the quantum regime is possible in such a system.

[1] E. Goldobin et al., Phys. Rev. B **72**, 054527 (2005).

TT 10.46 Mon 14:00 P4

Anomalous features in $I_c(H)$-patterns of multifacet Josephson junctions — •Sebastian Scharinger[1], Christian Gürlich[1], Roman G. Mints[2], Martin Weides[3], Hermann Kohlstedt[4], Edward Goldobin[1], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut-Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]The Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Israel — [3]National Institute of Standards and Technology, Boulder, Colorado, USA — [4]Nanoelektronik, Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany

Multifacet Josephson junctions (MJJs) with alternating 0 and π facets have been intensively investigated within the last years. The experimental dependence of their critical current on applied magnetic field $I_c(H)$ so far notoriously deviated from theoretical prediction. We have realized MJJs using superconductor-insulator-ferromagnet-superconductor heterostructures where 0 and π regions alternate 40 times. Here we show that anomalous features of $I_c(H)$ are caused by a non-uniform flux density parallel to the barrier resulting from screening currents in the electrodes in the presence of a (parasitic) off-plane field component. Further, we demonstrate that there is a specific "dead angle", which may be very close to in-plane field orientation. If the field applied by chance at the dead angle or close to it, the average flux density vanishes, resulting in very anomalous $I_c(H)$. This may lead to erroneous conclusions about the sample quality or even the physics investigated. This effect can also be observed in conventional junctions.

TT 10.47 Mon 14:00 P4

Triplet-superconductor-ferromagnet-triplet-superconductor junctions: Effects of finite width — •Bogusz Bujnowski, P.M.R. Brydon, and Carsten Timm — Institut für Theoretische Physik, Technische Universität Dresden, Germany

We study charge and spin transport in a junction involving triplet superconductors and ferromagnets. We analyze this system by using the Bogoliubov-de Gennes wavefunctions to construct the Green's function, from which we can obtain formulas for the Josephson currents in terms of the Andreev reflection coefficients. We investigate the occurrence of the 0-pi transition for a magnetic tunneling barrier of finite width, and examine the appropriateness of the usual delta-function approximation for the tunneling region.

TT 10.48 Mon 14:00 P4

Spin transport in diffusive ferromagnetic Josephson junctions with noncollinear magnetization — •Zahra Shomali[1], Malek Zareyan[1], and Wolfgang Belzig[2] — [1]Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45195, Iran — [2]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We numerically study the Josephson coupling of two s-wave superconductors which are connected through a diffusive contact made of two ferromagnetic domains with the magnetization vectors misoriented by an angle θ. The assumed superconducting leads are conventional s-wave type with the phase difference of φ. Using the quantum circuit theory, we find that in addition to the charge supercurrent, which shows a $0-\pi$ transition relative to the angle θ, the spin supercurrent with a spin polarization normal to the magnetization vectors will flow through the contact. Our results present a 0-π quantum phase transition as a function of the wave vector, $Q\xi$. Finally, we investigate the spin supercurrent in an extended magnetic texture with multiple domainwalls. We find the behavior of spin supercurrent is highly sensitive to the barrier. When asymmetric barriers don't change the value of the spin supercurrent, the symmetric ones decrease the value of it notably. We also investigate some other interesting effects for these systems. In addition, we present when $Q\xi$ is the even multiple of π, the spin-current which is penetrated into the nonhomogeneous ferromagnets is nearly zero, how ever the odd ones show the large amount of penetrated spin supercurrent.

TT 10.49 Mon 14:00 P4

Charge transport through 1D arrays of small capacitance Josephson junctions with uniform voltage bias — •Jochen Zimmer[1], Roland Schäfer[2], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruhe Institut of Technology — [2]Institut für Festkörperphysik, Karlsruhe Institut 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, described by 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 could be of metrological interest because they might offer access to very accurate frequency-to-current conversion (I = 2e f). In conventional setups, the bias voltage is only applied to the edges of the array, decaying exponentially from junction to junction. In order to achieve uniform force on charge carriers in the array, the voltage drop from junction to junction must be uniform. We present fabricated arrays with a uniform biasing scheme and first measurements thereof. We also show measurement results of similar arrays under rf radiation obtained at millikelvin temperatures.

TT 10.50 Mon 14:00 P4

Dynamical Coulomb blockade of nonlocal conductance in N/S hybrid structures — •Michael J. Wolf[1], Florian Hübler[1,2], Detlef Beckmann[1], and Hilbert v. Löhneysen[2,3] — [1]Institut für Nanotechnologie, KIT, 76021 Karlsruhe, Germany — [2]Institut für Festkörperphysik, KIT, 76021 Karlsruhe, Germany — [3]Physikalisches Institut, KIT, 76021 Karlsruhe, Germany

In multi-terminal N/S hybrid structures, crossed Andreev reflection and elastic cotunneling give rise to non-zero nonlocal conductance as it was investigated both experimentally and theoretically ([1], [2] and references therein).

We fabricated multi-terminal N/S hybrid structures by standard e-beam lithography and shadow evaporation techniques in order to gain further understanding of the nonlocal signal. The distance between the two contacts was chosen to be approximately 150 nm and care was taken to eliminate Josephson effects. Measurements were taken in a 4-probe setup using lock-in technique.

If non-zero bias voltages V_A and V_B are applied to both contacts, we observe a S-shaped nonlocal differential conductance dI_B/dV_A when sweeping V_A. These findings are consistent with recently published

calculations on the influence of Coulomb effects on the nonlocal conductance in N/S hybrid structures [2].
[1] J. Brauer et al., Phys. Rev. B **81**, 024515 (2010)
[2] D.S. Golubev and A.D. Zaikin, Phys. Rev. B **82**, 134508 (2010)

TT 10.51 Mon 14:00 P4

Quantum phase slip dynamics in Josephson junction chains — •Thomas Weissl[1], Iulian Matei[1], Ioan Mihai Pop[1], Florent Lecocq[1], Christoph Schenke[2], Gianluca Restelli[2], Frank W. Hekking[2], Olivier Buisson[1], and Wiebke Guichard[1] — [1]Institut Néel, CNRS/Université Joseph Fourier, Grenoble, France — [2]LPMMC, CNRS/Université Joseph Fourier, Grenoble, France

In contrast to Josephson Junctions (JJ) which show a tunneling of superconducting charge carriers, phase-slip junctions are characterized by a tunneling of the superconducting phase. It has been shown theoretically[1] that phase-slip junctions can be realized by including a JJ in a high impedance environment or by using a long chain of JJ's. Phase-slip junctions could have an important metrological application, as under microwave irradiation they are expected to show plateaus of constant current at multiples of the applied microwave frequency. This frequency to current conversion could be used to implement a current standard. We present measurements of the current voltage characteristics of JJ chains of different lengths. For shorter chains we observe a zero current state that we attribute to quantum phase-slip dynamics[2] in the chain. A superconducting like behavior is observed for longer chain that we understand by taking into account the excitation of standing electromagnetic waves in the chain.
[1] W.Guichard and F.W. Hekking Phys. Rev. B 81, 064508 (2010)
[2] I. Pop et al Nature Physics 6, 589-592 (2010)

TT 10.52 Mon 14:00 P4

Application of NbSi nanowires for quantum phase slip experiment — •Terhi T. Hongisto and Alexander B. Zorin — Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

A superconducting nanowire of sufficiently small (nanometer scale) cross section is expected to lose phase coherence due to the quantum phase slips (QPS) at low temperatures. The QPS nanowire combined with high impedance environment forms a system dual to the Josephson junction and is suggested to be applicable for a quantum current standard [1]. In analogy to the current-biased Josephson junction this QPS nanowire, biased by voltage below the critical value V_C, can be characterized by a washboard potential for the charge variable. Application of ac drive should result in the steps of current, $I = 2ef$, which are dual to Shapiro steps.

Using approach similar to ones described in [2, 3] we have developed technology of fabrication of NbSi nanowires with cross sections down to 15 nm by 8 nm integrated with high-ohmic Cr film resistors. The circuits have been characterized at mK temperatures and some of them exhibited characteristic Coulomb blockade behaviour.
[1] J. E. Mooij, Yu. V. Nazarov, Nature Phys. 2, 169 (2006).
[2] J. Romijn, PhD Thesis, Delft University, (1991).
[3] T. van der Sar, Master Thesis, Delft University, (2007).

TT 10.53 Mon 14:00 P4

Raman light scattering on $YBa_2Cu_3O_7/La_{2/3}Ca_{1/3}MnO_3$ Superlattices — •Nadir Omar Driza, Mohammed Bakr, Santiago Blanco Canosa, Soltan Soltan, Hanns-Ulrich Habermeier, Giniyat Khaliullin, Mathieu Le Tacon, and Bernhard Keimer — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Artificial superlattice (SL) structures offer a possibility of combining antagonistic order parameters such as superconductivity (SC) and ferromagnetism (FM). It was recently observed [1] that the interface between $YBa_2Cu_3O_7$ (YBCO) and $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) exhibits an unusual orbital reconstruction different than that of either YBCO or LCMO. Therefore, it is of fundamental interest to explore proximity and inverse-proximity effects that take place at the vicinity of the interface between the two systems using Raman scattering (RS). We have performed RS experiments on YBCO/LCMO SLs with different thicknesses of YBCO, i.e., 5-50 nm and constant thickness of LCMO (10 nm). We focus our study on the 230 cm^{-1} phonon, which arises from in-phase rotations of the MnO_6 octahedra and the 340 cm^{-1} mode originating from out-of-phase vibrations of the oxygen atoms in the CuO_2 planes of YBCO. Our T-dependence measurements revealed a strong anomaly in the phonon frequency and linewidth of these modes at the SC- and Curie transition temperatures. The anomaly we observe appears to be tied to a competition between electronic instabilities at the YBCO/LCMO interfaces and the bulk electronic properties of both layers.
[1] J. Chakhalian *et al.*, Nature Phy. **2**, 244 (2006).

TT 10.54 Mon 14:00 P4

FFLO like State in Bilayers and Trilayers of Superconductors and Ferromagnets: The Spin-Valve Core Structure — •Vladimir Zdravkov[1,2], Jan Kehrle[1], Günter Obermeier[1], Aladin Ulrich[1], Claus Müller[1], Roman Morari[2], Anatolie Sidorenko[2], Lenar Tagirov[3], Reinhard Tidecks[1], and Siegfried Horn[1] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]Institute of Electronic Engineering and Nanotechnologies ASM, MD 2028 Kishiniev, Moldova — [3]Solid State Physics Department, Kazan State University, 420008 Kazan, Russia

Critical temperature oscillations and reentrant superconductivity has been observed in thin film bilayers and trilayers made of Nb as superconducting (S) and $Cu_{41}Ni_{59}$ as ferromagnetic (F) metal, for increasing F-layer thickness. This effect is caused by the establishing of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) like state in these geometries, leading to interference effects of the superconducting pairing wave function. While in our former investigations S/F bilayers were investigated [1], we here report on F/S bilayers where the S-metal now is grown on top of the F-metal, and the combination of both building blocks to a F/S/F trilayer, i.e. the core structure of the superconducting spin valve [2].
[1] V. I. Zdravkov, J. Kehrle, G. Obermeier, et al. Phys. Rev. B 82, 054517 (2010)
[2] L. R. Tagirov, Phys. Rev. Lett. 83, 2058 (1999)

TT 10.55 Mon 14:00 P4

Spin-dependent boundary conditions for diffusive quasiclassical Green's functions at weakly polarised tunnel interfaces — •Peter Machon[1], Matthias Eschrig[1,2], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Royal Holloway, University of London, Egham Hill, EGHAM, TW20 0EX, UK

The quasiclassical Green's function method is a standard tool to describe the transport properties of diffusive superconducting heterostructures. Since this approach is not suited for heterostructures containing ferromagnets it has to be supplemented by spin-dependent boundary conditions [1]. Here we present a correction to the boundary conditions [1] for the case of weakly polarized tunnel interfaces. The resulting matrix current is described by a few parameters containing the spin-dependent interfacial phase shifts. We apply the new boundary conditions to a three terminal proximity system using a finite-element approach to study the influence of these parameters on the conductivities. Our setup consists of two ferromagnetic and a superconducting terminal coupled via tunneling barriers. We analyze the local and nonlocal spin-dependent currents and determine various ways to tune the resulting conductivities using the spin-dependent interface parameters.
[1] A. Cottet et al., Phys. Rev. B 80, 184511 (2009)

TT 10.56 Mon 14:00 P4

Hybrid Rings for circuit Quantum Electrodynamics — •E. Hoffmann[1], F. Deppe[1], T. Niemczyk[1], T. Wirth[2], E. P. Menzel[1], G. Wild[1], H. Huebl[1], F. Bilger[1], M. Mariantoni[1], A. Lukashenko[2], A. P. Zhuravel[3], A. Ustinov[2], A. Marx[1], and R. Gross[1] — [1]Walther-Meissner-Institut and TU München, Garching, Germany — [2]Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany — [3]B. I. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine

During the last years, superconducting circuit quantum electrodynamics (circuit QED) has attracted increasing interest. Experiments in this field require detection schemes for microwave signals on the single photon level. In particular, devices acting as microwave beam splitters are necessary. Using niobium thin films on silicon and sapphire substrates, we fabricated superconducting 180° microstrip hybrid ring couplers, acting as beam splitters with center frequencies of about 6 GHz. For the magnitude of the coupling and isolation we find -3.5 ± 0.5 dB and at least -15 dB, respectively, in a bandwidth of 2 GHz. We also investigate the effect of reflections at the contact between the superconducting hybrid ring and the normal conducting wiring using low temperature laser scanning microscopy. Our measurements indicates that our hybrid rings are well suited for on-chip applications in circuit quantum electrodynamics experiments.

We acknowledge financial support by the DFG via SFB 631, as well

as support by and CFN, EU project SOLID and the German Excellence Initiative via NIM.

TT 10.57 Mon 14:00 P4

Spatially-Resolved Single-Photon Detection in NbN Nanowires — •Philipp Jung[1], Alexander Lukashenko[1], Alexander P. Zhuravel[4], Stefan Wuensch[2,3], Matthias Hofherr[2], Konstantin Ilin[2], Michael Siegel[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Supported by the DFG-Center for Functional Nanostructures — [4]B. Verkin Institute for Low Temperature Physics & Engineering, Kharkov, Ukraine

We are investigating the mechanism of the single photon photoresponse in superconducting nanowires patterned from NbN thin-films on sapphire substrate. Current-biased close to their critical current, these nanowires are sensitive to small disturbances such as the absorption of a photon and are therefore used as single-photon detectors.

Although previous experiments on straight wires have shown their local critical currents to be quite inhomogeneous due to the existence of grain boundaries, meander shaped nanowire detectors exhibit a comparatively homogeneous spatial pattern of photon detection efficiency. To gain a deeper understanding of the relation between the local photon detection efficiency and the local critical current we are going to present comparative measurements of these two quantities acquired using a low temperature laser scanning microscope as well as a comparison of our results with existing theoretical predictions.

TT 11: Poster Session: Matter at Low Temperature

Time: Monday 14:00–18:00 Location: P4

TT 11.1 Mon 14:00 P4

Development of a large-area detector for position and energy resolving detection of molecular fragments — •Alexandra Kampkötter, Andreas Fleischmann, Loredana Gastaldo, Sebastian Heuser, Sebastian Kempf, Christian Pies, Jan-Patrick Porst, Philipp Ranitzsch, Sönke Schäfer, Sarah Vick, Thomas Wolf, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

The recombination of a molecular cation with a low-energy electron, followed by fragmentation, is a fundamental reaction process in cold and dilute plasmas. For polyatomic ions, it can yield molecular fragments in excited states. The construction of a cryogenic ($\sim 2\,\mathrm{K}$) storage ring to store molecular ions in their groundstate is in progress to be built at the Max-Planck Institute for Nuclear Physics in Heidelberg. For measurements in the ring the usage of a metallic magnetic calorimeter (MMC) is planned. A MMC consists of a particle absorber and a paramagnetic temperature sensor, placed in a weak magnetic field. According to the calorimetric detection principle, the deposition of energy in the absorber causes a rise in temperature of the detector. The resulting magnetization change of the sensor can be read out as a change in magnetic flux by a low-noise dc-SQUID-magnetometer. Additionally to an energy-resolution the detector for the application in the CSR shall give information about the position of a detected particle. Due to the diffusive expansion of heat in a large-area absorber, the impact location can be associated to the rise-time of the detector-signal for particles with energy of a few keV upwards.

TT 11.2 Mon 14:00 P4

Noise Contributions in Metallic Magnetic Calorimeters — •S. Heuser, S. Kempf, A. Fleischmann, L. Gastaldo, A. Kampkötter, C. Pies, J.-P. Porst, P. Ranitzsch, S. Schäfer, S. Vick, T. Wolf, and C. Enss — Uni Heidelberg, Heidelberg

Metallic magnetic calorimeters (MMCs) are particle detectors operated at a temperature below 100 mK. The energy deposited by an absorbed particle produces an increase of the detector temperature which induces a change of magnetization of the paramagnetic Au:Er temperature sensor sitting in a small magnetic field. Low-noise high-bandwidth dc-SQUIDs are used to detect the change of flux in a pick-up coil. In the last years MMCs showed a rapid progress both in the achieved energy resolution and in the reproducibility of the performance. Presently the energy resolution for x-rays is 2.8 eV (FWHM) at 6 keV. Detector modeling predicts sub-eV sensitivity for the next generation of devices. To achieve this goal, each noise source needs to be under control. The thermal fluctuation noise (TFN), dependent on the thermodynamical properties of the detector, is only finite intrinsic resolution limit. The read-out noise mainly depends on the properties of the SQUID and its coupling to the sensor. Magnetic Johnson noise is due to fluctuating current in normal metal in the vicinity of the pick-up coil. Finally we have observed a 1/f noise contribution caused by the sensor material, which can presently only be described empirically. In order to achieve optimal performance of MMCs, the last three noise contribution should be negligible in respect to the TFN. We discuss all these noise sources in detail and how they affect the detector performance.

TT 11.3 Mon 14:00 P4

Millikelvin-System for the investigation of solid state/cold atom hybrid devices — •Martin Knufinke, Petra Vergien, Helge Hattermann, Florian Jessen, Florian Karlewski, Daniel Bothner, Daniel Cano, Kai Buckenmaier, Tobias Gaber, Matthias Kemmler, Dieter Koelle, József Fortágh, and Reinhold Kleiner — Center for Collective Quantum Phenomena and their Applications, Eberhard Karls Universität Tübingen

The investigation of hybrid systems consisting of solid state devices coupled to ultracold atoms has a strong perspective towards fundamental physics. For example, in the context of cavity QED, strong coupling of cold atoms via a superconducting resonator or coupling between atoms and superconducting qubits should be feasible.

An appropriate setup has to meet the combined requirements of both the operation of superconducting devices and the ultracold atomic clouds. This demands for stable temperatures in the millikelvin regime even with thermal load from the magneto-optical trap used for the preparation of the atomic cloud, the radiation from the optical ports and the lasers. At the same time, excellent vacuum conditions and high quality optical access to the sample have to be provided. We report on the design, installation and testing of our dry dilution refrigerator. We show first measurements for the characterization of the system.

TT 11.4 Mon 14:00 P4

Mechanical dissipation in bulk silicon for precision measurements — •Gerd Hofmann[1], Christian Schwarz[1], Julius Komma[1], Daniel Heinert[1], Ronny Nawrodt[1], Giles Hammond[2], Alexander Grib[3], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institute for Solid State Physics, Helmholtzweg 5, D-07743 Jena, Germany — [2]University of Glasgow, Institute for Gravitational Research, Kelvinbuilding, University Avenue, G12 8QQ Glasgow, Scotland — [3]Kharkov National University, Physics Department, 61077 Kharkov, Ukraine

Low mechanical loss materials are of great interest in high precision lengths measurements like interferometric gravitational wave detectors or cavities for laser stabilisation. The Brownian thermal noise of a test mass is directly linked to its mechanical loss by means of the fluctuation dissipation theorem.

We present systematic loss measurements of silicon bulk materials in a temperature range from 5 to 300 K and a frequency range from 10 to 100 kHz. The mechanical loss is obtained at the resonance frequencies by a Q-factor measurement. Dissipation processes that cause the mechanical loss like thermo-elastic damping or impurity based damping in the silicon samples are discussed in detail. Especially, the influence of oxygen impurities introduced during crystal growth on the mechanical loss is discussed. A strong dissipation peak at around 113 K is linked directly to transitions within a siloxane complexe (Si-O-Si). Mechanical losses as low as 2×10^{-9} have been obtained around 5.6 K.

This work is supported by the DFG under contract SFB TR7.

TT 11.5 Mon 14:00 P4

Development of a CuBe cell for magnetostriction and thermal expansion measurements in the PPMS — •Thomas Bauer, Robert Küchler, Manuel Brando, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

Thermal expansion and magnetostriction of solids give important information about the temperature and magnetic-field dependence of sample properties. Here, we report on the development of a cell designed to perform such kinds of measurements in the Physical Property Measurement System (PPMS) by Quantum Design. Due to limited sample space the biggest challenge to face was the miniaturisation of the cell. An entirely new concept of fabrication has been used to assure maximum resolution, easy and fast applicability and simple accessibility. We could achieve sensitivities equal to those of presently established thermal expansion measurement cells, i.e., within the range of $\Delta L = 10^{-1}$ to 10^{-2} Å[1]. For better thermal coupling and less influence of induced currents by the magnetic field, CuBe has been chosen as the adequate material. First test measurements of thermal expansion as well as magnetostriction have been performed from room temperature to 5 K on single crystals of selected systems which show 1^{st} and 2^{nd} order phase transitions.

[1] R Pott and R Schefzyk 1983 *J. Phys. E: Sci. Instrum.* **16** 444

TT 11.6 Mon 14:00 P4

Cantilever-based ESR detection at frequencies up to 400 GHz — •D. Kamenskyi, A. Dankert, O. Ignatchik, J. Wosnitza, and S. Zvyagin — Dresden High Magnetic Field Laboratory (HLD), FZ Dresden-Rossendorf, D-01314 Dresden, Germany

We present our recent developments of a new technique to measure electron spin resonance (ESR) spectra by means of cantilever-torque magnetometry. By combining a modulation technique with the use of a capacitive cantilever, we successfully observed ESR spectra in Cu-based weekly anisotropic materials (including $CuSO_4{\cdot}5H_2O$ and $CuCl_2{\cdot}2H_2O$) at frequencies up to 400 GHz and magnetic fields up to 16 T. The experimental details, performance, and limitations of the used ESR setup will be described.

Part of this work has been supported by Deutsche Forschungsgemeinschaft and EuroMagNET (EU contract No. 228043).

TT 11.7 Mon 14:00 P4

Coherent broadband continuous-wave THz spectrometry at low temperatures — Jennifer Marx[1], •Ernesto Uldarico Vidal[1], Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Axel Roggenbuck[2], Anselm Deninger[2], Iván Cámara Mayorga[3], Rolf Güsten[3], Joachim Hemberger[1], and Markus 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 report on the implementation of a cryostat into a continuous-wave THz spectrometer which uses the principle of mixing the light of two NIR DFB diode lasers at a photomixer for generating THz radiation over a broad range from 60 GHz to 1.3 THz. The THz radiation is detected coherently by a second photomixer. In combination with a fiber stretcher, our compact fiber-based setup allows very reliable determination of both real and imaginary parts of the complex optical functions, eliminating the need for Kramers-Kronig transformation. Furthermore, photocurrent correction can be used to correct for instabilities such as thermal drifts. Here, we present some results on different solid-state samples as an illustration of the capability of the spectrometer in the temperature range from room temperature to 1.5 K.

TT 11.8 Mon 14:00 P4

Coherent broadband continuous-wave THz spectrometer: Implementation at low temperature and high magnetic field — •Malte Langenbach[1], Komalavalli Thirunavukkuarasu[1], Andreas Janssen[1], Holger Schmitz[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Axel Roggenbuck[3], Anselm Deninger[3], Markus Grüninger[1], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [2]Max-Planck-Institute for Radio Astronomy, Auf dem Hügel 69, D-53121 Bonn, Germany — [3]TOPTICA Photonics AG, Lochhamer Schlag 19,D-82166 Gräfelfing, Germany

Our high-resolution THz 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 fiber-based phase modulation allows simultaneous determination of THz amplitude and phase. The two photomixers (the source and the detector) offer a compact face-to-face spectrometer assembly. Recently, this assembly was successfully integrated in the commercial magnetic cryostats. The initial problem of a low temperature resistant coupling between laser fibers and photomixers was overcome with a better design. We will present some first results to illustrate the properties of our setup and the response of the antennas for different temperatures down to 3 K and magnetic fields up to 8 T. The integrated setup enables phase sensitive broadband transmission spectroscopy in the subphonon regime at low temperatures and in high magnetic fields facilitating the study of low energy excitations in complex materials.

TT 11.9 Mon 14:00 P4

Design and first results of a ultra low temperature scanning tunnelling microscope — •Danny Baumann[1], Martha Scheffler[1], Ronny Schlegel[1], Torben Haenke[1], Christian Hess[1], Marko Kaiser[2], Ralph Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

We present the design of a home build 300 mK, ultra high vacuum (UHV) scanning tunneling microscope (STM). The STM is equipped with a 9 T superconducting magnet, a home build xy-sample positioning system, in situ tip and sample exchange, radio frequency filter for all relevant signals as well as a three chamber UHV system to prepare, analyze and store tips and samples.

Furthermore, we show the results of energy calibration measurements with different tip-sample configurations using a Niobium BCS superconductor.

TT 11.10 Mon 14:00 P4

Setup of a STM Operating at milliKelvin Temperature — •Udai Raj Singh, Mostafa Enayat, Seth Cullen White, and Peter Wahl — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

We present the set-up of a dilution-refrigerator based spectroscopic imaging scanning tunneling microscope. The STM can operate at temperatures down to below 10mK and in magnetic fields up to 14T to allow for studies of unconventional superconductors and heavy fermion materials. The system provides a continuous measurement time on the order of 150 hours and allows for sample transfer and in-situ sample cleavage. We present first results obtained at $T_{MXC} \approx 9$ mK on a $NbSe_2$ sample. To determine the energy resolution we have measured the superconducting gap of Aluminum. By fitting a BCS gap function to the spectra we have found the electronic resolution of our STM to be around 150 mK.

TT 11.11 Mon 14:00 P4

Broadband magnetodielectric spectroscopy on quantum paraelectric materials in the millikelvin-regime — •Christoph Grams, Max Schalenbach, Daniel Niermann, Harald Kierspel, and Joachim Hemberger — 2. Physikalisches Institut, Universität zu Köln, Deutschland

Quantum paraelectric materials are characterized by an extended dielectric permittivity due to the vicinity to a ferroelectric transition which, however, is suppressed by quantum fluctuations down to lowest temperatures.

Using broadband dielectric spectroscopy from 10^{-2} Hz to 1 MHz we examine the polarization dynamics in quantum paraelectric materials by measuring the complex permittivity as a function of temperature and magnetic field.

We present our results on (Fe-doped) $SrTiO_3$ and $Dy_2Ti_2O_7$. For the latter compound special weight has been put on the investigation of the magneto-dielectric response within the spin-ice regime which previously has been discussed in connection with the formation of magnetic monopoles [1].*This work was supported by the DFG through SFB 608.*

[1] C. Castelnovo, R. Mössner, S. L. Sondhi, *Nature*, **451**, 06433 (2008)

TT 11.12 Mon 14:00 P4

Spectral Functions for Strongly Correlated Multi-Orbital Systems with full Coulomb Vertex — •German Ulm[1] and Alexander I. Lichtenstein[2] — [1]German Research School for Simulation Sciences and RWTH Aachen University, 52425 Jülich — [2]1. Institut für Theoretische Physik, Universität Hamburg

We present an efficient approach for calculating dynamical properties of solids with strong electron correlations. The fast cluster method, a finite temperature Lanczos method, is combined with Dynamical Mean-Field Theory (DMFT) in order to study orbital degenerate systems as function of temperature. The full local Coulomb interaction

is taken into account in all calculations. We analyze different double-counting correction schemes for systems with strong electron correlations. We show results of an extensive study of the charge transfer system NiO in the LDA+DMFT framework using quantum Monte Carlo and finite-temperature Lanczos impurity solvers.

TT 11.13 Mon 14:00 P4

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

The investigation of superconductivity in repulsively interacting electron-systems is complicated by the interplay between different interaction channels, which have to be treated on equal footing. We use the functional renormalization group (fRG) to investigate the low-energy properties of such systems with the aim of finding an efficient parametrization of the effective Nambu two-particle vertex in a singlet superconductor. We analyse general properties of the vertex and the renormalization group flow for a reduced model with pairing and forward scattering with the aim of investigating superconductivity in the Hubbard model. Using a decomposition of the vertex in various interaction channels, we manage to isolate singular momentum and frequency dependences in a way suitable for an efficient parametrization.

TT 11.14 Mon 14:00 P4

Strong-coupling expansion in the Hubbard model by a diagrammatic-combinatorial computer algorithm — •Martin Paech[1,2], Eva Kalinowski[2,3], Walter Apel[4,1], and Eric Jeckelmann[1] — [1]Leibniz Universität, Hannover, Germany — [2]Academy of Computer Science and Management, Bielsko-Biała, Poland — [3]Union IT Services GmbH, Frankfurt am Main, Germany — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Motivated by the efficient diagrammatic approach for the evaluation of high-order terms in the strong-coupling limit for the Hubbard model on the half-filled Bethe lattice with infinite coordination number we present an optimized and parallelized implementation of the underlying 'divide-and-conquer' algorithm. This new implementation is accompanied by a functional analysis of its recursive kernel and extended to systems away from half filling and finite-dimensional systems. As a first application, we study the ground-state energy and determine the critical coupling of the Mott-Hubbard transition from the radius of convergence of the series.

TT 11.15 Mon 14:00 P4

Abelian Z(N) topological order and its breakdown — •Marc Daniel Schulz[1], Julien Vidal[2], Sébastien Dusuel[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Otto-Hahn-Straße 4, D-44221 Dortmund, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France — [3]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France

In the last years, topologically ordered systems gained much interest. Typical phenomenology uses models like Wen's plaquette model or the Toric Code proposed by Kitaev, which are exactly solvable models exhibiting topologically ordered ground states. Excitations in these models are Z(2) Abelian anyons which are completely local because they are protected by conservation laws. Here we present a generic extension of these type of models to the Z(N) case which possess a richer ground state degeneracy and a richer excitation spectrum. The major aim is to understand the robustness of the highly-entangled topologically ordered states against local perturbations. To this end we study for the cases $N = 3, 4$ the effect of external magnetic fields which results in mobile and interacting anyonic excitations.

TT 11.16 Mon 14:00 P4

Optimization of evaporation trajectories in weightlessness — •Roman Nolte — TU Darmstadt

Evaporative cooling is the essential method for attaining quantum degeneracy. Nowadays, optimization of evaporative cooling is done in the laboratory as an iterative process. Speed and yield are important aspects but usually not system critical. Not so, in the QUANTUS experiment [1], which explores quantum gases in microgravity. There evaporation time as limited resource and should be as short as possible.

In this contribution, we examine in detail the nonequilibrium process of evaporation in time-dependent traps for a classical gas [2]. We compare solutions of the ergodic Boltzmann equation with N-particle molecular dynamics codes performed on graphic cards. Results of various numerical simulations of particular evaporation processes are compared for the purpose of optimizing yield and duration.

[1] T. van Zoest et al., Science 328, 1540 (2010).
[2] O. J. Luiten et al., Phys. Rev. A 53, 381-389 (1996)

TT 11.17 Mon 14:00 P4

Condensation of bound states and pairs in interacting Fermi gases — •Michael Maennel[1,2], Klaus Morawetz[1,3], Pavel Lipavsky[4,5], and Michael Schreiber[2] — [1]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [3]International Institute of Physics, Universidade Federal do Rio grande do Norte, 59.072-970 Natal-RN, Brazil — [4]Institute of Physics, Academy of Sciences, 16253 Prague 6, Czech Republic — [5]Faculty of Mathematics and Physics, Charles University, 12116 Prague 2, Czech Republic

We investigate a Fermi gas with finite-range interaction using a scheme to eliminate self interaction in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature, without the use of anomalous functions. We calculate the phase diagram, excitation spectrum and equation of state. While in the low-density limit we find a condensation of bound states, for high density there is pairing. In between there is the BCS-BEC crossover.

TT 11.18 Mon 14:00 P4

Non-Equilibrium Dynamics of two coupled 1D condensates of interacting atoms — •Clemens Neuenhahn[1,3], Florian Marquardt[1,2], and Anatoli Polkovnikov[3] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institut for the Science of Light, Günter-Scharoswky- Strasse 1/Bau 24,D-91058 Erlangen, Germany — [3]Boston University, 590 Commonwealth Avenue Boston, MA 02215, USA

Motivated by recent experiments, we investigate the non-equilibrium dynamics of two interacting one-dimensional condensates following a quench of the tunnel-coupling to finite values. These coupled condensates provide a realization of the quantum sine-Gordon model, whose non-linear time-evolution after turning-on the coupling is studied using the semiclassical truncated Wigner approximation. We analyze the amplification of initial quantum fluctuations of the relative phase and the emergence of localized phase structures.

TT 11.19 Mon 14:00 P4

Relaxation phenomena in ultracold atomic systems after quenching the external potential — •Akos Rapp, Stephan Mandt, and Achim Rosch — Institute f. Theoretical Physics, Uni Cologne, Cologne, Germany

In contrast to the subjects of traditional solid state physics, ultracold atoms offer ways to realize and study states of matter without the influence of background degrees of freedom, impurities, etc. Furthermore, one can change the shapes and strengths of external potentials relatively easy, to investigate dynamics out of equilibrium. We study how a cloud of ultracold atoms in equilibrium in a harmonic trap evolves after the potential is changed suddenly. Without an optical lattice, the physics is usually relatively simple. However, in a deep optical lattice the kinetic energy is bounded, leading to unexpected relaxation phenomena. Even by simply turning the confining potential off, the system evolves through a nontrivial interplay of diffusive and ballistic motion of the atoms [arXiv:1005.3545], while reversing the sign of the harmonic potential allows equilibration to negative absolute temperatures, $T<0$ [PRL 105, 220405 (2010)]. We discuss direct experimental consequences of different external potential quenches and the common aspects of these out of equilibrium processes.

TT 11.20 Mon 14:00 P4

Radiofrequency spectroscopy of a strongly interacting two-dimensional Fermi gas — •Enrico Vogt, Bernd Fröhlich, Michael Feld, Marco Koschorreck und Michael Köhl — Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

We have realized and studied a strongly interacting two-component atomic Fermi gas confined to two spatial dimensions using an optical

lattice. Using radio-frequency spectroscopy we measure the interaction energy of the gas. We find that the strong confinement to two dimensions induces scattering resonances and leads to the existence of confinement-induced molecules which have no counterpart in three dimensions.

TT 11.21 Mon 14:00 P4

Strongly correlated fermions in disordered optical lattices — •Denis Semmler[1], Krzysztof Byczuk[2,3], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

Strongly correlated fermions in binary and speckle disordered optical lattices are investigated. We numerically solve the Anderson-Hubbard model within the statistical dynamical mean-field theory, which incorporates fluctuations due to disorder as well as local correlations. Localization due to disorder is studied by means of the probability distribution function of the local density of states. In both cases, the paramagnetic ground state phase diagram is determined. Binary disordered fermions exhibit a Mott metal-insulator transition at non-integer filling. In contrast to box disordered fermions, the Anderson-Mott insulator and the Mott insulator are not continuously connected in the presence of speckle disorder.

TT 11.22 Mon 14:00 P4

Magnetorotons versus transverse magnetophonons of quasi twodimensional electrons in high magnetic fields — •Guenther Meissner and Uwe Schmitt — Theoretische Physik, Universitaet des Saarlandes, Postfach 151150, D-60041 Saarbruecken

The nature of two condensed phases: an incompressible quantum liquid of Bose-condensed charge-vortex composites and a 2D quantum solid with a lattice-periodic structure of the guiding centers of the Coulomb-interacting electrons, is investigated. Applying sum-rule techniques in a unified many-body approach, a finite gap (magnetorotons) due to correlations in the density fluctuations of the cyclotron orbits or no gap (magentophonons), because of broken magnetic translational invariance, are shown to exist rigorously in the long-wavelength limit of the low-lying collective modes. Effects of random disorder on the dispersion of the collective excitations of the two phases are investigated for a comparison with experimental results of systems exhibiting the fractional quantum Hall effect.

TT 12: Micro Mechanical Oscillator 2 (jointly with Q)

Time: Monday 14:30–15:15 Location: HSZ 02

TT 12.1 Mon 14:30 HSZ 02

Synchronization in optomechanical arrays — •Georg Heinrich[1], Max Ludwig[1], Jiang Qian[2], Björn Kubala[1], and Florian Marquardt[1,3] — [1]Institute for Theoretical Physics, University of Erlangen-Nuremberg, Germany — [2]Department of Physics, LMU Munich, Germany — [3]Max Planck Institute for the Science of Light, Erlangen, Germany

The motion of nano- and optomechanical systems can be coupled to electromagnetic fields. Beside the ultimate goal to measure and control the quantum state of mechanical motion, these systems allow to study elaborate dynamics due to the light-mechanics interaction. Recent developments have demonstrated systems comprising several coupled optical and vibrational modes, such as optomechanical crystals. Here we investigate the collective dynamics of arrays of coupled optomechanical cells, each consisting of a laser-driven optical and a mechanical mode. Beyond a certain threshold of the laser input power, each cell shows a Hopf bifurcation towards a regime of self-induced oscillations. We show that the phases of many such cells, even with different bare initial frequencies, can lock to each other, synchronizing the dynamics to a collective oscillation frequency. We present different regimes for the dynamics and describe the system in terms of an effective Kuramoto model. This allows to connect our optomechanical results to the general field of nonlinear science where synchronization constitutes an important, universal feature finding applications in fields ranging from physics over chemistry to biology.

TT 12.2 Mon 14:45 HSZ 02

Optomechanical entanglement and teleportation in a pulsed scheme — •Sebastian Hofer[1,2], Markus Aspelmeyer[1], and Klemens Hammerer[2] — [1]Faculty of Physics, University of Vienna, Austria — [2]Institute for Theoretical Physics and Institute for Gravitational Physics, Leibniz University Hannover, Germany

We analyze the creation of optomechanical EPR entanglement in a pulsed scheme. Furthermore we apply the standard CV teleportation protocol to optomechanical systems, analyze its Fidelity under the influence of thermal noise and determine the optimal parameter regime.

TT 12.3 Mon 15:00 HSZ 02

Quantum theory of light scattering for dielectric objects in optical cavities — •Anika C. Pflanzer, Oriol Romero-Isart, and J. Ignacio Cirac — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, 85748 Garching, Germany

We develop a full quantum theory to describe the coupling of light to the motion of general dielectric objects in high-finesse optical cavities. In particular, we derive a master equation to describe the center-of-mass motion of the dielectric object, the cavity mode and their coupling to the other modes of the electromagnetic field via photon scattering. Focusing on massive particles here, this general theory is in particular applied to the recent proposal of using an optically levitating dielectric as a cavity opto-mechanical system [1,2]. Furthermore, we explore the range of applicability of this theory with respect to the size of the dielectric object and investigate limitations on possible cavity-cooling schemes. By comparing our findings to results from classical Mie scattering theory, we investigate differences arising from a fully quantum mechanical treatment of the system.

[1]Romero-Isart, New J. Phys. 12:033015 (2010)
[2]Romero-Isart, Pflanzer et al., arXiv:1010.3109 (2010)

TT 13: Multiferroics I (jointly with DF, DS, KR, MA)

Time: Monday 14:45–17:00 Location: HSZ 04

TT 13.1 Mon 14:45 HSZ 04

DFT calculation of $ACrO_3$ perovskites using hybrid functionals — •Martin Schlipf[1], Alessandro Stroppa[2], Silvia Picozzi[2], and Marjana Ležaić[1] — [1]Forschungszentrum Jülich, Peter Grünberg Institut and JARA, Germany — [2]CNR-SPIN, L'Aquila, Italy

Density-functional theory (DFT) is a very powerful tool for understanding the properties of several crystals and molecules. Novel hybrid exchange-correlation functionals, which include a fraction of Hartree-Fock exchange, improved the predictive power of DFT further. In this contribution, we have studied the $ACrO_3$ (A = Ca, Sr, Pb) perovskite compounds by DFT. These materials have recently gained a renewed interest, because they offer a rich phase-space of electronic, magnetic and structural transitions. The origins of several of these transitions are not understood, yet. In $SrCrO_3$ different authors report different electronic (metal/insulator) and magnetic (Pauli paramagnetic/Curie Weiss) configurations. It is not clear yet what is the ground state of this compound. In $PbCrO_3$ theoretical calculations predict a conducting state whereas experimentally a metal is found. We use a multi-code approach and clarify these issues from first-principles.

We gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409.

TT 13.2 Mon 15:00 HSZ 04

Optical properties of $BiCrO_3$ — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], Silvia Bahmann[1], Kannan Vijayanandhini[2], Adreas Talkenberger[1], Christian Röder[1], Dietrich R.T. Zahn[3], Alexei A. Belik[4], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, D-06120 Halle — [3]TU Chemnitz, Semiconductor Physics, D-09107 Chemnitz — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

Multiferroic materials that simultaneously show polarization and magnetization ordering are envisaged to play a significant role in developing devices with large magnetoelectric coupling. An interesting candidate for intrinsic multiferroism is $BiCrO_3$ (BCO). In this work, the optical properties of polycrystalline BCO ceramics and epitaxial BCO films deposited on $NdGaO_3$(110) substrates are investigated by Raman spectroscopy and spectroscopic ellipsometry. The spectral changes seen in temperature-dependent Raman measurements correlate well to a structural phase transition from a monoclinic structure (space group *C2/c*) to an orthorhombic structure (space group *Pnma*) at about 420 K. The room temperature dielectric function of a 55 nm thick BCO film deposited on $NdGaO_3$ substrate is determined by analyzing ellipsometry data and exploited to estimate the BCO band-gap. The imaginary part of the dielectric function calculated by means of density functional theory shows good agreement with the experimental one. *This work was supported by the German Research Foundation DFG HI 1534/1-1.*

TT 13.3 Mon 15:15 HSZ 04

Pressure induced phase transitions in $MnTiO_3$: Insights from First Principles calculations — •Carmen Quiroga and Rossitza Pentcheva — Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich

$MnTiO_3$ crystallizes in the ilmenite structure at ambient conditions and remains stable at least up to 26 GPa [1]. A denser $LiNbO_3$ phase can be quenched from high pressure and high temperature experiments to ambient conditions [2]. Our density functional theory calculations, including an on-site Coulomb repulsion term (LDA/GGA+U), show a transition from the $LiNbO_3$ to the perovskite phase at 2.5 GPa in agreement with experiments [3]. A transition from perovskite to the post-perovskite phase ($CaIrO_3$-type) is predicted at pressures above 50 GPa. Furthermore, the magnetic coupling of the Mn ions and the possibility of spin transitions in the different phases are explored.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] X. Wu et al. Geoscience Frontiers, in press (2010).
[2] J. Ko and C.T. Prewitt. Phys. Chem. Minerals **15**, 355 (1988).
[3] N. Ross et al. Phys Chem Minerals **16**, 621 (1989).

TT 13.4 Mon 15:30 HSZ 04

Resonant Soft X-ray Scattering (RSXS) Studies on Multiferroic YMn2O5 — •Sven Partzsch[1], Stuart Wilkins[2], John Hill[2], Enrico Schierle[3], Eugen Weschke[3], Dmitri Souptel[1], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden — [2]BNL Upton — [3]Helmholz-Zentrum Berlin

Multiferroic RMn_2O_5 (R = Y, rare earth, Bi) displays a complex magnetic behavior with transition into a ferroelctric phase as a function of temperature. The intensity of the magnetic superlattice reflection $(1/2, 0, 1/4)$ displays a strong resonance at the Mn L_{23}-edge, due to the strongly increased magnetic sensitivity close to the absorption edge.

Surprisingly, we also observe that this magnetic peak also displays a strong resonance at the oxygen K-edge. The measured integrated intensity of this reflection at the Mn L_3-edge in the commensurate and incommensurate magnetic phase is essentially unchanged. At the oxygen K-edge, however, a strong drop of the temperature dependent integrated intensity is observed at the corresponding phase transition, which resembles the temperature dependence of the ferroelectric polarization. Therefore RSXS at the different edges might provide more information about the origin of ferroelectricity in these frustrated magnets.

The experimental data together with LSDA+U calculations provide evidence that magnetically driven charge transfer between oxygen and manganese plays an important role for the ferroelectricity in these frustrated magnets.

TT 13.5 Mon 15:45 HSZ 04

Dilatometric studies of the multiferroic $FeTe_2O_5Br$ — •Christian Balz[1], Mariano de Souza[1], Matej Pregelj[2], Helmuth Berger[3], Denis Arčon[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany — [2]Institute "Jozef Stefan", Jamova 39, 1000 Ljubljana, Slovenia — [3]Institute of Physics of Complex Matter, EPFL, 1015 Lausanne, Switzerland

We report on high-resolution directional dependent thermal expansion measurements of the novel multiferroic system $FeTe_2O_5Br$ [1]. Our results reveal two distinct phase transition anomalies centered at $T_{N1} = 11.0$ K and $T_{N2} = 10.6$ K, which coincide with the transitions observed in other quantities [2]. A rounded minimum in α_c shows that short-range magnetic correlations within the crystal layers start to develop already above T_N. At T_{N1}, the system undergoes a magnetic phase transition into the high-T incommensurate (HT-ICM) phase. Interestingly, at T_{N2}, a second phase transition into the low-T incommensurately modulated (LT-ICM) phase is observed, which is accompanied by a spontaneous electric polarization. When magnetic field is applied, the transition temperatures shift depending on the field orientation. In the case of $B \| b > 4.5$ T, the HT-ICM phase merges into the LT-ICM phase. Despite the pronounced lattice effects observed at T_{N2} at 6 T, the electric polarization is destroyed. The rich low-T magnetic phase diagram of $FeTe_2O_5Br$ will be discussed in details [2].

[1] M. Pregelj *et al.*, Phys. Rev. Lett. **103**, 147202 (2009).
[2] M. Pregelj *et al.*, Phys. Rev. B **82**, 144438 (2010).

TT 13.6 Mon 16:00 HSZ 04

Investigation of multiferroic order in M_3TeO_6 (M=Co, Mn, Ni) by second harmonic generation — •Vera Carolus[1], Thomas Lottermoser[1], Sergey A. Ivanov[2], Matthias Weil[3], Roland Mathieu[4], Matthias Hudl[4], Per Nordblad[4], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic Materials, Karpov' Institute of Physical Chemistry, Vorontsovo pole, 10 105064, Moscow K-64, Russia — [3]Institute of Chemical Technologies and Analytics, Vienna University of Technology, Austria — [4]Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden

Orthotellurates with the formula M_3TeO_6 are structurally well characterized and can be divided into six different structure types. According to this, these materials show a wide range of magnetic phases. Recently it was suggested, that in some of the orthotellurates multiferroic order is possible.

Among this are: Co_3TeO_6 (space group C2/c) and Mn_3TeO_6 ($R\bar{3}$) with two magnetic phase transitions as well as Ni_3TeO_6 (R3) with one magnetic phase transition. However, a direct proof of ferroelectricity has not been reported so far.

Here, we investigate the multiferroic order by second harmonic generation (SHG) spectroscopy. For Co_3TeO_6 we measured a intense SHG contribution in the low temperature phase below 18 K, which is a strong evidence for multiferroic order. This interpretation is supported by the observation of complex domain patterns using SHG imaging techniques.

TT 13.7 Mon 16:15 HSZ 04

Optical Spectroscopy on the triangular antiferromagnet $CuCrO_2$ — •Michael Schmidt, Zhe Wang, Franz Mayr, Vladimir Tsurkan, Joachim Deisenhofer, and Alois Loidl — Experimental Physics 5, Center for Electronic Correlations and Magnetism, Institute of physics, Augsburg University, Germany

$CuCrO_2$ belongs to the class of triangular lattice antiferromagnets and shows ferroelectricity below $T_{FE} \approx 24$ K [1] while the spins order in a proper screw [2]. Already a moderate magnetic field of 5.3 T can flop the plane of the spins and the polarization. A microscopic theory [3] explains this by the variation of the spin-orbit coupling with the metal-ligand (d-p) hybridization. Recently, electromagnons (magnetic excitations excited by electric field) have been detected in the related compound $Cu(Fe,Al)O_2$ [4] in the submillimeter range. We report on the optical excitation spectrum of $CuCrO_2$ including phonons, crystal-field excitations and magnon sidebands. The relation of magnon lifetime with the possible formation of Z_2 vortices in this system is discussed.

[1] K. Kimura et al., Phys. Rev. B 78, 140401 (2008)
[2] S. Seki et al., Phys. Rev. Lett. 101, 067204 (2008)
[3] T. Arima J. Phys. Soc. Jap. 76, 073702 (2007)
[4] S. Seki et al., Phys. Rev. Lett. 105, 097207 (2010)

TT 13.8 Mon 16:30 HSZ 04

New design for magnetoelectric switch from first principles — •Michael Fechner[1], Peter Zahn[2], Sergey Ostanin[1], and

Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

Saving information in a magnetic bit requires at least two stable magnetic states that can be distinguished. In conventional hard disks two opposite directions of the magnetization provide these two states. The magnetic state is changed by an external magnetic field thus writing information, whereas reading is performed by the usage of the GMR effect (giant magnetoresistance) [1]. Based on ab intio material design we propose a new hybrid magnetoelectric that allows this switching of the magnetic states by an applied electric field instead of the magnetic field. The switching in the proposed multilayer system is based on internal electronic couplings without any strain. Thus, it is a promising candidate for application in future magnetoresistive random access memory (MRAM).

[1] Baibich et al., PRL 61, 2472-2475, (1988)

15 min. break

TT 14: Multiferroics II (jointly with DF, DS, KR, MA)

Time: Monday 17:00–18:45 Location: HSZ 04

TT 14.1 Mon 17:00 HSZ 04

Tuning magnetism by epitaxial strain in biferroic $Fe_{70}Pd_{30}$ films — •Sandra Weiss[1], Markus Ernst Gruner[2], Jörg Buschbeck[1,3], Ludwig Schultz[1], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden — [2]University of Duisburg-Essen, Theoretical Physics, Lotharstraße 1, D-47048 Duisburg — [3]ECE Department, University of California, Santa Barbara

Due to combination of ferromagnetic and ferroelastic properties magnetic shape memory alloys can be considered as multiferrorics. For the magnetic shape memory alloy Fe-Pd we could demonstrate recently, that strained epitaxial film growth allows a variation of the tetragonal distortion by 27 % [J. Buschbeck et al., PRL 103, 2009, 216101]. Density functional calculations revealed a flat energy landscape along the Bain path, explaining this soft behaviour of $Fe_{70}Pd_{30}$. Here we show that tetragonal distortions up to 43 % are possible. This exceeds the Bain transformation path connecting bcc and fcc structure. $Fe_{70}Pd_{30}$ films are produced by coherent epitaxial growth on MgO substrates covered by different metallic buffer layers. By adjusting the tetragonal distortion intrinsic magnetic properties like Curie temperature, saturation magnetisation and magnetocrystalline anisotropy can be controlled. The relevance of two mechanisms for relaxation of epitaxial strain - misfit dislocations and adaptive martensite - is discussed.

TT 14.2 Mon 17:15 HSZ 04

Strain effect on the magnetic properties of $SrRuO_3$ thin films on ferroelectric PMN-PT substrates — •Andreas Herklotz, Mikko Kataja, Ludwig Schultz, and Kathrin Dörr — IFW Dresden, IMW, Helmholtzstrae 20, 01069 Dresden, Germany

We investigate a two-component multiferroic system consisting of a ferroelectric $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$ (PMN-PT) substrate and ferromagnetic $SrRuO_3$ (SRO) thin films. The inverse piezoelectric effect of the substrate is used to reversibly vary the strain state of the epitaxial SRO films in order to clarify the strain dependence of the magnetic film properties. Buffer films of $Sr_{1-x}Ba_xTiO_3$ are introduced to vary the as-grown state of the SRO films and to cover a wider range from compressive to tensile strain.

High resolution X-ray diffraction is deployed to structurally characterize the films and to determine Poisson's ratio of SRO, which is not known so far. SQUID magnetometry reveals that the Curie temperature is increasing with tensile strain, but starts to decrease again under high strain. Angular-dependent measurements provide that the easy axis orientation shows a complex dependence on strain and temperature. SQUID measurements on conventional substrates like $SrTiO_3$ and $LaAlO_3$ and electric transport measurements complete the data.

TT 14.3 Mon 17:30 HSZ 04

Strain effect on ferroelectric switching dynamics of epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ films — •Kathrin Dörr[1], Andreas Herklotz[1], Michael Biegalski[2], and Hans Christen[2] — [1]IFW Dresden, IMW, Helmholtzstr.20, Dresden — [2]CNMS, Oak Ridge National Laboratory, TN, USA

Elastic strain is known to change ferroic properties of thin films such as the remanent polarization. Less understood and little measured is the influence of the lattice strain induced by film-substrate mismatch on the switching dynamics. In this work, reversible biaxial strain has been applied to films on piezoelectric substrates for a study of their strain-dependent ferroelectric switching. $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) films have been epitaxially grown by pulsed laser deposition on piezoelectric substrates of $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$(001) (PMN-PT) buffered with a $SrRuO_3$/$SrTiO_3$ double layer. Four-circle x-ray diffraction has been employed to confirm the tetragonal symmetry and to measure the lattice parameters of the films. Measurements of the characteristic ferroelectric switching time at various temperatures and strains show an increase of several percent under compression, revealing a similarly strong strain sensitivity of the switching dynamics as that of the remanent polarization. We attempt to identify the strain dependence of the domain wall velocity.

TT 14.4 Mon 17:45 HSZ 04

Fabrication and multiferroic properties of $BiFeO_3$/$BiCrO_3$ perovskite heterostructures — •Vijayanandhini Kannan, Florian Johann, Alessio Morelli, Miryam Arredondo, Eckhard Pippel, and Ionela Vrejoiu — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle.

Bi-based multiferroic materials have attracted strong research interests due to the presence of sterochemical active $6s^2$ lone pair electrons in Bi^{3+} ions and high ordering temperatures, e.g., $BiMeO_3$ (Me = Fe, Cr, Mn, etc). In the present work, epitaxial films of $BiCrO_3$ and $BiFeO_3$ of different thickness (5 nm to 250 nm) were grown on $SrTiO_3$ (100) using pulsed laser deposition technique. Reciprocal space mapping XRD measurements showed that both $BiFeO_3$ (40 nm) and $BiCrO_3$ films (130 nm) are fully strained, having out-of-plane lattice constants of 4.075 Å, and 3.88 Å, respectively. The transmission electron microscopy (TEM) analysis of $BiCrO_3$(130nm)/$SrRuO_3$(16nm)/$SrTiO_3$ films revealed the presence of 45^o and 90^o domains along with the coexistence of three structurally different phases, (i) monoclinic (Space Group: C2/c) and (ii) orthorhombic (Space Group: Pnma) and (iii) an unknown monoclinic-like structure. $BiCrO_3$ film (160 nm) grown on $NdGaO_3$ (110) showed a coherent interface without any misfit dislocations or structural variants. A systematic approach on understanding the thickness evolution of these defects or strain induced structural variants of $BiCrO_3$/$SrRuO_3$/$SrTiO_3$ films is done. Furthermore, the fabrication and multiferroic properties of $BiCrO_3$/$BiFeO_3$ bilayers and multilayer heterostructures are investigated.

TT 14.5 Mon 18:00 HSZ 04

Microscopic Investigations of the Strain-Mediated Coupling in Magnetoelectric Ni/$BaTiO_3$ — •Robert Streubel[1], Denny Köhler[1], Lukas Eng[1], Rudolf Schäfer[2], Claudia Patschureck[2], Anja Wolter[2], Sebastian Gass[2], Stephan Geprägs[3], and Rudolph Gross[3] — [1]Institute of Applied Physics, Technische Universität Dresden — [2]Leibniz Institute for Solid State and Materials Research Dresden — [3]Walther-Meißner-Institute for Low Temperature Research

Coupling the (anti-)ferromagnetic and ferroelectric phases within magnetoelectrics allows affecting the magnetic properties by electric fields. Magnetoelectric heterostructures thus may be considered as prospective candidates for future nanoscale memory devices. However, since only a few single-phase room temperature magnetoelectrics exist with rather poor permeability values, simple composite materials, e.g. amorphous nickel on barium titanate (Ni/$BaTiO_3$) may be used for this purpose. While the macroscopic characterization by monitoring magnetic hysteresis and other effects has been thoroughly carried out, microscopic investigations elucidating the mechanism of ferroelectric/ferromagnetic coupling are still missing.

We report here on the nanoscale inspection of the Ni/$BaTiO_3$ system by PFM, MFM and MOKE. In addition, the saturation magnetization and magnetic anisotropy were measured by SQUID. Both stress and anisotropy within the amorphous Ni film have been modeled showing

an excellent agreement with experimental results.

TT 14.6 Mon 18:15 HSZ 04

Magnetoelectric properties of core-shell $CoFe_2O_4$-$BaTiO_3$ composites — •Vladimir Shvartsman[1], Firas Alawneh[2], Morad Etier[1], Shiwam Tiwari[1], and Doru Lupascu[1] — [1]Institut für Materilawissenschaft, Universität Duisburg-Essen — [2]The Hashemite University, Zarqa, Jordan

In recent years there has been growing interest in materials exhibiting the magnetoelectric (ME) effect. A large ME coupling has been achieved in composites, where a magnetostrictive phase is mechanically coupled to a piezoelectric phase. The magnitude of the ME effect in such systems depends on the properties of the phases and the type of connectivity. In particular, in core/shell-type structures, where the magnetostrictive core is surrounded by the piezoelectric shell, a large well-defined interface area should enhance the ME coupling.

We report on results of synthesis and ME characterization of $CoFe_2O_4$ - $BaTiO_3$ composites with the core-shell structure. The ceramic samples were prepared by covering cobalt ferrite nanoparticles by a shell of $BaTiO_3$ using a sol-gel technique. Scanning probe microscopy studies confirm formation of the core-shell structure with a magnetic core and piezoelectric shell. The ME effect was measured using a modified SQUID susceptometer. Though the relatively high conductivity of the samples prevents an efficient poling of the ferroelectric component, the obtained ME coefficients are comparable to those reported for similar systems. Effects of the microstructure and ratio between piezoelectric and magnetostrictive phases on ME performance are analysed.

TT 14.7 Mon 18:30 HSZ 04

Highly ordered multiferroic nanocomposite arrays: Fabrication and Properties — •Xiaoli Lu, Yunseok Kim, Silvana Goetze, Peter Werner, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

With the resurgence of interest in multiferroics, searching for materials with high coupling coefficient becomes more and more important from both fundamental and practical point of views. We report a new type of artificial nanocomposite, $BaTiO_3/CoFe_2O_4$ (BTO/CFO) heterostructured nanodot arrays. Using a stencil of ultra thin anodic aluminum oxide (AAO) membrane and pulsed laser deposition (PLD), BTO and CFO nanodots were epitaxially grown on top of each other. The size of the nanodots can be easily tuned from 60 to 400 nm. Piezoresponse force microscopy (PFM) and superconducting quantum interference device (SQUID) were used to study the nanocomposite. The local characterization of the piezoresponse and domain structure within single nanodots may shed new light on the strain-mediated magnetoelectric (ME) coupling. The epitaxial interface and reduced clamping from the substrate in this nanocomposite promise a better elastic coupling, which makes it a good prototype for nonvolatile ultrahigh-density memory unit with multi-state data storage capability.

TT 15: SC: Fabrication and Characterization

Time: Monday 16:30–18:00 Location: HSZ 301

TT 15.1 Mon 16:30 HSZ 301

Enhanced two-dimensional behavior of metastable T′-La_2CuO_4, the parent compound of electron-doped cuprate superconductors — •Alexander Buckow[1], Roland Hord[2], Hubertus Luetkens[3], Gwendolyne Pascua[3], Kathrin Hofmann[2], Jose Kurian[1], Vladimir Pomjakushin[4], Andreas Suter[3], Barbara Albert[2], and Lambert Alff[1] — [1]Institute of Materials Science, TU Darmstadt — [2]Eduard-Zintl-Institute, TU Darmstadt — [3]Laboratory for Muon Spin Spectroscopy, PSI — [4]Laboratory for Neutron Scattering, PSI

We synthesized crystalline bulk samples of lanthanum cuprate in the metastable T' phase using cesium hydroxide flux. Its crystal structure was determined as space group $I4/mmm$, no. 139, $a = 401.02$ pm, $c = 1252.66$ pm. Muon spin rotation reveals a gradual slowing down of magnetic order below $T_{N2} = 115$ K, in sharp contrast to La_2CuO_4 in the T structure where $T_{N1} \approx T_{N2} \approx 300$ K. Our result shows that the strikingly different magnetic behavior of the two parent compounds has its origin in the two crystal structure modifications. In addition, we find that T'-La_2CuO_4 has strongly reduced magnetic interactions compared to the other T' materials Nd_2CuO_4 and Pr_2CuO_4, where Nd^{3+} and Pr^{3+} are magnetic ions in contrast to the nonmagnetic La^{3+}.

[1] R. Hord, H. Luetkens, G. Pascua, A. Buckow, K. Hofmann, Y. Krockenberger, J. Kurian, H. Maeter, H.-H. Klauss, V. Pomjakushin, A. Suter, B. Albert, and L. Alff, Phys. Rev. B **82**, 180508(R) (2010).

TT 15.2 Mon 16:45 HSZ 301

Preparation and characterization of $YBa_2Cu_3O_{7-\delta}$ thin films on piezoelectric substrates — •Patrick Pahlke, Sascha Trommler, Ruben Hühne, Bernhard Holzapfel und Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, PO Box 270116, D-01171 Dresden, Germany

The electronic properties of superconducting materials are correlated to external strain. A suitable approach to study this interplay is the preparation of thin superconducting films on piezoelectric substrates. The lattice parameter of theses substrates can be tuned continuously by applying an electric field. Superconducting $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films were successfully prepared on single crystalline piezoelectric (001) $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ substrates using off-axis pulsed laser deposition. Transport measurements revealed a superconducting transition temperature of $T_{c,50} = 89$ K with a transition width of 1 K. By inducing a biaxial strain of 0.2 % in the a-b plane of YBCO a shift of the superconducting transition temperature of $\Delta T_{c,50} = 0.1$ K was observed for optimally doped YBCO. A significant larger effect was found for underdoped samples. We will present the results of these straining experiments and the detailed structural analysis of the grown films. Furthermore our investigations on low temperature properties of the used PMN-PT substrates, which are required for the evaluation of the applicable strain in this temperature region, will be discussed.

TT 15.3 Mon 17:00 HSZ 301

Electric and Magnetic Characterization of La-doped $Bi_2Sr_{2-x}La_xCuO_6$ single crystals — •Michael R Koblischka[1], Johannes Lillig[1], Michal Rames[2], Milos Jirsa[2], Huiqian Luo[3], Hai-Hu Wen[3], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, P.O.Box 151150, D-66041 Saarbrücken, Germany — [2]Institute of Physics, ASCR, Na Slovance 2, CZ-182 21 Prague, Czech Republic — [3]National Laboratory for Superconductivity, P.O.Box 603, Beijing, 100190, P.R.China

We present an exhaustive electric and magnetic characterization of La-doped $Bi_2Sr_{2-x}La_xCuO_6$ single crystals. The critical temperature, T_c, is varying from 27 K to 0 depending on the La content with a maximum at $x = 0.4$. For the measurements we selected samples with $x = 0.4$ (optimally doped) and $x = 0.6$ (slightly underdoped). The sample $x = 0.6$ shows an onset of superconductivity at 25 K and a transition width of 3.5 K. However, at temperatures lower than 20 K, a clear upturn of the resistance curve is found, which also depends on the applied field and the flowing current. The origin of this behavior is discussed.

TT 15.4 Mon 17:15 HSZ 301

Fabrication of superconducting MgB_2 thin films by magnetron co-sputtering on (001) MgO substrates — •Savio Fabretti, Patrick Thomas, Markus Meinert, and Andy Thomas — Bielefeld University, Germany

We fabricated superconducting MgB_2 thin films on (001) MgO substrates. The samples were prepared by magnetron rf and dc co-sputtering on heated substrates. They were annealed ex-situ for one hour at temperatures between 450°C and 750°C. We will show that the substrate temperature during the sputtering process and the post annealing temperatures play a crucial role in forming MgB_2 superconducting thin films. We achieved a critical onset temperature of 27.1 K for a film thickness of 30 nm. The crystal structures were measured by x-ray diffraction.

TT 15.5 Mon 17:30 HSZ 301

Gallium nanolayers featuring on-chip superconductivity in silicon — •Richard Skrotzki[1], Thomas Herrmannsdörfer[1], Jan Fiedler[1,2], Viton Heera[1], Matthias Voelskow[1], Arndt Mücklich[1], Bernd Schmidt[1], Wolfgang Skorupa[1], Gerhard Gobsch[2], Manfred Helm[1], and Joachim Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD) and Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 51 01 19, D-01314 Dresden, Germany — [2]Experimental Physics, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany

We demonstrate the feasibility of embedding superconducting Ga nanolayers in commercial (100) oriented silicon wafers and discuss the possibility of potential device applications [1]. Ion implantation and rapid thermal annealing, known as versatile tools of microelectronic technology, have been used for inserting and distributing a gallium dose of up to 4×10^{16} cm^{-2}. As proven by structural analysis, a 10 nm thin layer of amorphous Ga-rich precipitates forms during annealing at 600 - 700°C. These structures exhibit a superconducting transition at 7 K. Extended resistivity and magnetization measurements reveal in-plane critical fields around 14 T and critical current densities exceeding 2 kA/cm^2. In summary, we proceed with an optimistic outlook concerning the implementation of prospective microstructuring. After all, this would be the next step towards the development of novel semiconductor-based superconducting devices.
[1] R. Skrotzki et al., Appl. Phys. Lett. 97, 192505 (2010)

TT 15.6 Mon 17:45 HSZ 301

Structural characterization of buried superconducting Ga rich films in Si — •Jan Fiedler[1,2], Viton Heera[1], Richard Skrotzki[1], Thomas Herrmannsdörfer[1], Matthias Voelskow[1], Arndt Mücklich[1], Bernd Schmidt[1], Wolfgang Skorupa[1], Gerhard Gobsch[2], Manfred Helm[1], and Jochen Wosnitza[1] — [1]Institute of Ion Beam Physics and Materials Research and Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 51 01 19, D-01314 Dresden, Germany — [2]Experimental Physics, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany

Recently it has been shown that heavily p-doped group-IV semiconductors such as diamond, silicon and germanium can become superconducting at low temperatures. Here, we present a study of Ga-implanted Si that becomes superconducting due to precipitation after annealing. Ion implantation allows introducing a high Ga dose (4E16cm-2) in Si that leads to peak concentrations far beyond the solid solubility limit. Rapid thermal annealing (RTA) causes redistribution of the Ga and re-crystallization of the amorphous implanted Si layer. After annealing at temperatures up to 850°C the implanted layers are polycrystalline and contain Ga-rich precipitates. Structural investigations by means of RBS/C measurements and TEM demonstrate a high density of precipitates at the interface of a protective SiO2 layer and the silicon substrate. At optimized annealing conditions (600-700°C) such samples become superconducting with critical temperatures up to 7 K [1].
[1] Skrotzki R. et al. , Appl. Phys. Lett. 97 (2010) 192505

TT 16: TR: Nanoelectronics III - Molecular Electronics 1

Time: Monday 18:15–19:45 Location: HSZ 03

TT 16.1 Mon 18:15 HSZ 03

Thermal conductivity behavior in double-stranded molecular systems — •Elena Diaz, Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

The analysis of the mechanisms mediating energy flow in biomolecules is a fundamental issue for the understanding of many biologically relevant functions. Our interests focus on studying the energy and heat transport along biomolecular systems which present helix structures, i. e. alpha-helices in proteins or double-helix DNA. When dealing with such systems, the anomalous thermal properties of low dimensional systems must be taken into account. For instance, it is well known that one dimensional harmonic lattices are not able to present the proper thermal gradient in a non-equilibrium regime. Furthermore, even when anharmonicity is present in the system, Fourier's law is still not valid unless a local potential affects every site of the lattice. Biomolecular systems, specially those containing helix structures, can be considered as ladder models of coupled one-dimensional lattices. In this work we study how the thermal properties of isolated lattices are modified by introducing this coupling. We demonstrate that a harmonic lattice interacting with an anharmonic system is able to support a well defined thermal gradient for a large enough coupling. Our results show that by coupling two lattices with a different strength of anharmonicity heat rectification features can arise.

TT 16.2 Mon 18:30 HSZ 03

Electronic signatures of DNA with oxidative damage(8-oxoguanine) — •Myeong Lee[1], Giorgia Brancolini[2], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062, Dresden, Germany — [2]National Research Center on nanoStructures and bioSystems at Surfaces (S3) of INFM-CNR, Via Campi 213/A, 41100 Modena, Italy

8-Oxoguanine (8-oxoG) is the most common form of oxidative DNA damage found in human cells. When DNA polymerases encounter 8-oxoG, they frequently misincorporate adenine in preference to cytosine, leading to G:C → T:A transversion mutation which is commonly found in age-related diseases and human cancers. How DNA repair enzymes recognize 8-oxoG lesions within the entire genome is a long-standing question. Recent experiment by Markus *et al.* [1] suggests that electronic property of 8-oxoG might play a role in the mechanism of locating damage. In this talk we discuss the electronic structure and charge transfer characteristics of dsDNA sequence with 8-oxoG:C and 8-oxoG:A base pairs compared to the one with regular base pairs (G:C). We fully consider the effect of solvent environment and structural fluctuations [2] by combining molecular dynamics (MD) simulations and electronic structure calculations.
[1] T.Z. Markus *et al.*, J. Am. Chem. Soc. **131**, 89 (2008).
[2] P. B. Woiczikowski *et al.*, J. Chem. Phys. **130**, 215104 (2009); R. Gutierrez, *et al.*, Phys. Rev. Lett. **102**, 208102 (2009); M.H. Lee *et al.*, Phys. Rev. B **82**, 155455 (2010).

TT 16.3 Mon 18:45 HSZ 03

Conductance of DNA molecules: Effects of decoherence and bonding — •Matías Zilly[1], Orsolya Ujsághy[2], and Dietrich E. Wolf[1] — [1]Department of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Theoretical Physics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Budafoki út 8., 1521 Budapest, Hungary

The influence of decoherence and bonding on the linear conductance of single double-stranded DNA molecules is examined by fitting a phenomenological statistical model developed recently (Eur.Phys.J.B 68, 237 (2009)) to experimental results. The DNA molecule itself is described by a tight binding ladder model with parameters obtained from published ab initio calculations (J.Am.Chem.Soc. 127, 14894 (2005)). The good agreement with the experiments on sequence and length dependence gives a hint on the nature of conduction in DNA and at the same time provides a crucial test of the model.

TT 16.4 Mon 19:00 HSZ 03

Electrostatic Potential Profiles and Current Voltage Characteristics of Molecular Wires: Effects of Dephasing — •Thomas Stegmann, Matías Zilly, and Dietrich E. Wolf — Department of Physics and CeNIDE, University of Duisburg-Essen, D-47048 Duisburg, Germany

The transport properties of molecular wires are studied using a tight-binding Hamiltonian and non-equilibrium Green's function (NEGF) method. We have developed a statistical model for the effects of dephasing [1], that assumes coherent transport between a distribution of completely phase randomizing regions. Recently, this model has been applied successfully on the conduction of DNA molecules in zero-bias approximation [2].

Here we present the extension of our model to finite bias requiring to take Coulomb interactions into account. This is done by means of the

Hartree approximation where a self-consistent solution of both Poisson's equation and NEGF formalism has to be calculated. As a first application electrostatic potential profiles and current voltage characteristics of linear chains are shown. We demonstrate that the current depends sensitively on whether energy relaxation processes take place in the dephasing regions or not.
[1] M. Zilly, O. Ujsághy and D. E. Wolf, Eur. Phys. B, **68**:237 (2009)
[2] M. Zilly, O. Ujsághy and D. E. Wolf, Phys. Rev. B, **82**:125125 (2010)

TT 16.5 Mon 19:15 HSZ 03

Nonlinear effects of phonon fluctuations on transport through nanoscale junctions — •Daniel F. Urban[1], Remi Avriller[2], and Alfredo Levy Yeyati[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Departamento de Fisica de la Materia Condensada C-XII, Universidad Autonoma de Madrid, E-28049, Madrid, Spain

We analyze the effect of electron-phonon coupling on the full counting statistics of a molecular junction beyond the lowest order perturbation theory. Our approach allows to take into account analytically the feedback between the non-equilibrium phonon and electronic distributions in the quantum regime. We show that for junctions with high transmission and relatively weak electron-phonon coupling this feedback gives rise to increasingly higher nonlinearities in the voltage dependence of the cumulants of the transmitted charges distribution.
[1] D. F. Urban, R. Avriller, and A. Levy Yeyati, Phys. Rev. B **82**, 121414 (R) (2010).

TT 16.6 Mon 19:30 HSZ 03

Statistical analysis of the thermopower of metallic atomic contacts — •Fabian Pauly[1], Juan Carlos Cuevas[2], Markus Dreher[3], Peter Nielaba[3], and Janne K. Viljas[4] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid — [3]Fachbereich Physik, University of Konstanz — [4]Low Temperature Laboratory, Aalto University

We study theoretically the thermopower of Ag, Au, and Pt nanocontacts [1]. In our work, we employ classical molecular dynamics simulations to obtain structures during wire stretching and a tight-binding model for electric transport calculations. We find good agreement with experiment [2] for the evolution of the thermopower with increasing electrode separation and also the therompower histograms. The comparison between the monovalent metals (Ag, Au) shows qualitative differences to those for multivalent ones (Pt).
[1] F. Pauly, J.C. Cuevas, M. Dreher, P. Nielaba, J.K. Viljas (in preparation)
[2] B. Ludoph and J. M. van Ruitenbeek, Phys. Rev. B 59, 12290 (1999)

TT 17: SC: Fe-based Superconductors - 1111

Time: Monday 18:15–20:00 Location: HSZ 301

TT 17.1 Mon 18:15 HSZ 301

Structural trends from a consistent set of single-crystal data of *R*FeAsO (*R* = La, Ce, Pr, Nd, Sm, Gd, and Tb) — •Fabian Nitsche[1], Anton Jesche[2], Ellen Hieckmann[3], Thomas Doert[1], and Michael Ruck[1,2] — [1]Department of Chemistry and Food Chemistry, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [3]Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

A new crystal growth technique for single crystals of RFeAsO (R = La, Ce, Pr, Nd, Sm, Gd, and Tb) using NaI/KI as flux is presented. Crystals with a size up to 300 μm were isolated for single-crystal X-ray diffraction measurements. Lattice parameters were determined by LeBail fits of X-ray powder data against LaB_6 standard. A consistent set of structural data is obtained and interpreted in a hard-sphere model. Effective radii for the rare-earth metal atoms in RFeAsO are deduced. The relation of the intraplane and interplane distances of the arsenic atoms is identified as limiter of the phase formation, and its influence on T_c is discussed.

TT 17.2 Mon 18:30 HSZ 301

Ferromagnetic correlations and Pauli limit behavior of As-deficient $LaO_{0.9}F_{0.1}FeAs_{1-\delta}$ — •V. Grinenko[1], G. Fuchs[1], K. Nenkov[1], F. Hammerath[1], B. Holzapfel[1], K. Kikoin[2], and S.-L. Drechsler[1] — [1]IFW-Dresden, D-01171 Dresden, Germany — [2]Tel Aviv University, Tel Aviv, Israel

The field and T-dependence of the static magnetic susceptibility χ of As-deficient $LaO_{0.9}F0_{0.1}FeAs_{1-\delta}$ (with δ 0.05-0.1) and $LaO_{0.9}F_{0.1}FeAs$ is analysed basing on recent ^{75}As NMR spectroscopy data [1]. The analysis of the Curie-like contribution to the spin-lattice relaxation rate T_1 and $\chi(T)$ together with specific heat data reveals that As vacancies induce local moments. We ascribe the appearance of uncompensated magnetic moment to reconstruction of valence bonds with 4 Fe atoms neighboring to the As-vacancy. These local moments do not suppress superconductivity (T_c increases compared to $LaO_{0.9}F_{0.1}FeAs$) but contribute to the Pauli susceptibility χ_P via an enhanced Stoner factor. We estimated an enhanced χ_P for $LaO_{0.9}F_{0.1}FeAs_{1-\delta}$ by a factor of 3-4 in the clean reference sample. This high χ_P is responsible for the Pauli limiting (PL) behavior observed in As-deficient $LaO_{0.9}F_{0.1}FeAs_{1-\delta}$ [2]. A thermodynamic critical field $B_c(0) \approx$1T was estimated for $LaO_{0.9}F0_{0.1}FeAs_{1-\delta}$, using the measured χ and the PL field $B_p(0)$=88 T from $B_{c2}(T)$ data. In contrast, no PL was found for stoichiometric $LaO_{0.9}F_{0.1}FeAs$ which is consistent with its small Pauli susceptibility.
[1] F. Hammerath *et al.*, Phys. B. **88**, 140504(R) (2010).
[2] G. Fuchs *et al.*, Phys. Rev. Lett. **101**, 237003 (2008).

TT 17.3 Mon 18:45 HSZ 301

Gd^{3+} electron spin resonance spectroscopy on $LaO_{1-x}F_xFeAs$ 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], A. Köhler[1], G. Behr[1], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Universität Zürich, CH-8057 Zürich, Schweiz

In this work we have studied by means of electron spin resonance (ESR) spectroscopy polycrystalline samples of $LaO_{1-x}F_xFeAs$ (x = 0, 0.1) with small levels of Gd doping (2% and 5% with respect to La). The Gd^{3+} ion is an established spin probe to study local magnetic and charge environments in the crystal lattice. In the parent compound the Gd ESR signal is found to be sensitive to the magnetic phase transition from the paramagnetic to the spin density wave (SDW) state taking place at a temperature $T_{SDW} \sim$ 130 K. Here, the analysis of the low-T ESR spectra gives evidence for the occurrence of magnetically non-equivalent Gd sites and possibly sites with different local charge environments. In the case of the superconducting samples with 10% of the F doping (T_c = 25 K) the Gd ESR gives no indication of the SDW order.

TT 17.4 Mon 19:00 HSZ 301

Inelastic neutron scattering on iron arsenide high T_c superconductor $CaFe_{1-x}Co_xAsF$ — •Stephen Price[1], Yixi Su[2], Yinguo Xiao[1], Shibabrata Nandi[1], Ranjan Mittal[3], and Thomas Brueckel[1,2] — [1]Institute of Solid State Research Forschungszentrum Jülich , Jülich, Germany — [2]Jülich Centre for Neutron Science IFF Forschungszentrum Jülich , Jülich, Germany — [3]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai, India

Recent discoveries of iron pnictide superconductors such as $LaFeAsO_{1-x}F_x$ and $Ba_{1-x}K_xFe_2As_2$ have generated a huge amount of interest in the studies of high-T_c superconductivity. In a way very similar to cuprates, superconductivity in iron pnictides is in the proximity to magnetism. Prominent features in the spin excitation spectra such as the *spin gap* and *spin resonance* are characteristic to this class of high-T_c superconductors and therefore are believed to be intimately connected to superconductivity. Here we present our recent results on studies of the magnetic excitation spectrum of Co doped $CaFe_{1-x}Co_xAsF$, a member of the 1111-family of pnictide high-T_c superconductors, obtained via time of flight neutron spectroscopy on powder samples. We successfully detected the resonance mode of the short range two dimensional spin dynamics in superconducting $CaFe_{0.88}Co_{0.12}AsF$ and therefore can report the first direct observation of this characteristic feature for a member of oxygen-free 1111

pnictide superconductors.

TT 17.5 Mon 19:15 HSZ 301

Nanoscale electronic order and ground-state coexistence in iron pnictides — •Guillaume Lang[1], Hans-Joachim Grafe[1], Dalibor Paar[1,2], Franziska Hammerath[1], Katarina Manthey[1], Alexey Alfonsov[1], Ferenc Murányi[1], Richard Zahn[1], Vladislav Kataev[1], Günter Behr[1], Jochen Werner[1], Saicharan Aswartham[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dept. of Physics, Faculty of Science, Univ. of Zagreb, P.O. Box 331, HR-10002 Zagreb, Croatia

Controversial issues in the iron-based superconductors are the extent to which static magnetism and superconductivity can coexist, and whether intrinsic electronic inhomogeneities can show up as in related transition metal oxides. Using nuclear quadrupole resonance at the arsenic sites, we investigated the local charge distribution in "1111" pnictides [1]. Underdoped samples are shown to present systematically two different local charge environments, irrespective of the ground state. Spin-lattice relaxation measurements show their coexistence at the nanoscale. Together with the quantitative variations of the spectra with doping, they point to an intrinsic local electronic order, which is likely to impact the interplay of static magnetism and superconductivity. The latter will also be briefly discussed from the point of view of high-field ESR measurements revealing short-range spin correlations [2].

[1] G. Lang *et al.*, Phys. Rev. Lett. **104**, 097001 (2010)
[2] A. Alfonsov *et al.*, arXiv:1010.5070

TT 17.6 Mon 19:30 HSZ 301

Critical current density and scaling behavior of oxypnictide thin films — •Martin Kidszun, Silvia Haindl, Jens Hänisch, Alexander Kauffmann, Thomas David Thersleff, 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) and SmFeAs(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 these iron oxypnictides. The anisotropy of the irreversibility field was determined using a combination of resistive measurements in high magnetic fields and critical current density measurements. We have demonstrated that critical current densities can be scaled using the approach described by the anisotropic GL formalism.

TT 17.7 Mon 19:45 HSZ 301

Epitaxial thin films of arsenic free pnictide superconductors grown by molecular beam epitaxy — •Alexander Buckow, Jose Kurian, and Lambert Alff — Institute of Materials Science, TU Darmstadt

Within the family of superconducting pnictides, arsenic containing compounds not only are the largest in number, but also the materials with the highest critical temperatures, T_c, obtained so far (up to 55 K). However, from the viewpoint of applications As free superconductors are more desirable, and from the fundamental point of view, the role of other pnictogens is of interest. For Bi as pnictogen, 1111 structure bulk superconductors have been found with T_c up to 9 K [1]. Here we report on the growth of arsenic free superconducting thin films by reactive molecular beam epitaxy as a generic synthesis route. Besides the successful growth of superconducting thin films of LaONiBi, we have also grown the 122 phase $LaNi_2Bi_2$. These thin films were fabricated on MgO substrates from elemental sources in a custom designed UHV chamber ($\approx 10^{-8}$ mbar). A streaky RHEED pattern during deposition clearly indicates epitaxial growth. The observed Laue oscillations in the X-ray diffraction patterns reveal the high crystallinity of the films. So far, however, we could not observe superconductivity in the Bi based 122 epitaxial thin films.

[1] V. L. Kozhevnikov *et al.*, JETP Lett. **87**, 649 (2008).

TT 18: CE: Low-dimensional Systems - Materials 1

Time: Monday 18:30–20:00 Location: HSZ 201

TT 18.1 Mon 18:30 HSZ 201

Magnetic models from DFT cluster calculations - an alternative to supercell computations? — •Stefan Lebernegg[1], Miriam Schmitt[2], Ulrike Nitzsche[3], and Helge Rosner[2] — [1]Universität Salzburg, 5081 Salzburg, Austria — [2]MPI CPfS Dresden, 01187 Dresden, Germany — [3]IFW Dresden, 01171 Dresden, Germany

For the treatment of strong electron correlation two standard approaches are commonly used: In principle, quantum chemistry can deal with strong correlations exactly, but only for small clusters. On the other hand, periodic 3D compounds can be calculated reliably in DFT codes, but the correlations are treated in a very approximate manner, often including external parameters like in the LSDA+U method. The far goal of this work is to find a way to construct reliable clusters capable to describe local properties of solids. In a first step toward this aim, magnetic properties of simple Cu^{2+} compounds with different ligands (N,O,F,Cl,Br) that exhibit edge sharing chains as their central building blocks are systematically studied. For the model clusters, effects of their finite size, embedding and termination as well as the substitution of Cu by formally nonmagnetic cations (broken chain) are investigated. The calculations are carried out within a full potential DFT code and are compared with corresponding known periodic 3D compounds (CuNCN, Li_2CuO_2, $CuCl_2$, $CuBr_2$). The presented cluster approach not only enables the application of highly accurate computational methods but might be used instead of elaborated supercell calculations. Moreover, additional degrees of freedom can provide deeper insight into magneto-structural correlations.

TT 18.2 Mon 18:45 HSZ 201

A microscopic magnetic model for the spin-1/2 Heisenberg piezoelectric ferrimagnet Cu_2OSeO_3 — •Oleg Janson, Alexander Tsirlin, and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

We present the results of band structure calculations for the piezoelectric ferrimagnet Cu_2OSeO_3. Below the $T_C = 60$ K, the compound exhibits sizable magnetocapacitance and stays metrically cubic, which excludes lattice strain from possible magnetoelastic mechanisms [1]. The crystal structure of Cu_2OSeO_3 comprises two inequivalent positions of magnetic Cu^{2+} atoms: 4 Cu(1) atoms are locally coordinated by a trigonal bipyramid of O atoms, while 12 Cu(2) atoms have a distorted 4-fold coordination, typical for cuprates. The net magnetization in the ferrimagnetically ordered ground state results from the antiparallel arrangement of Cu(1) and Cu(2) sublattices [2] and amounts to one-half of the saturation value. Based on DFT calculations, we disclose different magnetically active orbitals for Cu(1) and Cu(2) and five relevant magnetic couplings that form a complex, albeit non-frustrated 3D spin lattice. The role of quantum fluctuations will be discussed in the context of the reduced ordered moment on Cu atoms amounting to $0.61\,\mu_B$ [1] and a low $T_C/J \approx 0.6$.

[1] J.-W. G. Bos *et al.*, Phys. Rev. B 78, 094416 (2008).
[2] M. Belesi *et al.*, Phys. Rev. B 82, 094422 (2010).

TT 18.3 Mon 19:00 HSZ 201

Ferromagnetic versus helical order in edge sharing CuO_2 chains - a computational study — •Helge Rosner[1], Ulrike Nitzsche[2], Roman Kuzian[2], and Stefan-Ludwig Drechsler[2] — [1]MPI CPfS Dresden — [2]IFW Dresden

The magnetic ground state of edge sharing CuO_2 spin 1/2 Heisenberg chains with ferromagnetic nearest neighbor exchange J_1 and antiferromagnetic second neighbor exchange J_2 depends delicately on structural details of the crystal structure, like Cu-O-Cu bond angles, Cu-O distances and the position of the cations. Without taking into account a renormalization by the interchain coupling, a critical ratio $\alpha = -J_2/J_1 = 1/4$ separates a ferromagnetic from a helical ground state (FM for $\alpha < 1/4$, helical for $\alpha > 1/4$). Here, we present a density functional based band structure study that investigates the different influences of various structural parameters for Li_2CuO_2 as example compound. We find that the ferromagnetic and antiferromagnetic contributions develop rather differently for the same structural changes. Therefore, the key parameter α for the ground state is especially sensi-

tive to small structural changes that might be induced by temperature or pressure variation.

TT 18.4 Mon 19:15 HSZ 201

The influence of inter-chain couplings on the thermodynamics of the strongly frustrated chain cuprate Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R.O. Kuzian[2], S. Nishimoto[1], S. Petit[3], Y. Skourski[4], N. Wizent[1], R. Klingeler[5], and B. Büchner[1] — [1]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Inst. f. Problems of Materials Science, Kiev, Ukraine — [3]Laboratoire Léon Brillouin, Saclay, France — [4]Hochfeld-Magnetlabor Dresden(HLD), FZ-Dresden-Rossendorf, Dresden, Germany — [5]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany

We report on detailed experimental and theoretical studies on the magnetic properties of Li_2CuO_2. This compound serves as a simple, but representative model system for spin-chain materials in which strong nearest-neighbor ferromagnetic interactions in the chain which are frustrated by an antiferromagnetic (afm) coupling to next-nearest-neighbors. The competition of interactions can induce incommensurate correlations in the chain. On the example of Li_2CuO_2 we illustrate, that relatively weak inter-chain couplings can prevent incommensurate long-range order and determine solely the saturation field. The inter-chain coupling derived from the saturation field are in excellent agreement with inelastic neutron scattering data [1,2]. The absence of bound magnon states in Li_2CuO_2 is explained in terms of the inter-chain couplings exceeding a critical value of a few meV, only.

[1] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).
[2] S. Nishimoto *et al.*, arXiv:1004.3300v2 (2010).

TT 18.5 Mon 19:30 HSZ 201

Evidence for the opening of a spin gap in the Ca-doped S=1/2 spin chain compound $SrCuO_2$ probed by NMR — •Franziska Hammerath, Satoshi Nishimoto, Hans-Joachim Grafe, A.U.B. Wolter, Christian Hess, Vladislav Kataev, Patrick Ribeiro, S.-L. Drechsler, and Bernd Büchner — Institute for Solid State Research, IFW Dresden,

We present ^{63}Cu Nuclear Magnetic Resonance (NMR) measurements on undoped $SrCuO_2$ and Ca-doped $Sr_{0.9}Ca_{0.1}CuO_2$ single crystals. The crystal structure contains one dimensional CuO_2 double chains that are magnetically decoupled due to frustration. For $SrCuO_2$ the spin lattice relaxation rate T_1^{-1} is temperature independent as it is expected for a one dimensional S=1/2 Heisenberg spin chain. Doping with nonmagnetic, isovalent Ca takes place on the Sr sites outside the spin chains, and should not affect the magnetic properties of the compound. It is therefore very surprising that we do observe a decrease of T_1^{-1} in the Ca-doped sample for temperatures below 80K that clearly evidences the opening of a gap in the spin excitation spectrum. Density Matrix Renormalization Group (DMRG) calculations are presented to discuss the origin of this spin gap.

TT 18.6 Mon 19:45 HSZ 201

Low temperature ballistic spin transport in the $S = 1/2$ antiferromagnetic Heisenberg chain compound $SrCuO_2$ — H. Maeter[1], A.A. Zvyagin[1,2], H. Luetkens[3], G. Pascua[3], Z. Shermadini[3], C. Hess[4], N. Hlubek[4], B. Büchner[4], R. Saint-Matin[5], A. Revcolevschi[5], and •H.-H. Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Kharkov, 61103, Ukraine — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [5]Laboratoire de Physico–Chimie de L'Etat Solide, ICMMO, UMR 8182, Universite Paris-Sud, 91405 Orsay, France

For one-dimensional quantum spin chain systems recent experimental and theoretical studies indicate unexpectedly large, in some cases diverging spin and heat transport coefficients. Local probes, like e.g. muon spin relaxation (μSR) can indirectly characterize the spin transport properties of low dimensional systems via the magnetic field dependence of the spin lattice relaxation rate $\lambda(B)$. For diffusive spin transport $\lambda \propto B^{-0.5}$ is expected. For the ground state of the isotropic spin-1/2 antiferromagnetic Heisenberg chain the eigenstates of the Heisenberg Hamiltonian dominate the spin transport, which is then *ballistic*. Using the Müller ansatz $\lambda \propto B^{-1}$ is expected in this case. For $SrCuO_2$ we find $\lambda \propto B^{-0.9(3)}$. This result is temperature independent for 5 K$\leq T \leq$ 300 K. Within conformal field theory and using the Müller ansatz we conclude *ballistic* spin transport in $SrCuO_2$.

TT 19: CE: Quantum Impurities, Kondo Physics

Time: Monday 18:45–19:45 Location: HSZ 304

TT 19.1 Mon 18:45 HSZ 304

Phase transitions in the multichannel Anderson model with pseudogap density of states — •Imke Schneider[1], Adel Benlagra[1], Lars Fritz[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, TU Dresden — [2]Institut für Theoretische Physik, Universität zu Köln

We consider a multichannel Anderson model with a pseudogap density of states $\rho(\omega) \propto |\omega|^r$. Using analytical and numerical renormalization group techniques we study the phase diagram and associated observables. In particular, we apply an expansion in the hybridization strength to access the quantum phase transition near $r = 1$. We relate our findings to experimental results on graphene.

TT 19.2 Mon 19:00 HSZ 304

Exact Crossover Green Function In 2-Channel Kondo Effect — •Eran Sela, Andrew Mitchell, and Lars Fritz — Universitaet zu Koeln

The non Fermi liquid critical point of the two-channel Kondo model and related multi impurity models is unstable with respect to symmetry breaking perturbations, which lead to a crossover into Fermi liquid behavior. We use an analogy between this crossover and one occurring in the boundary Ising model to calculate the crossover Green function analytically. In remarkable agreement with our numerical renormalization group calculations, the exact function applies for arbitrary mixture of the relevant perturbations of the critical point such as magnetic field or channel asymmetry, leading to rich behavior which can be observed in quantum dot or tunneling experiments.

TT 19.3 Mon 19:15 HSZ 304

RG analysis of a Spin-1 Kondo dot out of equilibrium — •Christoph Hörig, Sabine Andergassen, and Dirk Schuricht — RWTH Aachen, Germany

We study the spin-1 Kondo dot in a magnetic field and at finite bias voltage by using the real-time renormalization group in frequency space [1].

Based on a systematic expansion in the reservoir-system coupling, we integrate out the reservoir degrees of freedom and solve the resulting two-loop RG equations in the weak-coupling regime. We derive analytic expressions for the dot magnetization and for the current through the dot in the stationary state. We show that any initial spin anisotropy is strongly enhanced by renormalization effects.

Furthermore, we determine the relaxation and decoherence rates governing the time evolution into the stationary state, where an additional rate with respect to the spin-1/2 case emerges [2].

[1] H. Schoeller, Eur. Phys. J. Special Topics 168, 179 (2009).
[2] H. Schoeller and F. Reininghaus, Phys. Rev. B 80, 045117 (2009).

TT 19.4 Mon 19:30 HSZ 304

Molecular DMFT calculations of Co dimers in metal nanocontacts — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06108 Halle, Germany

Using our recently developed Molecular Dynamical Mean-Field Theory method [1,2] we study the electronic structure and transport properties of two Co atoms suspended between the tips of a metal nanocontact. Due to the competition between Kondo screening of the magnetic moments of the two Co atoms by the conduction electrons and the mutual antiferromagnetic coupling between the Co atoms, the spectral density and the concomitant low-bias conductance spectrum strongly changes in dependence of the distance between the two Co atoms.

[1] D. Jacob, K. Haule, and G. Kotliar, Phys. Rev. Lett. **103**, 016803

(2009).
[2] D. Jacob, K. Haule, and G. Kotliar, Phys. Rev. B **82**, 195115 (2010).

TT 20: Focused Session: 50 Years of Flux Quantization

Time: Tuesday 10:30–13:10 Location: HSZ 03

Invited Talk TT 20.1 Tue 10:30 HSZ 03
The discovery of fluxoid quantization: 2e or not 2e — •Dietrich Einzel — Walther-Meißner-Institut, D-85748 Garching

The year 2011 is quite remarkable because it allows us to celebrate not only the centennial of the discovery of superconductivity by Heike Kamerlingh–Onnes in 1911 but also the half–centennial of the discovery of what is referred to as *fluxoid quantization* in superconductors by Robert Doll and Martin Näbauer and, independently, by Bascom S. Deaver Jr. and William Fairbank. The experimental proof of the quantization of magnetic flux (or more accurately fluxoid) in hollow superconducting cylinders actually supports two important theoretical concepts, namely the pairing hypothesis formulated in the BCS theory of superconductivity and the concept of macroscopic phase coherence of the pair condensate. This talk is devoted to a discussion of the physics behind the Doll–Näbauer Deaver–Fairbank discoveries and is intended to review historically the chain of events which motivated these talented experimentalists and which led to their independent discoveries at quite remote points of the earth.

Invited Talk TT 20.2 Tue 11:00 HSZ 03
Fluxoid Quantization and the Superconducting Quantum Interference Device — •John Clarke — University of California, Berkeley CA USA

The observation of fluxoid quantization by Doll and Näbauer and by Deaver and Fairbank in 1961 and the observation of Josephson tunneling by Anderson and Rowell in 1963 laid the foundation for the demonstration by Jaklevic, Lambe, Silver and Mercereau in 1964 of quantum interference between two Josephson junctions interrupting a superconducting loop. Early types of SQUIDs (Superconducting Quantum Interference Devices) are briefly reviewed. Today, most SQUIDs are fabricated from thin films on silicon wafers in a square washer design, and are based on Nb-AlO_x-Nb tunnel junctions. Two applications of SQUIDs are briefly described. The first is the use of a near-quantum-limited SQUID amplifier in a detector to search for the axion, a candidate particle for cold dark matter. This amplifier potentially increases the axion search rate by as much as three orders of magnitude compared with a semiconductor amplifier. The second application is the use of a SQUID to detect the signal in an ultralow field magnetic resonance imaging (ULFMRI) system operating at 5.6 kHz. At this frequency, there is a significantly higher contrast between different tissue types compared with conventional MRI. ULFMRI may have applications in imaging cancer.

10 min. break

Invited Talk TT 20.3 Tue 11:40 HSZ 03
Flux Quantization driving Fractional Flux Quantum Generation — •Hans Hilgenkamp — University of Twente and Leiden University, The Netherlands

The single-valuedness of the superconducting wave function has peculiar consequences in ring structures in which phase-shifting elements are introduced. It namely demands that such phase-shifts are compensated to an integer multiple of 2π, for which the spontaneous generation of a corresponding/complementary fraction of a magnetic flux quantum by the ring is one possible option.

For example, in rings containing an element with a phase-shift of π, a spontaneous flux of a half the regular flux quantum is to be expected as the energetic ground state. This half flux quantum can have either up or down polarity, mimicking in a way the electron spin in a macroscopic structure.

This remarkable effect was key to proving the d-wave symmetry of the high-T_c superconductors, in the famous Tsuei-Kirtley tricrystal ring experiment in the early 1990's.

By connecting high-T_c superconductors with their s-wave low-T_c counterparts it became possible to generate and couple a multitude of fractional flux quanta on a single chip. Similar developments are taking place using other forms of phase-shifters, such as Superconductor-Ferromagnet-Superconductor Josephson junctions. Besides for basic studies, such spontaneous-flux generating structures have proven to be of interest as new building blocks for superconducting (quantum)-electronics.

Invited Talk TT 20.4 Tue 12:10 HSZ 03
Quantum information with quantized fluxoids: flux qubits — •Johan E. Mooij — Kavli Institute of Nanoscience, Delft University of Technology

A closed superconducting ring which contains one or more Josephson junctions can exist in a quantum superposition of two states with different fluxoid number, when it is biased near half a flux quantum. The ring behaves as a two-level system and can be manipulated with microwave pulses. With three or four junctions in the ring, the size can be as small as several micrometers. The level splitting can be tuned with the applied magnetic flux, in addition one of the junctions can be converted into a SQUID leading to tunable quantum coupling between the fluxoid states . Relative to other types of superconducting quantum bits, flux qubits have the advantage that the next-higher level is separated by a high energy. Quantum operations can be performed in nanoseconds, coherence times go up to microseconds. Readout is performed with a SQUID that senses the generated flux of order 0.001 flux quantum. Inductive coupling between qubits is typically h times 200 MHz, allowing the realization of quantum entanglement. With flux qubits it is possible to achieve ultrastrong coupling between a two-level system and a harmonic oscillator.

Invited Talk TT 20.5 Tue 12:40 HSZ 03
Flux quantization and the quantum Hall effect — •Klaus von Klitzing — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart

The combination of electrons with flux quanta is an important ingredient for discussions of phenomena related to quantum Hall physics. Especially the introduction of composite fermions (an electron accompanied by an even number of fluxes) is very successful in discussing the fractional quantum Hall effect on the basis of the integer quantum Hall effect. The talk summarizes experimental phenomena in quantum Hall physics where the flux quantization plays an important role.

TT 21: TR: Nanoelectronics III - Molecular Electronics 2

Time: Tuesday 10:30–13:00 Location: HSZ 301

TT 21.1 Tue 10:30 HSZ 301
Spatio-Temporal description of Quantum Transport — •Björn Oetzel[1,2], Friedhelm Bechstedt[1,2], and Karsten Hannewald[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]European Theoretical Spectroscopy Facility, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

We present a numerical method for the calculation of time-dependent transport properties of non-periodic systems connected to electron reservoirs. The approach is based on the solution of the time-dependent Schrödinger equation combined with the emitting boundary conditions using plane waves as modeling of the leads.

Using the approach we are able to simulate the temporal evolution of wave packets through potential barriers. Within the quasi-stationary limit the method can be associated with the Landauer Formalism.

Transmission functions are calculated directly from the transmitted and reflected currents for the insertion of a single plane wave. Beyond the calculation of transmission functions the approach is also capable of field-dependent transport properties such as current voltage characteristics. Those can be calculated independently of the transmission functions including by direct treatment of time-dependent potentials and electrical fields, in contrast to the Landauer approach. The success of the method is demonstrated by 1D-model calculations for single and double barriers including modifications due to applied electrical fields.

TT 21.2 Tue 10:45 HSZ 301

Highly controllable fabrication of horizontally aligned single walled carbon nanotubes — •Imad Ibrahim[1,2], Alicja Bachmatiuk[2], Jan Blüher[1], Felix Börrnert[2], Mark H. Rümmeli[2,3], Bernd Büchner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, TU-Dresden, 01062 Dresden, Germany — [2]Institute for Solid State Research, IFW Dresden, 01171 Dresden, Germany — [3]Department of Physics, TU-Dresden, 01062 Dresden, Germany

Single-walled carbon nanotubes (SWCNTs) are considered a promising material for future nanoelectronics because of their excellent electronic and physical properties. Their electronic properties strongly depend on their diameter and chiral angle. SWCNTs are divided into metallic and semiconductor SWCNTs. High yield semiconductor horizontally well-aligned SWCNT are essential for molecular electronics applications, in which one needs to fabricate parallel active devices, such as diodes and transistors. In this study, well-defined protocols have been developed for growing horizontally well-aligned carbon nanotubes in high yield via chemical vapor deposition. The developed route provides a high degree of control of various aspects, such as the tube length, yield, quality and the alignment of the tubes. The as-grown CNT are characterized with different techniques; scanning electron microscopy, atomic force microscopy, Raman spectroscopy and transmission electron microscopy.

TT 21.3 Tue 11:00 HSZ 301

Interference and transport through π-conjugated molecules in an STM set-up — •Sandra Kolmeder, Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We develop a general STM transport theory for π-conjugated molecules, based on the density matrix formalism. The focus is on STM experiments which measure electronic properties of individual molecules deposited on ultra-thin insulating films on metal substrates, where the insulating film allows to electronically decouple the molecule from the metallic 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. Applied to a benzene molecule we find that angular momentum conservation rules allow to express the STM tunneling current in terms of few relevant "angular momentum channels". In the tunneling the molecule changes free energy F and angular momentum l. In turn the tunneling rate changes of several orders of magnitude depending on ΔF and Δl. We will show that current blocking occurs as an interference effect, because of involved orbitally degenerate states.

TT 21.4 Tue 11:15 HSZ 301

Electron transport through π-conjugated molecules anchored via carboxilate groups to Cu(110) electrodes — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Nowadays, carboxilate-Cu bonds[1] are recognized as an alternative to the thiolate-Au bonds to be used in future molecular electronic devices. As a consequence, a clear understanding of the electron transport properties is highly desirable and, in particular, *ab initio* simulations are used to elucidate and design the functionality of specific molecules in a given organic-metal electrode environment.

Here we report on the transmission properties of three aromatic molecules anchored via carboxyliate groups to the Cu(110) electrodes. In our approach, the scattering wave functions are computed by solving the Lippmann-Schwinger equation.

While thiolate-Au systems show both sharp and broad transmissions peaks, the electron transmissions of the aromatic carboxilates-Cu molecular systems exhibit only sharp peaks. This implies that the molecular system with carboxilate-Cu bonds are more sensitive to change in bias voltage as compared to that with thiolate-Au ones. Furthermore, we demonstrate that the switching property of the molecules can be locally controlled by replacing a CH group of the aromatic ring with an N atom since the transmissions peaks are shifted to lower energies keeping the peak-peak distance.

[1] M. C. Lennartz *et al.*, Langmuir, **25**, 856 (2009).

TT 21.5 Tue 11:30 HSZ 301

Conformational changes in biphenyl under applied voltage — •Lars Kecke and Joachim Ankerhold — Institut für theoretische Physik, Universität Ulm

The usual way to calculate the transmission of a molecule is to calculate the transmission matrix of an isolated molecule and then to add the leads. We show that, especially in case of molecules with intrinsic switching probabilities, this procedure leads to massively incorrect conductivities. We have used a Born-Oppenheimer-like master-equation approach to calculate the energy profile of the torsional degree of freedom in a molecule of biphenyl in the presence of two electrodes and found the torsional angle snapping from a roughly 45-degree position at low voltage to zero, accompied by a quantization of current, in a pattern reminiscent of Coulomb diamonds.

15 min. break

TT 21.6 Tue 12:00 HSZ 301

Coherent transport and the effects of strong correlations in cobalt-benzene sandwich molecules — •Michael Karolak[1], David Jacob[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We study the impact of dynamical correlations on the electronic structure and coherent transport properties of cobalt-benzene sandwich molecules (see e.g. [1]) hosted in a copper nanocontact. The interactions of the Co 3d electrons are fully taken into account by combining density functional calculations with a dynamical treatment of the strong correlations in the Co 3d shell in the one-crossing approximation [2]. We find that depending on the geometry of the contact region the hybridization of the Co 3d shell with the benzene ring states and dynamical correlations give rise to the Kondo effect and thus lead to Fano-like features in the coherent transport characteristics.

[1] T. Kurikawa et al. J. Phys. Chem. 99, 16248 (1995)
[2] D. Jacob et al. Phys. Rev. Lett. 103, 016803 (2009)

TT 21.7 Tue 12:15 HSZ 301

Ab initio Anderson-Hubbard model of molecular junctions — •Dmitry Ryndyk and Klaus Richter — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Electron-electron interaction plays an important role in transport through single-molecule junctions, controlling a position of resonant levels and leading to Coulomb blockade and Kondo effect in the case of weak coupling to the leads. The methods of many-body theory are necessary to explain nonequilibrium correlation effects. On the other hand ab initio approach is required to take into account realistic geometry and electronic structure of molecular junctions. The task of modern theory is to combine ab initio and many-body quantum transport methods. We developed a theoretical approach to describe single-molecule junctions in terms of Anderson-Hubbard Hamiltonian in the basis of localized molecular orbitals. The matrix elements of the effective Hamiltonian are calculated by GAMESS and Firefly (former PC GAMESS) quantum chemistry codes. The transport at finite voltage is described in the framework of nonequilibrium Green function or generalized master equation approaches. The systems, to which we apply the method, include oligophenyl (benzene, biphenyl, terphenyl an other) junctions and metal-phtalocyanines.

TT 21.8 Tue 12:30 HSZ 301

How Vibrations Generate Electrical Current: Decoherence in Single-Molecule Junctions — •Rainer Härtle, Michael Butzin, and Michael Thoss — Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Employing a nonequilibrium Green's function approach [1,2], we analyze quantum interference effects and decoherence mechanisms in single-molecule junctions. Quantum interference effects have been found to be of importance in coherent electron transport for different

types of nanostructures [3,4], in particular for single-molecule junctions [5]. These effects may result in a suppression of the electrical current due to destructive interference. In the presence of electronic-vibrational coupling, however, this suppression may not fully develop or completely disappears, especially if the vibrational degrees of freedom are highly excited. This is demonstrated for a generic model system and for a realistic model of a biphenyl-acetylene-dithiolate molecular junction, where strong dephasing results from a multitude of vibrational modes. The currents are significantly larger than without electronic-vibrational coupling. In other words, vibrations generate electrical current by quenching of desctructive interference.

[1] R. Härtle *et al.*, Phys. Rev. B 77, 205314 (2008).
[2] R. Härtle *et al.*, Phys. Rev. Lett. 102, 146801 (2009).
[3] B. Kubala, J. König, Phys. Rev. B 65, 245301 (2002).
[4] A. Donarini *et al.*, Phys. Rev. B 82, 125451 (2010).
[5] G. C. Solomon *et al.*, Nano Lett. 6, 2431 (2006).

TT 21.9 Tue 12:45 HSZ 301

Vibration-assisted tunneling through a molecular level with competing phonon modes — •Federica Haupt[1,2], Johannes Buelte[1], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52074 Aachen, Germany

We investigate the electronic transport properties of a single electronic level weakly coupled to leads and interacting with two different phonon modes. We consider the interplay between the two phonon modes under the assumption that tunneling induces a non–equilibrium vibrational distribution and compare to the opposite limit of strong relaxation of the vibrations due to some dissipative environment. We show that in the presence of non–equilibrium the tunneling electrons mediate an effective interaction between the two phonon modes. This results in characteristic features in the transport properties of the device such as sub-threshold excitation of one phonon mode and the appearance of negative differential conductance in a wide range of parameters.

TT 22: CE: Low-dimensional Systems - Materials 2

Time: Tuesday 10:30–13:00 Location: HSZ 304

TT 22.1 Tue 10:30 HSZ 304

Peculiar high-field quantum magnetism in the frustrated s = 1/2 spin chain cuprate linarite — •M. Schäpers[1], A. U. B. Wolter[1], S.-L. Drechsler[1], S. Nishimoto[1], Y Skourski[2], M. Uhlarz[2], M. Schmitt[3], H. Rosner[3], K. C. Rule[4], S. Süllow[5], G. Heide[6], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]MPI-CPfS, Dresden, Germany — [4]HZB für Materialien und Energie, Berlin, Germany — [5]IPKM, TU Braunschweig, Braunschweig, Germany — [6]TU Bergakademie Freiberg, Freiberg, Germany

We present an experimental and theoretical study of the quasi-one-dimensional s = 1/2 Heisenberg magnet linarite $PbCuSO_4(OH)_2$, with competing ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions. It includes magnetization and NMR studies as well as theoretical simulations for the determination of the leading exchange couplings, which are about an order of magnitude higher as determined previously.[1] Furthermore, a manifold of field-induced phases are probed, from which we draw a preliminary phase diagram. Notably, spin-lattice relaxation investigations indicate that linarite might undergo a magnetic quadrupolar spin liquid phase transition as recently predicted for such materials.[2]

[1] M. Baran, et al., Phys. Stat. Sol. (c) 3, 220 (2006).
[2] M. Sato, T. Momoi, A. Furusaki, Phys. Rev. B 79, 060406(R) (2009).

TT 22.2 Tue 10:45 HSZ 304

Magnetism in the Diamond Spin Chain Azurite — •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, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Institute for Solid State Research, IFW, D-01069 Dresden, Germany — [3]Physikalisches Institut, J.W. Goethe Universität, D-60438 Frankfurt (Main), Germany — [4]SμS, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Azurite is a mineral, which has been proposed as a model substance for a 1D spin-$\frac{1}{2}$-Heisenberg-diamond-chain. Specific heat [1] indicated a magnetic phase transition at 1.8K, where the coupling between the 1D Cu-chains sets in. At 0.5K indications of another phase transition, with yet unknown nature, were observed [3]. Due to the small magnetic moments and the complex structure of azurite, the magnetic ground state is yet not well understood.
We performed μSR measurements at PSI on a single crystal and a powdered sample, in extension of already published μSR-data [4]. Our measurements revealed a critical behaviour of the transversal damping approaching T_c as well as clear evidence of static magnetic order below T_c. The phase transition at 0.5K is observable as well, and can be related to an alteration in the local environment of the Cu^{2+} monomers.

[1] H. Kikuchi et al., Phys. Rev. Lett. 94, 227201 (2005).
[2] B. Gu and G. Su, Phys. Rev. Lett. 97, 089701 (2006).
[3] P.T. Cong et al., J. Phys.: Conf. Ser. 200, (2010).
[4] M.C.R. Gibson et al., Phys. Rev. B 81, 140406 (2010).

TT 22.3 Tue 11:00 HSZ 304

Magnetic coupling and dynamics in the 1D quantum magnet azurite $Cu_3(CO_3)_2(OH)_2$ as determined from inelastic neutron scattering. — •Kirrily Rule[1], Alan Tennant[1,2], Mark Telling[3], Sebastian Gerischer[1], Stefan Suellow[4], and Michael Lang[5] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut fuer Festkoerperphysik, TU Berlin, Berlin, Germany — [3]ISIS, Rutherford Appleton Laboratories, Chilton, UK — [4]Institut fuer Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [5]Goethe Universitat, Frankfurt(M), SFB/TR 49, Germany

Low dimensional magnetic systems, in particular, copper oxides are interesting subjects of study due to the novel physics that can arise in such systems at low temperatures. Both a natural mineral and quantum magnet, $Cu_3(CO_3)_2(OH)_2$ is a candidate model of the so-called Distorted Diamond Chain system. Early studies of this material imply the presence of an ordered antiferromagnetic phase below $T_N \sim 1.9$ K while magnetization measurements have revealed a 1/3 magnetization plateau. Most recently the interactions and magnetic exchange couplings have been hotly debated. We will present our analysis of the inelastic neutron scattering data, highlighting the temperature and field dependence of the low energy spin chain excitations. We will also reveal information about the as yet unseen higher energy magnetic excitations. Finally we would like to consolidate this data by presenting a model to describe this intriguing 1D quantum magnet.

TT 22.4 Tue 11:15 HSZ 304

Distinct magnetic regimes through site-selective atom substitution in the frustrated quantum antiferromagnet $Cs_2CuCl_{4-x}Br_x$ — •Bernd Wolf[1], Pham Thang Cong[1], Mariano de Souza[1], Natalie Krüger[1], Amir Haghighirad[1], Franz Ritter[1], Wolf Assmus[1], Ingo Opahle[2], Kataryna Foyevtsova[2], Roser Valentí[2], Harald Jeschke[2], Leonore Wiehl[3], and Michael Lang[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt — [2]Institut für theoretische Physik, Goethe Universität Frankfurt — [3]Institut für Geowissenschaften, Goethe Universität Frankfurt

We report on a systematic study of the magnetic properties on single crystals of the solid solution $Cs_2CuCl_{4-x}Br_x$ ($0 \leq x \leq 4$), which include the two known end-member compounds Cs_2CuCl_4 and Cs_2CuBr_4, classified as quasi-two-dimensional quantum antiferromagnets with different degrees of magnetic frustration. By comparative measurements of the magnetic susceptibility $\chi(T)$ on as many as eighteen different Br concentrations, we found that the in-plane and out-of-plane magnetic correlations do not show a smooth variation with x. Rather three distinct concentration regimes can be identified, which are separated by critical concentrations $x_{c1} = 1$ and $x_{c1} = 2$. This unusual magnetic behavior can be explained by considering the structural peculiarities of the materials, especially the distorted Cu-halide tetrahedra, which support a site-selective replacement of Cl^- by Br^- ions.

TT 22.5 Tue 11:30 HSZ 304

Ultrasonic investigation in the vicinity of the quantum-critical point in Cs_2CuCl_4 — •P. T. Cong, B. Wolf, S. Belz, N. Krüger, F. Ritter, W. Assmuss, and M. Lang — Physikalisches Institut, Goethe Universität-Frankfurt, SFB/TR 49, D-60438 Frankfurt(M)

The insulator Cs_2CuCl_4 is a quasi-two-dimensional triangular lattice (*bc* plane) spin-1/2 antiferromagnet (AFM) with a weak interlayer coupling. This material has been considered as one of the prime example for studying the phenomenon of Bose-Einstein condensation (BEC) of magnetic excitations [1]. The long-range antiferromagnetic order ($T_N = 0.6$ K at B = 0) 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). Anomalous physical properties at finite temperature are expected to be observed at B_c due to quantum-critical fluctuations. Here we present a detailed investigation of the elastic constants c_{11}, c_{22} and c_{33} together with the 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. At low temperature and around B_c, the ultrasonic attenuation of the all three modes exhibits a pronounced double peak structures, indicating two anomalies of different origin. While one of them is very sharp, strongly temperature dependent and coinciding with $T_N(B)$, the other one is distinctly broader and located at slightly higher fields. Upon cooling both features merge and extrapolate to $B_c \sim 8.5$ T for $T \to 0$.

[1] T. Radu *et al.*, Phys. Rev. Lett. **95**, 127202 (2005).

15 min. break

TT 22.6 Tue 12:00 HSZ 304

Spin-spin correlation of the spin-1/2 Heisenberg-chain compound CuPzN measured by magnetostriction — •Jens Rohrkamp[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

The spin-1/2 Heisenberg chain is one of the rare examples of quantum-spin Hamiltonians, which can be solved analytically exact. An experimental realization of this Hamiltonian is found in copper pyrazine dinitrate $Cu(C_4H_4N_2)(NO_3)_2$ (or CuPzN). The weak coupling constant $J \approx 10$ K in this compound leads to a critical magnetic field of about 14 T, which is accessible in typical superconducting laboratory magnets. At this field the system undergoes a quantum phase transition from the gapless Luttinger-liquid state to the fully saturated state with a finite excitation gap. As recently shown in [1] the field- and temperature-induced length changes are proportional to the spin-spin correlation function $\langle S_i S_j \rangle$. We present high-resolution measurements of thermal expansion and magnetostriction and compare these to calculations performed via Bethe ansatz.

[1] Anfuso *et al.* PRB **77**, 235113 (2008)

This work was supported by the DFG through SFB 608.

TT 22.7 Tue 12:15 HSZ 304

Competing ground states in a novel Ni based hybrid $S = 1$ chain investigated with Electron spin resonance spectroscopy — •F. Lipps[1], H. Maeter[2], A. H. Arkenbout[3], H. Luetkens[4], G. Pascua[4], Z. Shermadini[4], T.T.M. Palstra[3], H.-H. Klauss[2], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Zernike Institute, University of Groningen, The Netherlands — [4]PSI, Villigen, Switzerland

A new hybrid material that comprises arrays of one dimensional (1D) chains of $NiCl_6$ octahedra separated by a framework of organic molecules is investigated with different methods. The $Ni^{2+}(3d^8)$ ions in the $NiCl_6$ chain possess an integer spin $S = 1$. The temperature dependence of the static susceptibility shows a broad maximum suggesting an AFM coupling with a nearest neighbour exchange constant around 25 K. The ESR signal consists of a single lorentzian line at a g-factor of 2.2 typical for Ni^{2+}. The ESR spectrum is isotropic proofing the absence of a single ion anisotropy. This indicates a good realization of the Haldane conjecture which predicts a non-magnetic ground state for an isotropic AFM Heisenberg $S = 1$ chain and a gapped spin excitation spectrum. In contrast to this, a magnetic ordering is observed at temperatures below 10 K with ESR and μsr. In the low temperature regime the static susceptibility and ESR measurements reveal an anisotropic behaviour for the magnetic field applied along and perpendicular to the chain. We discuss a possible ground state and spin dynamics of the studied compound.

TT 22.8 Tue 12:30 HSZ 304

Nature of electronic correlations in strongly doped Na_xCoO_2 — •Christoph Piefke[1], Lewin Boehnke[1], Antoine Georges[2], and Frank Lechermann[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]CPHT, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France

With the combination of the rotationally invariant slave-boson mean-field theory (RISB) [1,2] and the local-density approximation (LDA) to density functional theory, the phase diagram of layered sodium cobaltate Na_xCoO_2 is investigated in the high-doping regime close to zero temperature [3]. This system represents one of the rare natural examples of a dopable strongly correlated triangular lattice. Utilizing a tailored realistic single-band approach in a cellular-cluster framework, we investigate the effect of electronic correlations with doping until the band-insulating (x=1) limit. The experimentally verified [4] in-plane crossover from antiferromagnetic tendencies at low x towards ferromagnetic order for x>0.75 is revealed with an on-site Hubbard interaction. Relevant charge-ordering physics in the system is modelled via an additional inter-site Coulomb interaction V on an effective kagomé lattice, as observed in experiment [5].

[1] T. Li *et al.*, PRB **40**, 6817 (1989).
[2] F. Lechermann *et al.*, PRB **76**, 155102 (2007).
[3] C. Piefke *et al.*, PRB **82**, 165118 (2010).
[4] G. Lang *et al.*, PRB **78**, 155116 (2008).
[5] H. Alloul *et al.*, EPL **85**, 47006 (2009).

TT 22.9 Tue 12:45 HSZ 304

Implications of Choosing the Local Coordinate Frame for the Understanding of Magnetism in Highly Anisotropic Co^{II} Clusters — •Joscha Nehrkorn[1], Sven Pfirrmann[2], Yanhua Lan[2], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut für anorganische Chemie, Universität Karlsruhe, KIT, Germany

Molecular nanomagnets containing Co^{II} ions are currently of much interest, because they provide large magnetic anisotropy and hence potentially superior magnetic properties. However, only relatively few examples can be found in the literature, which might be due to the complications in describing the magnetic properties of such clusters.

Here we report our studies of the magnetic properties in a polynuclear $Co_2^{III}Co_6^{II}$ complex. An effective low-temperature model reproduces excellently our magnetic data at the lowest temperatures and the general trend at higher temperatures. However, the derived exchange parameters are maximally anisotropic, while the energy spectrum is typical for the strong exchange limit, in which anisotropy is weak. This will be explained by noting the implications of the freedom to choose the local coordinate frame at will. The consequences thereof, which are potentially of general interest, will be discussed.

TT 23: CE: Quantum-Critical Phenomena 2

Time: Tuesday 10:30–13:00 Location: HSZ 105

TT 23.1 Tue 10:30 HSZ 105

Electrical transport properties of single-crystal $Nb_{1-y}Fe_{2+y}$ — •Max Hirschberger[1,2], William Duncan[3], Andreas Neubauer[2], Manuel Brando[4], Christian Pfleiderer[2], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Physik-Department E21, Technische Universität München, Garching, Germany — [3]Department of Physics, Royal Holloway, University of London, Egham, UK — [4]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

The Laves phase system $Nb_{1-y}Fe_{2+y}$ displays a marginal Fermi liquid breakdown close to the critical composition $y_c = -0.015$ [1]. For $y > -0.015$ various bulk properties suggest the formation of hitherto unidentified electronic order at low temperatures akin a spin-density-

wave (SDW) state. We have grown large single crystals of $Nb_{1-y}Fe_{2+y}$ by means of a bespoke image furnace. We present a study of the electrical transport properties of single-crystal $Nb_{1-y}Fe_{2+y}$ for three different compositions y and for a wide range of field orientations. All samples display strong anisotropy of the magnetoresistance between fields along the magnetically easy c-axis and the magnetically hard ab-plane. In a slightly iron-rich sample ($y = 0.006$) we observed a pronounced peak in the magnetoresistance for magnetic fields perpendicular to the c-axis in a temperature range from 10 to 30 K. We discuss possible explanations for this behaviour, such as the emergence of complex magnetic textures near the border of ferromagnetic quantum criticality.

[1] M. Brando et al, Phys. Rev. Lett. **101**, 026401 (2008); D. Moroni-Klementowicz et al., Phys. Rev. B **79**, 224410 (2009).

TT 23.2 Tue 10:45 HSZ 105

Uniform lattice distortion in the nematic phase of $Sr_3Ru_2O_7$ — •Christian Stingl and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen

In the itinerant metamagnet $Sr_3Ru_2O_7$, a first order metamagnetic transition is suppressed to a quantum critical end point (QCEP) at $T = 0$ by applying a magnetic field $\mu_0 H_c = 7.85$ T along the c-axis. Quantum critical behaviour is observed in thermal expansion and can be explained in terms of 2d ferromagnetic fluctuations [1].

Below 1 K, a new phase with a strongly enhanced residual resistivity forms in the vicinity of the QCEP. When H has a small in-plane component, the resistivity becomes anisotropic, which is discussed in terms of formation of an electronic nematic fluid organized into domains [2].

We present in-plane thermal expansion and magnetostriction measurements obtained by high-resolution capacitive dilatometry. Our findings suggest that inside the nematic phase, the four-fold symmetry is broken by a uniform lattice distortion with $\Delta L/L$ of the order of 10^{-6}. The results are discussed in the context of a recent model [3] for domain formation via partial orbital ordering.

This work is in collaboration with F. Weickert, R. Küchler, R.S. Perry and Y. Maeno and supported by the DFG through SFB602.

[1] P. Gegenwart et al., PRL **96**, 136402 (2006)
[2] R.A. Borzi et al., Science **315**, 214-217 (2007)
[3] W.-C. Lee and C. Wu, arXiv:1008.2486

TT 23.3 Tue 11:00 HSZ 105

Short range magnetic order close to a ferromagnetic quantum critical point in CeFePO — •Stefan Lausberg, Anton Jesche, Cornelius Krellner, Alexander Steppke, Luis Pedrero, Manuel Brando, Christoph Geibel, and Frank Steglich — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The compound $CeFeAs_{1-x}P_xO$ combines strong 3d and 4f correlation effects. At $x = 0$ two antiferromagnetic (AFM) transitions were found. Iron orders at $T_{N,Fe} = 145$ K and cerium at $T_{N,Ce} = 3.7$ K. Increasing the chemical pressure by phosphorus substitution leaves $T_{N,Ce}$ almost unaffected while it shifts $T_{N,Fe}$ towards lower temperatures until it vanishes above $x = 0.35$. Further increasing phosphorus content induces ferromagnetic (FM) order of cerium at $T_c \approx 9$ K which is believed to suppress a superconducting state found in other iron pnictides when the iron AFM disappears. For $x \geq 0.6$, T_c decreases and finally vanishes in CeFePO which was reported to be a paramagnetic heavy fermion system close to a FM instability. However, tiny differences in sample preparation lead to the onset of short range magnetic order.

In this contribution we present low-temperature magnetization, specific heat and ac-susceptibility measurements of a polycrystaline CeFePO sample. The ac-susceptibility shows a peak at $T_f = 620$ mK which shifts towards higher temperatures by increasing the measuring frequency. We compare our results with the Kondo cluster glass $CePd_{1-x}Rh_x$ and discuss its properties in the frame of the quantum Griffiths phase scenario.

TT 23.4 Tue 11:15 HSZ 105

Thermodynamics of the spin-dimer $NiCl_2$-4SC$(NH_2)_2$ system at the magnetic-field-induced quantum phase transition — •Alexander Steppke[1], Robert Kuechler[1], Luis Pedrero[1], Manuel Brando[1], Armando Paduan-Filho[2], Christian Batista[3], Franziska Weickert[3], Vivien Zapf[3], Marcelo Jaime[3], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil — [3]Los Alamos National Laboratory, Los Alamos, USA

The concept of universality class in magnetic systems undergoing a quantum phase transition (QPT) can be tested in so-called quantum magnets, where the local spins are coupled forming ladders ($TlCuCl_3$), planes of dimers ($BaCuSi_2O_6$) or weakly coupled chains of $S = 1$ Ni atoms, as in the organic system $NiCl_2$-4SC$(NH_2)_2$ (DTN). In DTN the Ni^{2+} single ion anisotropy $D = 8.9$ K opens an energy gap between the $S_z = 0$ ground state and the $S_z = \pm 1$ first excited state. At a magnetic field $Hc_1 \approx 2$ T the gap closes and a transition into an XY-antiferromagnetic ordered state is induced at low temperatures. Such a QPT belongs to the $d = 3$ and $z = 2$ universality class and the following theoretical laws are predicted: The magnetization $M \propto T^{d/z}$, the phase boundary line $(H - Hc_1) \propto T_c^{d/z}$, the thermal and magnetic Grüneisen ratios are expected to follow T^{-1}. We have investigated the temperature and field dependences of all these thermodynamic quantities in the temperature range $0.05 \leq T \leq 5$ K.

TT 23.5 Tue 11:30 HSZ 105

Spinon continuum and the ground state of the quantum kagome system — •Dirk Wulferding[1], Peter Lemmens[1], Shaoyan Chu[2], Tianheng Han[2], Young S. Lee[2], Yoshihiko Okamoto[3], Hiroyuki Yoshida[4], Zenji Hiroi[3], and Reizo Kato[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]MIT, Massachusetts, USA — [3]ISSP, Tokyo, Japan — [4]NIMS, Tsukuba, Japan — [5]IPCR, Riken, Japan

We present a temperature dependent Raman study on different kagome lattice systems. At low temperatures, volborthite shows signs of structural distortions, while in the vesignieite spectra a low energy excitation appears that could be assigned to an emergent magnetic mode. We compare our results to the kagome model system herbertsmithite and discuss the effects of antisite disorder and lattice distortions.

Work supported by DFG, IGSM and NTH.

15 min. break

TT 23.6 Tue 12:00 HSZ 105

Electron self-energy near a nematic quantum critical point — •Markus Garst[1] and Andrey V. Chubukov[2] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — [2]Department of Physics, University of Wisconsin, Madison, 1150 University Avenue, Madison, Wisconsin 53706-1390, USA

We consider an isotropic Fermi liquid in two dimensions near a nematic instability in the charge channel [1]. Previous studies have found that such a system exhibits multiscale quantum criticality with two different energy scales associated with the different dynamics of the two polarization of the nematic order parameter [2]. We study the impact of the multiple energy scales on the electron Green's function. Apart from the common singular local self-energy of non-Fermi liquid form, we also find a logarithmically singular renormalizations of the quasiparticle residue Z and the vertex Γ. We derive and solve renormalization-group equations for the flow of Z and Γ , and show that the system develops an anomalous dimension at the nematic quantum critical point. As a result, the spectral function at a fixed ω and varying k has a non-Lorentzian form.

[1] M. Garst and A. V. Chubukov, Phys. Rev. B 81, 235105 (2010)
[2] M. Zacharias. P. Wölfle, and M. Garst, Phys. Rev. B 80, 165116 (2009)

TT 23.7 Tue 12:15 HSZ 105

Compressible Quantum Critical Metamagnetism — •Mario Zacharias[1], Indranil Paul[2], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institut Neel, CNRS/UJF, 25 avenue des Martyrs, BP 166, 38042 Grenoble, France

The coupling of critical fluctuations to the crystal lattice results in unusual dilatometric phenomena close to quantum phase transitions like, e.g., a diverging Grüneisen parameter. In certain cases, however, strong critical fluctuations are generically able to induce a distortion of the crystal lattice such that the quantum critical point gets preempted by a first-order structural transition. We argue that this applies for quantum critical metamagnetism as discussed in the context of $Sr_3Ru_2O_7$ and $CeRu_2Si_2$. Within an effective Ginzburg-Landau theory for itinerant quantum critical metamagnetism we discuss the resulting phase diagram and the experimental consequences.

TT 23.8 Tue 12:30 HSZ 105

Field-induced gap in a quantum spin-$\frac{1}{2}$ chain in a strong

magnetic field — •M. Ozerov[1], J. Wosnitza[1], E. Čižmár[2], R. Feyerherm[3], S.R. Manmana[4,5], F. Mila[5], and S.A. Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Dresden, Deutschland. — [2]Centre of Low Temperature Physics, P.J. Šafárik University, Košice, Slovakia. — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany. — [4]JILA, Department of Physics, University of Colorado, Boulder, Colorado, USA. — [5]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.

Magnetic excitations in copper pyrimidine dinitrate, a spin-$\frac{1}{2}$ antiferromagnetic chain with alternating g-tensor and Dzyaloshinskii-Moriya interaction, that exhibits a field-induced spin gap, are probed by means of pulsed-field electron spin resonance spectroscopy. In particular, we report on a minimum of the gap in the vicinity of the saturation field $B_{sat} = 48.5$ T associated with a transition from the sine-Gordon region (with soliton-breather elementary excitations) to a fully spin-polarized state (with magnon excitations). This interpretation is fully confirmed by quantitative the agreement with DMRG calculations for a spin-$\frac{1}{2}$ Heisenberg chain with staggered transverse field.

Part of this work has been supported by EuroMagNET under the EU contract N.228043.

TT 23.9 Tue 12:45 HSZ 105

Quantum phase transition in the paired spin-boson model — •André Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, Campus, 66123 Saarbrücken

We study the quantum phase transitions occurring in a system of two two-level degrees of freedom (e.g. spin-1/2) each coupled to a bath of oscillators, denoted as the paired spin-boson model. Even in the absence of a direct interaction between the two spin-1/2s the dissipative bath establishes an effective interaction causing both mutual coherence effects and disspation. We perform large scale quantum Monte Carlo simulations based on a cluster algorithm in continuous imaginary time, which we applied already successfully to the single spin-boson model [1], to determine the phase diagram in the Ohmic and sub-Ohmic regime and use finite temperature scaling to determine the critical exponents. The extension to multiple spin-1/2 degrees of freedom and an infinite spin-1/2-chain coupled to a single dissipative bosonic bath are discussed.

[1] A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. 102, 030601 (2009)

TT 24: Multiferroics III (jointly with DF, DS, KR, MA)

Time: Tuesday 10:15–10:45 Location: HSZ 04

Invited Talk TT 24.1 Tue 10:15 HSZ 04

Search for a permanent electric dipole moment of an electron: Multiferroics bring us a step closer — •Marjana Ležaić — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

Although it is conjectured that the Big Bang created equal amounts of matter and antimatter, the Universe that we know consists only of matter. It is not yet clear why the Nature treats matter and antimatter in a different way. One possibility that is being intensively explored lies in the existence of a permanent electric dipole moment (EDM) of an electron. Electron's EDM would violate time-reversal symmetry leading to charge-parity symmetry violation and as a consequence, would act as a source of the matter-antimatter asymmetry. The talk will present a multidisciplinary study [1] including theoretical solid state design, consequent synthesis and characterization of a multiferroic material, (Eu,Ba)TiO_3, with characteristics optimized for a search for electron's EDM.

[1] K. Z. Rushchanskii, S. Kamba, V. Goian, P. Vaněk, M. Savinov, J. Prokleška, D. Nuzhnyy, K. Knížek, F. Laufek, S. Eckel, S. K. Lamoreaux, A. O. Sushkov, M. Ležaić and N. A. Spaldin, Nature Mater. **9** 649 (2010).

TT 25: Multiferroics IV (jointly with DF, DS, KR, MA)

Time: Tuesday 10:45–12:15 Location: HSZ 04

TT 25.1 Tue 10:45 HSZ 04

Polarization and magnetization dynamics of a field-driven multiferroic structure — •Alexander Sukhov[1], Chenglong Jia[1], Paul P. Horley[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle/Saale, Germany — [2]Centro de Investigation en Materiales Avanzados, S.C. (CIMAV), 31109 Chihuahua, Mexico

A multiferroic chain with a linear magnetoelectric coupling induced by electrostatic screening at the ferroelectric/ferromagnet interface [1] is considered. We study theoretically the dynamic ferroelectric and magnetic response to external magnetic and electric fields by utilizing an approach based on coupled Landau-Khalatnikov and finite-temperature Landau-Lifshitz-Gilbert equations. Additionally, we make comparisons with Monte Carlo calculations. It is demonstrated [2] that for material parameters corresponding to $BaTiO_3$/Fe the polarization and the magnetization are controllable by oscillating external magnetic and electric fields, respectively.

[1] T. Cai, S. Ju, J. Lee, N. Sai, A.A. Demkow, Q. Niu, Z. Li, J. Shi and E. Wang, Phys. Rev. B **80**, 140415(R) (2009). [2] A. Sukhov, C.L. Jia, P.P. Horley and J. Berakdar, J. Phys.: Condens. Matter **22**, 352201 (2010).

TT 25.2 Tue 11:00 HSZ 04

Rare-earth induced magnetoelectric effect in multiferroic $TbMn_2O_5$ — •Naëmi Leo[1], Dennis Meier[2], Roman V. Pisarev[3], Sang-Wook Cheong[4], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]UC Berkeley, USA — [3]Ioffe Institute, St. Petersburg — [4]Rutgers University, USA

The presence of magnetic frustration and multi-dimensional magnetic order parameters leads to remarkable effects like magnetically induced ferroelectricity. Such a particularly interesting compound is $TbMn_2O_5$ due to the associated magnetic-field controllable electric polarization. The gigantic magnetoelectric coupling originates in the presence of three independent ferroelectric contributions, which can be separatedly accessed by optical second harmonic generation (SHG). Two of these contributions are related to the manganese Mn^{3+} and Mn^{4+} magnetism. The third one is attributed to the spin arrangement of the Tb^{3+} sublattice which also mediates the intricate field-dependent cross-coupling. We confirm this model by measurements taken on isostructural YMn_2O_5 with non-magnetic Y^{3+} ions.

Also we perform spatially resolved domain topography to show that the magnetic-field induced polarization reversal in $TbMn_2O_5$ does not include domain wall motion but is indeed due to a reversal of only one ferroelectric contribution.

This work was supported by the DFG through SFB 608.

TT 25.3 Tue 11:15 HSZ 04

Three-dimensional distribution of protected ferroelectric vortices in multiferroic hexagonal $YMnO_3$ — Tobias Jungk[1], •Martin Lilienblum[2], Ákos Hoffmann[1], Manfred Fiebig[2], and Elisabeth Soergel[1] — [1]PI, Universität Bonn, Wegelerstraße 8, 53115 Bonn, Germany — [2]HISKP, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Multiferrroics are a rich source for "unusual" forms of ferroelectric order. The spontaneous polarizations is induced by magnetism, charge order, geometric effects, etc., and may lead to novel domain states and functionalities. Here we show by piezoresponse force microscopy that ferroelectric domains in hexagonal multiferroic $YMnO_3$ form vortex-like structures around the direction of polarization. Although one would intuitively associate the sixfold character of the domain vortices to the uniaxial hexagonal structure, sixfold vortices are also present

perpendicular to the direction of the spontaneous polarization. We will explain the intriguing topology on the basis of a simple geometric model. In addition, we will show how individual domain vortices are affected by application of an electric field applied along the polarization axis.

TT 25.4 Tue 11:30 HSZ 04

Poling of ferrotoroidic domains in $LiCoPO_4$ with toroidal fields — •Anne S. Zimmermann[1], Jean-Pierre Rivera[2], Hans Schmid[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic, Analytical and Applied Chemistry, University of Geneva, Switzerland

Ferrotoroidicity denotes a fourth, space- and time-asymmetric form of ferroic order with a spontaneous uniform alignment of magnetic vortices. Space and time asymmetry also relates ferrotoroidic materials to multiferroics and magnetoelectrics. After ferrotoroidic domains have been observed in $LiCoPO_4$ by second harmonic generation (SHG) experiments [1] controlled manipulation of these ferrotoroidic domains is the next step in demonstrating the ferroic nature of the toroidal state. This can be achieved by a toroidal field, i.e., a field behaving asymmetric under space inversion and time reversal, which can be realized by crossed electric and magnetic fields.

Here we report on the behaviour of ferrotoroidic domains in applied toroidal fields. The ferrotoroidic domain structure in various field experiments was investigated by phase-sensitive SHG. We demonstrate that it is possible to orient and switch the ferrotoroidic domains with an appropriate toroidal field. Furthermore the critical field strengths required to orient the ferrotoroidic domains and the relation of ferrotoroidic poling with magnetoelectric annealing are discussed. - Work supported by the SFB 608.

[1] B. B. Van Aken et. al., Nature 449, 702 (2007)

TT 25.5 Tue 11:45 HSZ 04

Time resolved measurements of the multiferroic switching in MnWO4 — •Max Baum[1], Thomas Finger[1], Jeannis Leist[2], Karin Schmalzl[3], Louis-Pierre Regnault[4], Petra Becker[5], Ladislav Bohatý[5], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Georg-August-Universität Göttingen — [3]Jülich Centre for Neutron Science (JCNS) at ILL, Grenoble — [4]Institut Nanosciences et Cryogénie, CEA-Grenoble — [5]Institut für Kristallographie, Universität zu Köln

Multiferroic materials or compounds with a strong magnetoelectric effect posses a large application potential in data storage techniques. Quite recently, systems with a peculiar spiral magnetic order were shown to directly induce a spontaneous electric polarisation and to exhibit giant magnetoelectric and magnetocapacitance effects, among them MnWO4. Neutron scattering with spherical polarisation analysis gives direct access to the chiral component of the magnetic structure which is directly linked to the electric polarisation and thus may be tunable by an electric field. In MnWO4 it is possible to drive multiferroic hysteresis loops at constant temperature as a function of the electric field. We broadened our investigations in this topic and present time resolved measurements of magnetoelectric switching. We applied stroboscopic techniques in order to investigate how fast the chiral component of the magnetic structure adapts to an instantaneously switched electric field. The time scale of the response is remarkable slow, in the range of 3 - 20 ms.

TT 25.6 Tue 12:00 HSZ 04

Time resolved reversal of spin-spiral domains by an electric field in multiferroic $MnWO_4$ — •Philip Thielen[1], Tim Hoffmann[1], Petra Becker[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]University Bonn, HISKP, Germany — [2]Institut für Kristallographie, Universität zu Köln

The interaction of magnetic and ferroelectric order is intrinsically strong in spin-spiral multiferroics. Here the complex magnetic long range order breaks inversion symmetry and induces a spontaneous electric polarization. The interaction allows for switching of the magnetization by means of an applied electric field and is thus of great interest for possible applications. So far there exists little information on the time scale and dynamics of the actual switching process. Here we report time resolved measurements of the reversal of spin-spiral domains in multiferroic $MnWO_4$ by optical second harmonic generation. Magnetic single-domain states are created by the application of an electric field. By reversing its polarity, a reversal of the magnetic domain state occurs. The time scale of the dynamic switching process is found to be in the ms region. Images of the domain-reversal process are obtained. The dynamic domain pattern differs substantially from that of quasi-statically switched multi domain structures.

TT 26: TR: Fluctuations and Noise

Time: Tuesday 14:00–15:30 Location: HSZ 301

Invited Talk TT 26.1 Tue 14:00 HSZ 301

Quantum paradoxes in quantum transport — •Wolfgang Belzig[1] and Adam Bednorz[1,2] — [1]Fachbereich Physik, Universiät Konstanz, D-78457 Konstanz, Germany — [2]Institute of Theoretical Physics, University of Warsaw, Hoza 69, PL-00681 Warsaw, Poland

The impossibility of measuring non-commuting quantum mechanical observables is one of the most fascinating consequences of the quantum mechanical postulates, relevant for correlation measurements of the electric current [1]. Hence, to date the investigation of quantum measurement and projection is a fundamentally interesting topic. We propose to test the concept of weak measurement of non-commuting observables in mesoscopic transport experiments, using a quasiprobablistic description [2]. As first example of a paradox, we derive an inequality for current correlators, which is satisfied by every classical probability but violated by high-frequency fourth-order cumulants in the quantum regime for experimentally feasible parameters [3]. Further paradoxes can be used to detect nonlocal quantum correlations (entanglement) in mesoscopic junctions far beyond the regime covered by the usual Bell inequalities.

[1] A. Bednorz and W. Belzig, Phys. Rev. Lett. 101, 206803 (2008).
[2] A. Bednorz and W. Belzig, Phys. Rev. B 81, 125112 (2010).
[3] A. Bednorz and W. Belzig, Phys. Rev. Lett. 105, 106803 (2010).

TT 26.2 Tue 14:30 HSZ 301

A Full Counting Statistics with the 2nd-order-von-Neumann approach — •Philipp Zedler[1], Tomáš Novotný[2], Clive Emary[1], and Tobias Brandes[1] — [1]Technische Universität Berlin — [2]Univerzita Karlova v Praze

We formulate a (Non-Markovian) master equation with counting fields which generalizes the 2nd-order-von-Neumann approximation. The approach can also be considered as a resonant tunneling approximation in real time diagramatics or can be derived using Liouvillian perturbation theory. We apply the formalism to the well-understood single resonant level model to make statements about its accuracy in the presence of counting fields.

TT 26.3 Tue 14:45 HSZ 301

Semiclassical dynamics of a NEMS oscillator — •Anja Metelmann and Tobias Brandes — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, Berlin D-10623, Germany

We investigate the dynamics of a single phonon (oscillator) mode linearly coupled to an electronic few–level system in contact with external particle reservoirs (leads). A stationary electronic current through the system generates non–trivial dynamical behaviour of the oscillator [1]. Using Feynman–Vernon influence functional theory, we derive a Langevin equation for the oscillator trajectory that is non–perturbative in the system–leads coupling. For the case of two coupled electronic levels, we discuss various regimes of the oscillator dynamics.

[1] R. Hussein, A. Metelmann, P. Zedler, and T. Brandes, Phys. Rev. B **82**, 165406 (2010).

TT 26.4 Tue 15:00 HSZ 301

Factorial cumulants reveal interactions in counting statistics — •Dania Kambly, Christian Flindt, and Markus Büttiker — Département de Physique Théorique, Université de Genève, CH-1211 Genève, Switzerland

Full counting statistics concerns the stochastic transport of electrons in mesoscopic structures. Recently it has been shown that the charge

transport statistics for non-interacting electrons in a two-terminal system is always generalized binomial: it can be decomposed into independent single-particle events and the zeros of the generating function are real and negative. Here we investigate how the zeros of the generating function move into the complex plane due to interactions and demonstrate that the positions of the zeros can be detected using high-order factorial cumulants. As an illustrative example we consider electron transport through a Coulomb blockade quantum dot for which we show that the interactions on the quantum dot are clearly visible in the high-order factorial cumulants. Our findings are important for understanding the influence of interactions on counting statistics and the characterization in terms of zeros of the generating function provides us with a simple interpretation of recent experiments, where high-order statistics have been measured.

TT 26.5 Tue 15:15 HSZ 301

Thermal noise due to electron interactions in networks of disordered wires — •Maximilian Treiber[1], Christophe Texier[2], Oleg M. Yevtushenko[1], Jan von Delft[1], and Igor V. Lerner[3] — [1]Ludwig-Maximilians-Universität, Physics Department, ASC, CeNS, Theresienstrasse 37, D-80333 Munich, Germany — [2]Université Paris-Sud, CNRS, LPTMS, UMR 8626, Bat. 100, F-91405 Orsay, France — [3]University of Birmingham, School of Physics and Astronomy, Birmingham, B15 2TT, UK

At sufficiently low temperatures, electron interactions govern dephasing in mesoscopic samples. Thus, a theory of dephasing requires the knowledge of the correlation function of Johnson-Nyquist (electronic) noise. This function is well-known, for example, for quasi-1d wires. Recent experiments address dephasing in substantially inhomogeneous systems consisting of multiply-connected wires, such as metallic grids or connected rings. Motivated by these experiments, we study the spatial dependence of the noise correlation function in networks of disordered wires with arbitrary boundary conditions.

Using the fluctuation-dissipation theorem and the random-phase approximation, we derive a real-space integro-differential equation for the correlation function. In the case of sufficiently strong screening, this equation reduces to a time-integrated diffusion equation which has to be solved for the given boundary conditions (such as connections to leads). We show how a solution can be found efficiently for networks of wires, by using a method based on the spectral determinant.

TT 27: SC: Fe-based Superconductors - LiFeAs

Time: Tuesday 14:00–15:30 Location: HSZ 304

TT 27.1 Tue 14:00 HSZ 304

Nuclear Magnetic Resonance study of pure and Ni/Co doped LiFeAs — •Hans-Joachim Grafe, Seung-Ho Baek, Franziska Hammerath, Uwe Gräfe, Yannic Utz, Luminita Harnagea, Claudia Nacke, Saicharan Aswartham, Sabine Wurmehl, and Bernd Büchner — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

We present Nuclear Magnetic and Nuclear Quadrupole Resonance (NMR/NQR) measurements on pure, Ni and Co doped LiFeAs single crystals. The parent compound LiFeAs exhibits unconventional superconductivity with a transition temperature of about 17 K. Unlike other Fe based superconductors, where superconductivity is induced or stabilized by Co or Ni doping, replacement of Fe by these elements leads to a suppression of the superconducting transition temperature in LiFeAs. In case of Ni doping, a bulk magnetic order is induced below about 160 K. In contrast, for Co doping, the superconducting transition temperature is only reduced, but no magnetic order is observed. We discuss the nature and the origin of this magnetic order and its relation to unconventional superconductivity in pure LiFeAs.

TT 27.2 Tue 14:15 HSZ 304

Influence of doping on the physical properties of LiFeAs — •Luminita Harnagea[1], Claudia Nacke[1], Igor Morozov[1,2], Dirk Bombor[1], Anne Bachmann[1], Uwe Gräfe[1], Yannic Utz[1], Mahmoud Abdel-Hafiez[1], Seung-Ho Baek[1], Ulrike Stockert[1,3], Rüdiger Klingeler[1,4], Anja U.B. Wolter[1], Hans-Joachim Grafe[1], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Institute for Solid State Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Moscow State University, Moscow 119991, Russia — [3]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [4]Kirchhoff Institute for Physics, Heidelberg University, D-69120 Heidelberg, Germany

Single crystals of $LiFe_{1-x}M_xAs$ (M = Cr, Rh, Ni) were grown using the self-flux method. The parent compound LiFeAs is an unconventional superconductor with a transition temperature of about 17 K. Upon doping on the Fe site with Rh, Ni or Cr the superconductivity is suppressed, which is reflected in different physical properties. This observation is in contrast to the effect of doping in the NaFeAs homologous and in other Fe-based superconductor families, where the superconductivity is induced or/and stabilized by replacing Fe either by Rh or Ni.

TT 27.3 Tue 14:30 HSZ 304

Suppressed superconductivity in charge doped $Li(Fe_{1-x}Co_x)As$ single crystals — •Saicharan Aswartham[1], Günter Behr[1], Luminita Harnagea[1], Dirk Bombor[1], Igor V. Morozov[1,2], Anne Bachmann[1], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, D 01069 Dresden, Germany — [2]Moscow State University, Moscow 119991, Russia

Single crystals of the new unconventional superconductor $LiFe_{1-x}Co_xAs$ with x =0, 0.025, 0.05 were grown by a new approach using the self-flux technique. Superconducting properties have been studied by means of temperature dependent resistivity and magnetic susceptibility. The superconducting transition temperature was found to decrease upon Co-doping at the Fe site. Charge doping in LiFeAs supresses superconductivity, in contrast to the effects of charge doping in other Fe-As compounds, where charge doping supresses the spin density wave and establishes superconductivity. We present crystal growth and superconducting properties of $LiFe_{1-x}Co_xAs$.

TT 27.4 Tue 14:45 HSZ 304

Theory for Magnetism and Triplet Superconductivity in LiFeAs — Philip Brydon[1], •Maria Daghofer[2], Carsten Timm[1], and Jeroen van den Brink[2] — [1]Institut für Theoretische Physik, TU Dresden — [2]IFW Dresden

Superconducting pnictides are spin-singlet superconductors, where superconductivity is found near an antiferromagnetic (AF) phase. The AF order is believed to be largely driven by Fermi surface nesting. The band structure of LiFeAs, which does not have to be doped to become superconducting, differs from the other pnictides by two distinct features; it shows poorer nesting and has hole pockets that are much more shallow than he electron pockets. We incorporate these specific features into a three-band model and study the resulting magnetic order and pairing instabilities. We find that they are markedly different from the results for models with better nesting. The magnetic susceptibility shows a peculiar ring-shaped feature around $(0,0)$ instead of peaks at $(\pi,0)$ and $(0,\pi)$, as one would expect in the AF phase. These "almost FM" fluctuations are found to promote triplet superconductivity with a p-wave symmetry.

TT 27.5 Tue 15:00 HSZ 304

Quasiparticle interference of superconducting LiFeAs — •Torben Hänke, Steffen Sykora, Ronny Schlegel, Danny Baumann, Sabine Wurmehl, Igor Morozov, Luminita Harnagea, Christian Hess, Jeroen van den Brink, and Bernd Büchner — IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

We performed scanning tunneling spectroscopy measurements on the iron pnictide superconductor LiFeAs in the superconducting state. After cleavage of the crystal, we observe atomically flat surfaces which contain several defects in the field of view (FOV) of about 20×20 nm^2. Already in topographic images, pronounced spatial modulations of the integral density of states are present, which are particular strong in the vicinity of the defects. We recorded full $\mathrm{d}I/\mathrm{d}V(V)$ spectroscopy maps to determining the energy dependent quasiparticle interference in the FOV. The Fourier transform of the $\mathrm{d}I/\mathrm{d}V$ maps exhibits a rich structure which has a strong resemblance of constant energy cuts through

the experimental band structure. We will compare the experimental data with theoretically calculated quasiparticle interference using a realistic three-band model which is consistent with recent ARPES experiments.

TT 27.6 Tue 15:15 HSZ 304

Transport properties of LiFeAs — •Gerhard Kolland[1], Oliver Heyer[1], Stephanie Orbe[1], Volodymyr Zabolotnyy[2], Daniil Evtushinsky[2], Sergiy Borisenko[2], Igor Morozov[2], Luminita Harnagea[2], Sabine Wurmehl[2], Christian Hess[2], Bernd Büchner[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Leibniz-Institute for Solid State Research, IFW-Dresden, Germany

LiFeAs is unique among the broad family of FeAs-based superconductors, because it is the only stoichiometric compound that is superconducting at a rather large $T_c \simeq 18\,\mathrm{K}$ under ambient conditions. We studied electrical and thermal transport on high-quality single crystals. The low-temperature resistivity shows quadratic temperature dependence above T_c giving evidence for strong electron-electron scattering, while there is a tendency towards saturation around room temperature. The Hall constant is negative and changes with temperature, what most probably arises from a van Hove singularity close to the Fermi energy in one of the holelike bands. From the anisotropic magnetic-feld dependence of T_c we extrapolate the correlation lengths ξ_i and derive a moderate anisotropy $\xi_a/\xi_c \simeq 2.2$. The thermal conductivity κ shows a shoulder below T_c. This feature is strongly suppressed by an applied magnetic field whereas below 1 K the thermal conductivity increases with increasing field.

Supported by the DFG through SFB 608 and SPP1458.

TT 28: CE: (General) Theory 2

Time: Tuesday 14:00–15:30 Location: HSZ 105

TT 28.1 Tue 14:00 HSZ 105

Enhancement of the Na_xCoO_2 thermopower due to electronic correlations — •Karsten Held, Philipp Wissgott, and Alessandro Toschi — Institute for Solid State Physics, TU Wien

Climate change and the prospective oil peak necessitate the discovery of new green energy sources. One possibility in this context is to convert hithero unused excess heat into electrical energy using thermoelectrics. For a real breakthrough and a widespread application of this technology however, better materials are needed. Using the merger of local density approximation and dynamical mean field theory, we show how electronic correlations increase the thermopower of $Na_0.7CoO_2$ by 200%. The newly revealed mechanism is an asymmetric shift of (quasi) electrons and holes away from the Fermi level, concurrent with an asymmetry of the respective (group) velocities. Exploiting this effect in bandstructure and correlation engineering may lead to a substantial increase of the thermoelectric figure of merit.

TT 28.2 Tue 14:15 HSZ 105

Phase diagram and criticality of the three dimensional Hubbard model in the Dynamical Vertex Approximation — •Georg Rohringer[1], Alessandro Toschi[1], Andrey Katanin[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Institute of Metal Physics, Ekaterinburg, Russia

Inclusion of spatial correlations on all length scales beyond the dynamical mean field theory (DMFT) induces two relevant changes to the phase-diagram of the three dimensional Hubbard model: i) a sizable reduction of the Néel temperature (T_N) for the onset of antiferromagnetic long-range order; (ii) a deviation from then mean-field critical behavior for $T \sim T_N$. Both effects are well captured by means of the recently developed[1] Dynamical Vertex Approximation (DΓA) applied to the half-filled Hubbard model: We find[2] a reduction of the Néel temperature of $\sim 30\%$, which agrees with previous cluster calculations in the intermediate-to-strong coupling regime. Furthermore we observe a temperature region of deviation from the mean field criticality, which increases with the interaction strength U. Remarkably, the critical exponents extracted for the highest U values well agree with those of the three-dimensional Heisenberg universality class. Finally, DΓA also allows for a quantitative estimation of the errors stemming from the purely local nature of DMFT, when it is applied to a (realistic) finite dimensional case.

[1] A. Toschi, A. Katanin, K. Held, Phys. Rev. B 75, 045118 (2007) & Phys. Rev. B 80, 075104 (2009).
[2] G. Rohringer, A. Toschi, A. Katanin, K. Held in preparation.

TT 28.3 Tue 14:30 HSZ 105

Calculation of dynamical susceptibilities in the 2d Hubbard model: A dynamical cluster approximation study — •David J. Luitz and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

We calculate dynamical susceptibilities of the 2d Hubbard model within the dynamical cluster approximation (DCA). We use the weak coupling continuous time quantum Monte Carlo method which allows the unbiased calculation of the two particle irreducible vertex Γ on the cluster by virtue of the Bethe Salpeter equation. Γ is identified with the coarse grained vertex of the lattice thus yielding dynamical susceptibilities of the lattice within DCA. We will discuss technical details of the approach and present preliminary results of the dynamical spin susceptibility.

TT 28.4 Tue 14:45 HSZ 105

Phase diagram of an extended classical dimer model — •Daniel Charrier — Max Planck Institut fuer Physik Komplexer Systeme, Noethnitzer Strasse 38, 01187 Dresden

Dimer models have attracted the interest of researchers in various branches of physics, ranging from statistical and condensed matter physics to high-energy physics. Their distinctive properties essentially result from the close-packing condition, which imposes that on a lattice, each site should be part of one and only one dimer. This strict condition generates strong correlations between degrees of freedom, even when interactions are absent from the system. Some years ago, it has been proposed that these systems could also sustain non-Landau phase transitions, i.e, transitions that are not easily described by the conventional theory of critical phenomena. We present here some new results obtained from an extensive numerical study of the attractive dimer model on the cubic lattice. The phase diagram of the model is discussed and the peculiarity of each phase is exposed. It is confirmed that the universality class of the phase transitions does not match critical exponents of conventional Landau theories. Moreover, the critical exponents seem to be related to the ones observed in exotic transitions in frustrated quantum magnets.

TT 28.5 Tue 15:00 HSZ 105

Electronic correlations at the α-γ structural phase transition in paramagnetic iron — •Ivan Leonov[1], Alexander I. Poteryaev[2], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]TP III, Center for Electronic Correlations and Magnetism, Uni 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]. 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 the equilibrium crystal structure and phase stability of *paramagnetic* iron at the α(bcc)-γ(fcc) phase transition as a function of temperature [2]. 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. The magnetic correlation energy is found to be an essential driving force behind the *bcc-fcc* structural phase transition in paramagnetic iron. The phonon dispersion curves calculated for paramagnetic iron at the *bcc-fcc* structural phase transition show good agreement with experimental data.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **101**, 096405 (2008); I. Leonov *et al.*, Phys. Rev. B **81**, 075109 (2010).
[2] I. Leonov *et al.*, arXiv:1008.4342 (2010).

TT 28.6 Tue 15:15 HSZ 105

Thermalization of Interacting Fermions and Delocalization in Fock space — •Clemens Neuenhahn[1] and Florian Marquardt[1,2] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institut for the Science of Light, Günter-Scharoswky-Strasse 1/Bau 24,D-91058 Erlangen, Germany

By means of exact diagonalization, we investigate the onset of 'eigenstate thermalization' and the crossover to ergodicity in a system of 1D fermions with increasing interaction. We show that the fluctuations in the expectation values of the momentum distribution from eigenstate to eigenstate decrease with increasing coupling strength and system size. It turns out that these fluctuations are proportional to the inverse participation ratio of eigenstates represented in the Fock basis. The latter decays exponentially with increasing interaction strength before one enters the chaotic regime. We found good numerical evidence that in the thermodynamic limit eigenstate thermalization should set in even for vanishingly small perturbations.

TT 29: Poster Session: Quantum Information Systems, Quantum Coherence (jointly with SAMOP)

Time: Tuesday 18:00–21:00 Location: P1

TT 29.1 Tue 18:00 P1

Temperature Dependence of Driven Duffing Oscillators — •Lingzhen Guo[1,3], Michael Marthaler[1,2], Stephan André[1,2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [3]Department of Physics, Beijing Normal University, Beijing 100875, China

A broad class of physical systems such as Josephson junctions, trapped electrons, and nanomechanical oscillators, can be well described by the Duffing oscillator under proper conditions. A driven Duffing oscillator (DDO) can exhibit many profound features, such as dynamical bifurcation. Near the bifurcation point, the oscillator state is highly sensitive to perturbation. This property can be exploited for applications such as sensing devices, amplifiers, and logic devices. In the light of nanomechanics, the quantum properties of the driven Duffing oscillator gained renewed interest in the past years, such as resonant tunneling and photon-assisted tunneling and the switching rate between thebistable states near the bifurcation point due to quantum and/or thermal fluctuations. In the bistable region of a DDO, the stationary probability distribution in phase space (i.e., Wigner function) or the distribution over energy levels of DDO in the finite temperature is also an important and interesting problem. Based on simulating a Lindblad-type master equation, we investigate the relationship of the statiobary probability distribution and the temperature.

TT 29.2 Tue 18:00 P1

The effect of solid-state noise sources on three-level systems — •Nicolas Vogt[1], Michael Marthaler[1], Jared H. Cole[1], 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

We investigate the behaviour of a three level quantum system in contact with a two level fluctuator. There are a number of established ways to treat the TLF as a noise source and obtain an equation of motion for the three level system, for example Bloch-Redfield theory. We compare such perturbative methods with the fully coherent treatment of the TLF in a parameter regime where the assumptions made in the derivation of these perturbative methods are no longer guaranteed to hold. Using these results, we consider the effect of intrinsic decoherence sources on the process of stimulated Raman adiabatic passage, within a three-level system.

TT 29.3 Tue 18:00 P1

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

Spins on surfaces of superconductors are currently believed to be responsible for the 1/f flux noise in SQUIDs and Josephson qubits [1,2,3,4,5]. In recent experiments the spin contribution to the inductance of superconducting wires was measured [6]. This inductance describes the response to a current, which polarizes spins by creating magnetic fields on the surface. In particular low frequency fluctuations of the complex inductance were observed with roughly a 1/f noise spectrum. We provide an analysis of inductance noise in analogy to the well known theory of "noise of noise" and analyze some microscopic models that could explain these experiments.
[1] F. C. Wellstood et al., Appl. Phys. Lett. 50, 772 (1987).
[2] S. Sendelbach et al., Phys. Rev. Lett. 100, 227006 (2008).
[3] H. Bluhm et al., Phys. Rev. Lett. 103, 026805 (2009).
[4] R. H. Koch et al., Phys. Rev. Lett. 98, 267003 (2007).
[5] L. Faoro and L. B. Ioffe, Phys. Rev. Lett. 100, 227005 (2008).
[6] S. Sendelbach et al., Phys. Rev. Lett. 100, 227006 (2008).

TT 29.4 Tue 18:00 P1

Two Level Fluctuators in Josephson qubits — •Daniel Mischek[1], Clemens Müller[1,2], and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruhe, Germany

Spectroscopic analysis of superconducting qubits often shows clear signatures of avoided level crossings, indicating the presence of microscopic two-level fluctutors (TLFs) coupling to the qubit[1].

Within "direct coherent control" method it was possible for the first time to investigate coherence times and temperatures properities of single TLFs[2].

Measurements of relaxation time shows unusual behaviour of temperature dependence. Within Bloch Redfield formalism we analyse the influence of higher qubit levels on the resonance shape of relaxation time.
[1] R.W.Simmonds et al., Phys. Rev. Lett. 93, 077003 (2004)
[2] J.Lisenfeld et al., arXiv: 1008.0337

TT 29.5 Tue 18:00 P1

Dispersive readout scheme for a Josephson phase qubit — •Tobias Wirth, Jürgen Lisenfeld, Alexander Lukashenko, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology and DFG Center for Functional Nanostructures, 76128 Karlsruhe, Germany

A vital ingredient of experiments on quantum bits is a detection tool to efficiently read out the state of a qubit. This detector must introduce as little back-action as possible, while showing a large measurement contrast; it should have negligible dissipation and offer fast operation.

The standard method to read out a Josephson phase qubit is to record the dc bias current at which the SQUID switches to its non-superconducting state. This process generates heat directly on the chip and quasi-particles in the circuitry. Both effects are responsible for a relatively long cool-down time of about 1-2 ms required after each switching event. Together with the time needed to ramp up the bias current of the SQUID, this limits the repetition rate of the experiment.

We present experimental results on a dispersive scheme for reading out a Josephson phase qubit. A capacitively shunted dc-SQUID is used as a nonlinear resonator which is inductively coupled to the qubit. The flux state of the qubit is detected by measuring the amplitude and phase of a microwave pulse reflected from the SQUID resonator. By this low-dissipative method, the qubit state measurement time is reduced to 25 μs, which is much faster than the conventional readout.

TT 29.6 Tue 18:00 P1

Light Effects on High Q-Resonators for Hybrid Quantum Systems — •Christian Koller, Robert Amsüss, Tobias

Nöbauer, Matthias Schramböck, Jörg Schmiedmayer, and Johannes Mayer — Atominstitut, TU Wien, Stadionalle 2, 1020 Wien, Österreich

Over the last years hybrid quantum systems have drawn attention in the field of quantum information processing, because of their ability to combine the advantages of different quantum worlds. A number of proposals for the combination of systems with long coherence times (e.g. atoms, cold molecules, nitrogen vacancies (NV) in diamond, ...) with solid-state systems featuring fast manipulation (e.g. Cooper-pair boxes, flux qubits, transmons, ...) have been made.

The heart of these hybrid systems are planar resonators with high quality factors (on the order of one million) formed by superconducting coplanar microwave transmission lines. The properties of these resonators under the influence of light is crucial, since many of the hybrid applications involve laser light, for example imaging and manipulation of cold atoms and molecules as well as the initialization and read-out of NV centers.

We will present measurements of the shift of resonator frequency as a function of the applied light power. Furthermore, we show the effects on the Q value due to the generation of quasi particles and the saturation of two-level fluctuators in the superconducting thin films. We will also put these facts in perspective with resent measurements of resonators strongly coupled to an ensemble of NV centers.

TT 29.7 Tue 18:00 P1

Dual-path state reconstruction scheme for propagating quantum microwaves — Edwin P. Menzel[1], Frank Deppe[1], •Peter Eder[1], Matteo Mariantoni[1], Miguel Angel Araque Caballero[1], Alexander Baust[1], Thomas Niemczyk[1], Elisabeth Hoffmann[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

Weak propagating microwave signals on the quantum level can be characterized using two amplification chains and suitable correlations between their outputs. In such a dual path setup all quadrature moments of an input signal can be determined, although the noise added by each individual amplifier chain can be larger than the microwave signal to be measured [E.P. Menzel et al., PRL 105, 100401 (2010)]. This allows for a full quantum tomography of propagating microwaves. As a possible application of the dual-path method, we discuss detecting squeezed states generated by a superconducting Josephson parametric amplifier or other circuit QED setups.

This work is supported by SFB 631, NIM, Basque Government IT4720-10, Spanish MICINN FIS2009-12773-C02-01, and EU project SOLID.

TT 29.8 Tue 18:00 P1

Characterization of flux-driven Josephson parametric amplifiers — •Alexander Baust[1], Edwin P. Menzel[1], Thomas Niemczyk[1], Elisabeth Hoffmann[1], Max Haeberlein[1], Friedrich Wulschner[1], Frank Deppe[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-shi, Japan — [4]NEC Corporation, Tsukuba, Japan

Phase sensitive linear amplifiers receive increasing interest for applications in the field of circuit QED as they allow for the amplification of one signal quadrature without, in principle, adding noise. The flux-driven Josephson parametric amplifier characterized in this work is formed by a SQUID-terminated transmission line resonator with resonant frequency that can be varied by applying an ac magnetic flux signal through the SQUID. We have characterized two Josephson parametric amplifiers with different design parameters with respect to the center frequency and quality factor of the resonator, phase-dependent and phase-independent gains, as well as compression points and bandwidths.

This work is supported by SFB 631, NIM, Basque Government IT4720-10, Spanish MICINN FIS2009-12773-C02-01, and EU project SOLID.

TT 29.9 Tue 18:00 P1

The influence of noise on the measurement of the Berry phase in superconducting circuits — •Vera Gramich and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, D-89069 Ulm

Motivated by recent experiments of Cooper pair pumping in a novel type of a phase-biased charge pump ('Cooper pair sluice'), we study the influence of noise on the measurement of the Berry phase for such a configuration embedded in a superconducting loop. In the adiabatic regime a master equation beyond the RWA (Rotating Wave Approximation) for an open two level quantum system is derived taking consistently into account the combined effect of drive and dissipation. This also includes the driving and friction induced Lamb-shifts. Their impact on the steady state density matrix, which determines the pumped charge, is analyzed for an experimental set-up. Strategies to measure the Lamb-shift in a condensed matter environment are discussed.

TT 29.10 Tue 18:00 P1

Different types of integrability and their relation to decoherence in central spin models — •Bjoern Erbe and John Schliemann — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

In a large variety of nanostructures spins couple to a bath of other spin degrees of freedom. Important examples are given by semiconductor and carbon nanotube quantum dots, phosphorus donors in silicon, nitrogen vacancy centers in diamond and molecular magnets. Commonly such systems are described by so-called central spin models [1,2].

We present recent results on the relation between integrability and decoherence in central spin models with more than one central spin [3]. We show that there is a transition between integrability ensured by Bethe ansatz and integrability ensured by complete sets of commuting operators. This has a significant impact on the decoherence properties of the system, suggesting that it is not necessarily integrability or non-integrability which is related to decoherence, but rather its type or a change from integrability to non-integrability.

[1] J. Schliemann, A. Khaetskii, and D. Loss, J. Phys.: Condens. Mat. 15, R1809 (2003).
[2] W. A. Coish and J. Baugh, phys. stat. sol. B 246, 2203 (2009).
[3] B. Erbe and J. Schliemann, Phys. Rev. Lett. 105, 177602 (2010).

TT 29.11 Tue 18:00 P1

Non-Equilibrium Transport Properties of a Tunnel Junction Coupled to an Harmonic Oscillator in the Non-Markovian Regime — •Stefan Walter and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We are interested in the true quantum behavior of the coupled system of a quantum harmonic oscillator and a tunnel junction beyond Born and Markov approximation. The non-equilibrium transport properties of the tunnel junction (I-V characteristics and finite frequency noise) are perturbatively calculated in the tunneling Hamiltonian using the Keldysh formalism. We find that the transport properties of the tunnel junction significantly depend on the properties of the oscillator.

For a non-stationary oscillator, we find a complex noise (in second order in the tunnel amplitudes) which complements the proposal for a momentum detector in Ref. [1].

We further investigate the noise signatures of the oscillator to fourth order in the tunneling similar to Ref. [2]. As in Ref. [1] we additionally include an arbitrary relative phase between the tunnel amplitudes, allowing for the detection of the oscillator's momentum. The non-equilibrium treatment permits us to extend previous results to the non-Markovian regime.

[1] C. B. Doiron, B. Trauzettel, and C. Bruder., *Phys. Rev. Lett.* **100**, 027202 (2008)
[2] J. Wabnig, J. Rammer, and A. L. Shelankov, *Phys. Rev. B* **75**, 205319 (2007)

TT 30: TR: Quantum Coherence and Quantum Information Systems 1 (jointly with MA and HL)

Time: Wednesday 10:30–13:00 Location: HSZ 03

TT 30.1 Wed 10:30 HSZ 03

Lasing without Inversion in Circuit Quantum Electrodynamics — •Michael Marthaler[1], Yasuhiro Utsumi[2], Dmitry Golubev[3], Alexander Shnirman[4], 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]Department of Physics Engineering, Faculty of Engineering, Mie University 1577, Kurimamachiya-cho, Tsu, Mi-e, 514-8507, Japan — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology,D-76021 Karlsruhe, Germany — [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology,D-76021 Karlsruhe, Germany

We study photon generation in a pumped qubit coupled to a transmission line oscillator under the influence of a dissipative electromagnetic environment. It has been demonstrated previously that if population inversion can be produced a lasing state is created in the oscillator. Further effects known from quantum electrodynamics (QED) have also been demonstrated in these circuit QED systems. Here we show that the circuit can also exhibit the effect of "lasing without inversion". This arises since the coupling to the dissipative environment favors photon creation as compared to annihilation, similar to the recoil effect which was predicted for atomic systems. While the recoil effect is very weak and so far elusive the effect predicted here should be readily observable.

TT 30.2 Wed 10:45 HSZ 03

Coherent dynamics of two microscopic defect states coupled via a phase qubit — •Grigorij J. Grabovskij[1], Pavel Bushev[1], Jared H. Cole[2,3], Clemens Müller[4,3], Jürgen Lisenfeld[1], Alexander Lukashenko[1], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [3]DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany — [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

We report on the experimental demonstration of induced coherent interaction between two intrinsic two-level defect states (TLSs) via a phase qubit. During the implementation of the pulse sequence the tunable qubit serves as a quantum shuttle communicating quantum information between the two TLSs. We present a detailed comparison between experiment and theory and find excellent agreement over a wide range of parameters. We then use the theoretical model to study the creation and movement of entanglement between the three components of the system.

TT 30.3 Wed 11:00 HSZ 03

On Superradiant Phase Transitions and Effective Models in Circuit QED — •Oliver Viehmann[1], Jan von Delft[1], and Florian Marquardt[2] — [1]Department of Physics, ASC, and CeNS, LMU München, Germany — [2]Institute for Theoretical Physics, FAU Erlangen-Nürnberg, Germany

Circuit QED systems of artificial atoms interacting with microwaves have been proved to behave in many respects analogously to their counterparts with real atoms in cavity QED. However, it has been predicted recently that the analogy fails if a large number of (artificial) atoms couple strongly to the electromagetic radiation [1]: Whereas for real atoms a no-go theorem rules out the possibility of a superradiant quantum phase transition as the coupling is increased [2], the standard description of circuit QED systems by an effective model based on macroscopic quantities [1,3] does allow it.

We investigate the possibility of a superradiant quantum phase transition in circuit QED systems from a microscopic point of view. Our analysis shows that also circuit QED systems are subject to the no-go theorem. It hence restores the analogy of circuit QED and cavity QED and challenges the applicability of the standard description of circuit QED systems in the regime under concern. In the light of this analysis, the no-go theorem is scrutinized and confirmed in a way more adequate for realistic physical systems.

[1] P. Nataf and C. Ciuti, Nature Commun. **1**, 72 (2010).
[2] K. Rzążewski *et al.*, Phys. Rev. Lett. **35**, 432 (1975).
[3] A. Blais *et al.*, Phys. Rev. A **69**, 062320 (2004).

TT 30.4 Wed 11:15 HSZ 03

Hybrid Quantum System: Coupling Color Centers to Superconducting Cavities — •Robert Amsüss[1], Christian Koller[1], Tobias Nöbauer[1], Stefan Rotter[2], Matthias Schrammböck[1], Jörg Schmiedmayer[1], and Johannes Majer[1] — [1]Atominstitut, TU Wien, Stadionallee 2, 1020 Wien, Österreich — [2]Institut für Theoretische Physik, TU Wien, Wiedner Hauptstraße 8-10, 1040 Wien

Circuit quantum electrodynamics is a system that allows us to carry out new experiments in quantum optics using a superconducting integrated circuit on a chip. In circuit QED, microwave photons are guided and confined by superconducting transmission lines and cavities, and can then be coherently coupled to a transmon qubit. The very small mode volume allows to couple spins of atoms and molecules to the resonator. In that way it becomes possible to couple an ensemble of nitrogen vacancy defects to a superconducting resonator.

TT 30.5 Wed 11:30 HSZ 03

Pulse Sequences for Exchange-Based Quantum Computation — •Daniel Zeuch[1], Robert Cipri[2], Guido Burkard[1], and Nicholas Bonesteel[2] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Department of Physics and NHMFL, FSU, Tallahassee, Florida, USA

A CNOT-gate is one of the possible fundamental two-qubit gates for universal quantum computation. We consider a system where two qubits are encoded in any three spins of value 1/2 (arranged in a row), where each pair of neighboring spins can interact via the Heisenberg interaction. This could be realized by six quantum dots, each occupied by one excess electron. Electrons can virtually tunnel from one quantum dot to a neighboring dot, which switches on the interaction. Numerically a composition of 19 spin-interactions has been found leading to a quantum gate locally equivalent to a CNOT[1]. This has shown that universal quantum computation in such an *exchange-only* scheme is feasible if the experimental requirements can be met. Here we present a different sequence that consists of a larger number of pulses, but is less restrictive on the preparation of the qubits. One assumption of the former sequence is that the total spin of the system was set to be 1, for which reason one can turn on a magnetic field aligning certain spins during initialization. The new solution works for a total spin of 0 and 1 thus making the magnetic field unnecessary. The new sequence consists of approximately 40 pulses. It was found analytically, which will be the main focus of the talk.

[1] DiVincenzo et al. Nature **408**, 339 (2000)

15 min. break

TT 30.6 Wed 12:00 HSZ 03

Nuclear spin cooling using Overhauser field selective coherent population trapping — •Eric Matthias Kessler[1], Mena Issler[2], Géza Giedke[1], Susanne Yelin[3], Ignacio Cirac[1], Mikhail Lukin[4], and Atac Imamoglu[2] — [1]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [2]Institute of Quantum Electronics, ETH-Zürich, CH-8093 Zürich, Switzerland — [3]Department of Physics, University of Connecticut 2152 Hillside Road, U-3046 Storrs, CT 06269-3046, USA — [4]Department of Physics, Harvard University, Cambridge, MA 02138, USA

We show that a quantum interference effect in optical absorption from two electronic spin states of a solid-state emitter can be used to prepare the surrounding environment of nuclear spins in well-defined states, thereby suppressing electronic spin dephasing. The coupled electron-nuclei system evolves into a coherent population trapping state by optical-excitation-induced nuclear spin diffusion for a broad range of initial optical detunings. The spectroscopic signature of this evolution where the single-electron strongly modifies its environment is a drastic broadening of the dark resonance in optical absorption experiments. The large difference in electronic and nuclear timescales allows to verify the preparation of nuclear spins in the desired state.

TT 30.7 Wed 12:15 HSZ 03

Edge State, Entanglement Entropy Spectra and Critical Anisotropic Honeycomb Lattice Hopping Coupling of —

•Ming-Chiang Chung[1,2], Yi-Hao Jhu[3], Pochung Chen[3], and Sungkit Yip[2] — [1]Physics Division, National Center for Theoretical Science, Hsinchu, 30013, Taiwan — [2]Institute of Physics, Academia Sinica, Taipei 11529, Taiwan — [3]Physics Department, National Tsing Hua University, Hsinchu, 30013, Taiwan

For a bipartite honeycomb lattice, we show that the Berry phase depends not only on the shape of the system but also on the hopping couplings. Using the entanglement entropy spectra obtained by diagonalizing the block Green's function matrices, the maximal entangled state with the eigenvalue $\lambda_m = 1/2$ of the reduced density matrix is shown to have one-to-one correspondence to the zero energy states of the lattice with open boundaries, which depends on the Berry phase. For the systems with finite bearded edges along x-direction we find critical hopping couplings: the maximal entangled states (zero-energy states) appear pair by pair if one increases the hopping coupling h over the critical couplings h_cs.

TT 30.8 Wed 12:30 HSZ 03

Towards ultrastrong coupling of superconducting transmission line resonators — •Frank Deppe[1,2], Thomas Weissl[1,2], Elisabeth Hoffmann[1,2], Max Haeberlein[1,2], Alexander Baust[1,2], Jan Goetz[2], Manuel J. Schwarz[1], Thomas Niemczyk[1], Edwin P. Menzel[1], Achim Marx[1], David Zueco[3], Juan-Jose Garcia Ripoll[4], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Garching, Germany — [2]TU Muenchen, Garching, Germany — [3]CSIC-Universidad de Zaragoza, Zaragoza, Spain — [4]Institutio de Fisica Fundamental, CSIC, Madrid, Spain

Coupled superconducting transmission line resonator systems have potential applications in quantum information processing and fundamental quantum mechanics. Experimentally, high coupling strengths are desirable for a clear demonstration of quantum effects. We achieve coupling strengths of more than 10% of the resonator frequency (ultrastrong coupling) by distributed coupling. We find that, differently from the case of point-like coupling, the normal modes are no longer arranged symmetrically with respect to the single resonator frequency. Nevertheless, a detailed theoretical analysis shows that the system can still be described by a beam splitter Hamiltonian for two effective resonators. We expect that this result will allow for straightforward experimental access to exciting effects such as thermal entanglement in our samples.

This work is supported by the Deutsche Forschungsgemeinschaft via SFB 631, the German Excellence Initiative via NIM, FIS2008-01240, and FIS2009-13364-C02-0 (MICINN).

TT 30.9 Wed 12:45 HSZ 03

Qubit-oscillator system under ultrastrong coupling and extreme driving — •Johannes Hausinger and Milena Grifoni — Universität Regensburg, Germany

We present our recent study on the time-dependent qubit-oscillator Hamiltonian beyond the driven Jaynes-Cummings model [1]. We include counter-rotating terms for both the coupling of the two-level system to the quantized oscillator mode and to the external classical driving. Thus, the dynamics of the qubit can be examined analytically in the ultrastrong coupling regime, where the ratio g/Ω between coupling strength and oscillator frequency approaches unity or goes beyond, and simultaneously for driving strengths much bigger than the qubit energy splitting (extreme driving). Both qubit-oscillator coupling and external driving lead to a dressing of the qubit tunneling matrix element of different nature: the former can be used to suppress specifically certain oscillator modes in the spectrum [2], while the latter can yield coherent destruction of tunneling (CDT). We show that CDT is robust even in the case of ultrastrong coupling. Our findings are within the reach of present experimental superconducting setups for quantum information processing.

[1] J. Hausinger, and M. Grifoni, arxiv:1009.1485
[2] J. Hausinger, and M. Grifoni, arxiv:1007.5437, PRA (in press)

TT 31: TR: Nanoelectronics II - Spintronics and Magnetotransport 1 (jointly with HL and MA)

Time: Wednesday 10:30–13:00 Location: HSZ 301

Invited Talk TT 31.1 Wed 10:30 HSZ 301

New insights into the spin Hall effect — •Peter Schwab — Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The spin Hall effect allows to generate spin polarized currents without the need of magnetic materials or magnetic fields. Despite intensive theoretical and experimental efforts over the last years the microscopic mechanism that is responsible for the effect is in many cases not clear. Within a kinetic euqations approach we studied in detail the coupled dynamics of spin and charge currents in the two-dimensional electron gas and found that, surprisingly, the spin Hall effect and the inverse spin Hall effect are of different microscopic origin [1,2]. Recent experiments aim for an all-electrical measurement of the spin Hall effect. We will comment on an attempt to detect the spin Hall effect through the non-local voltage in H-shaped nanostructures, where an unexpected sign-change of the non-local voltage was observed when lowering the temperature.

[1] R. Raimondi, P. Schwab, EPL **87**, 37008 (2009)
[2] P. Schwab, R. Raimondi, C. Gorini, EPL **90**, 67004 (2010).

TT 31.2 Wed 11:00 HSZ 301

Geometric Correlations and Breakdown of Mesoscopic Universality in Spin Transport — •Klaus Richter[1], Inanc Adagideli[2], Philippe Jacquod[3], Matthias Scheid[1], Mathias Duckheim[4], and Daniel Loss[5] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Istanbul, Turkey — [3]Physics Department, University of Arizona, Tucson, USA — [4]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [5]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

We construct a unified semiclassical theory of charge and spin transport in chaotic ballistic and disordered diffusive mesoscopic systems with spin-orbit interaction [1]. Neglecting dynamic effects of spin-orbit interaction, we reproduce the random matrix theory results that the spin conductance fluctuates universally around zero average. Incorporating these effects in the theory we show that geometric correlations generate finite average spin conductances, but that they do not affect the charge conductance to leading order. The theory, which is confirmed by numerical transport calculations, allows us to investigate the entire range from the weak to the previously unexplored strong spin-orbit regime, where the spin rotation time is shorter than the momentum relaxation time.

[1] I. Adagideli et al., Phys. Rev. Lett., in print (2010); arXiv:1008.4656

TT 31.3 Wed 11:15 HSZ 301

Direct observation of band-gap closure for a semiconducting carbon nanotube in a large parallel magnetic field — •Sungho Jhang[1], Magdalena Margańska[1], Yurii Skourski[2], Milena Grifoni[1], Joachim Wosnitza[2], and Christoph Strunk[1] — [1]University of Regensburg, Germany — [2]Dresden High Magnetic Field Laboratory, Germany

We have investigated the magnetoconductance of semiconducting carbon nanotubes (CNTs) in pulsed, parallel magnetic fields up to 60 T, and report the direct observation of the predicted band-gap closure and the reopening of the gap under variation of the applied magnetic field. We also highlight the important influence of mechanical strain on the magnetoconductance of the CNTs.

TT 31.4 Wed 11:30 HSZ 301

Spin and charge transport in magnetically modulated 2DEGs — •Tobias Dollinger[1], Henri Saarikoski[1], Michael Wimmer[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universtität Regensburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, The Netherlands

We investigate transport properties of disordered mesoscopic conductors in the presence of periodically modulated magnetic field textures. The focus of the work lies on examining the effects due to the resulting spin superstructure which is of relevance in transport experiments on magnetic semiconductor systems with giant Zeeman interaction. Observables like transmission and local spin densities have been calculated by means of a Recursive Greens Function Technique. The numerical

results are interpreted within a semiclassical picture. Furthermore, the influence of adiabaticity on the observed transport features such as an anomalous peak in the magnetoconductance, is discussed.

15 min. break

TT 31.5 Wed 12:00 HSZ 301

Transport of Dirac fermions in HgTe quantum wells: Mobility anomaly and weak antilocalization — •G. Tkachov and E. M. Hankiewicz — Würzburg University, Germany

Recent studies of the quantum Hall effect and the minimal conductivity in HgTe quantum wells [1] have shown that this electronic system exhibits a single-valley Dirac fermion spectrum. In this work, we investigate further manifestations of the Dirac fermion transport in HgTe quantum wells: nonmonotonic carrier-density-dependent mobility and weak antilocalization effects. We demonstrate both theoretically and experimentally [2] that the carrier mobility has a maximum due to the competition of two disorder scattering mechanisms, viz. scattering by charged impurities and by quantum-well-width fluctuations which induce a fluctuating band gap, or, equivalently, fluctuating Dirac mass. Using the cooperon description of quantum interference effects, we also analyze how the symmetry breaking due to the finite band gap (Dirac mass) influences the weak antilocalization correction to the Drude conductivity.

[1] B. Büttner, C.X. Liu, G. Tkachov, E.G. Novik, C. Brüne, H. Buhmann, E.M. Hankiewicz, P. Recher, B. Trauzettel, S.C. Zhang and L. W. Molenkamp, *Single-valley Dirac fermions in zero-gap HgTe quantum wells*, to appear in Nature Physics; arXiv:1009.2248.

[2] G. Tkachov, C. Thienel, V. Pinneker, B. Büttner, C. Brüne, H. Buhmann, L. W. Molenkamp, and E. M. Hankiewicz, *Backscattering of Dirac fermions in finite gap HgTe quantum wells*, submitted to Physical Review Letters (2010)

TT 31.6 Wed 12:15 HSZ 301

Magnetotransport measurements of Bi(111) thin films on Si(111) — •Daniel Lükermann[1], Sergii Sologub[2], Christoph Tegenkamp[1], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover — [2]Academy of Science, Ukraine, 54 Volodymyrska St., Kiev, Ukraine

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as the low carrier concentration and a large mobility of the carriers. Furthermore, the surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown on Si(111) substrates.

In this talk the magnetotransport properties of epitaxially grown Bi(111) thin films in the range of 10 to 40 bilayers (BL) on Si(111) will be presented. The films show positive magnetoresistance, i.e. decreasing conductance with magnetic field. The amplitude of the effect depends on the film thickness. We could observe different contributions from the surface state and the bulk in the magnetotransport measurements. A sharp peak in the magnetoconductance in the low B-field regime can be attributed to bulk holes and electrons with high mobility. For higher B-fields a nearly linear decrease of the conductance was found, stemming from carriers within the surface states. Measurements of the Hall-resistance show that mainly electrons contribute to the conductance of the surface state. The hole density is around two orders of magnitude smaller. As it turns out, even Bi films as thick as 40 BL are not fully charge compensated.

TT 31.7 Wed 12:30 HSZ 301

Spin and density response of interacting particles with spin-orbit coupling — •Klaus Morawetz[1,2], Janik Kailasvuori[3], and Ozgur Bozat[2] — [1]University of Applied Science Münster, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Universidade Federal do Rio grande do Norte - UFRN, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Linearizing the appropriate kinetic equation, the density and spin response functions of an interacting particle system coupled to an external magnetic field is derived. Special attention is paid to the spin-orbit coupling. Different known cases are contained in the obtained expression, among them magnetized plasmas in high magnetic fields, quasi two-dimensional graphene with interband coupling and spin-polarized electrons interacting with impurities. The interplay between collective spin and charge phenomena dependent on the interaction and the magnetic field is presented and the resulting transport coefficients are calculated.

TT 31.8 Wed 12:45 HSZ 301

Spin transfer torques in chiral magnetic structures — •Karin Everschor[1], Markus Garst[1], Rembert Duine[2], Achim Rosch[1], Florian Jonietz[3], Sebastian Mühlbauer[3,4], Christian Pfleiderer[3], Andreas Neubauer[3], Wolfgang Münzer[3], Andreas Bauer[3], Tim Adams[3], Robert Georgii[3,4], Peter Böni[3], Michael Wagner[3], and Tomek Schulz[3] — [1]Inst. für Theoretische Physik, Universität zu Köln — [2]Inst. for Theoretical Physics, Utrecht University, Netherlands — [3]Physik-Department E21, Technische Universität München — [4]FRM II, Technische Universität München

We investigate the influence of electric currents on magnetic structures in bulk materials. In magnets without inversion symmetry, weak spin-orbit coupling leads to the formation of magnetic helices with a long pitch. These helices pin only weakly to disorder and the underlying crystalline lattice. Another weakly pinned, non inversion symmetric phase is the 2d Skyrmion lattice which appears for example in MnSi. Electrons traversing the topolocially stable knots pick up a Berry phase, which leads to an effective Lorentz force acting on the electrons. Via a "topological" contribution to the Hall effect this Lorentz force can be observed. The counter force, which is a Magnus force, acts together with additional drag forces on the Skyrmion lattice. A gradient in these forces (induced by a small temperature gradient) results in a net torque that can be observed with neutron scattering.

The coupling of the Skyrmion lattice to inhomogeneous spin currents is very efficient, leading to an ultra-low electrical threshold current of $j = 10^6 A/m^2$ to observe spin transfer torques.

TT 32: SC: Fe-based Superconductors - Theory

Time: Wednesday 10:30–13:00 Location: HSZ 304

TT 32.1 Wed 10:30 HSZ 304

Optical spectra and bandstructure in the SDW phase of the iron pnictides using density functional theory — •Johannes Ferber, Yu-Zhong Zhang, Kateryna Foyevtsova, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe- Universität Frankfurt

Understanding the antiferromagnetic (SDW) phase of the iron pnictides is important as superconductivity in these systems arises from either doping or pressurizing the antiferromagnetic parent compounds. However, density functional calculations in these systems are known to largely overestimate the magnetic moments. In our calculations, we suppress the moments to reasonable values and analyse the optical conductivity and bandstructure, finding that a number of features observed in experiments can be reproduced in this way. In addition, we consider the effect of spin excitations on the optical conductivity. Whereas the static antiferromagnetic order is commonly taken into account in DFT calculations, spin flip terms which lead to spin excitations (magnons) are not considered. Using a high-quality tight-binding model, we include the coupling of the electrons to the magnons into the calculation of the optical conductivity.

TT 32.2 Wed 10:45 HSZ 304

Effect of Impurities and Effect of Ellipticity on the Spin Resonance in Iron-Based Superconductors — •Johannes Knolle[1], Saurabh Maiti[2], Ilya Eremin[3], Andrey Chubukov[2], and Mike Norman[4] — [1]Max-Planck-Institut fur Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Department of Physics, University of Wisconsin-Madison, Madison,Wisconsin 53706, USA — [3]Institut fur Theoretische Physik III, Ruhr-Universitat Bochum, D-44801 Bochum, Germany — [4]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439-4845, USA

Iron-based superconductors are believed to have an unconventional or-

der parameter with $s\pm$ symmetry. Due to the sign change of the superconducting gap a spin resonance develops below the superconducting transition temperature. Based on an effective four-band model we analyze the doping dependence of this spin resonance and its sensitivity to non-magnetic, as well as, magnetic impurities. For zero ellipticity of the electron pockets the resonance becomes incommensurate at a critical doping δ_c, and, overall, the dispersion forms a so-called X-shape. For finite ellipticity, ϵ, the resonance splits into two incommensurate peaks and δ_c increases with increasing ϵ.

Both non-magnetic and magnetic impurities broaden the resonance. Its position depends on the interplay between the two impurity kinds and their intra- and inter-band scattering components. We find that the ratio between ω_{res}/T_c increases with the strength of the inter-band impurity scattering which is consistent with available experimental data.

TT 32.3 Wed 11:00 HSZ 304

Self-consistent spin wave theory in the collinear phase and its application to iron pnictides — •Daniel Stanek[1], Michael Holt[2], Oleg P. Sushkov[2], and Götz S. Uhrig[1] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

A possibility to describe magnetism in the iron pnictide parent compounds in terms of the two dimensional frustrated Heisenberg J_1-J_2 model has been actively discussed recently. However, neutron scattering studies have revealed the three dimensional character of the magnetism in the iron pnictides and an anisotropy between the exchange perpendicular and parallel to the spin stripes. Based on these observations, we study the J_1-J_2-J_c model as the three dimensional generalization of the J_1-J_2 model for $S = 1$ and $S = 1/2$. Using self-consistent spin wave theory, we present a detailed description of the staggered magnetization and magnetic excitations in the collinear state. Interestingly, two qualitatively distinct ways are found how the collinear, magnetically long-range ordered phase becomes unstable. Either the magnetization or one of the spin wave velocities vanishes. In addition, we discuss the relevance of a biquadratic exchange, which explains a part of the anisotropy between the effective in-plane exchange constants on the level of self-consistent spin wave theory.

In the application for the 122 iron pnictides, the experimentally measured spin wave dispersion is compared to the one derived within our model.

TT 32.4 Wed 11:15 HSZ 304

Doping dependence of antiferromagnetism in the pnictides — •Jacob Schmiedt[1], P.M.R. Brydon[1], Maria Daghofer[2], and Carsten Timm[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Various models have been proposed to describe the antiferromagnetic phase in iron pnictides. Models that take into account five d-orbitals are expected to contain all necessary information that is needed for the explanation of this phase. Based on RPA and mean-field calculations we investigate the doping dependence of the AFM phase in several different five-orbital models. In each of them a strong enhancement of the critical temperature is found for hole doping. We seek to understand this behavior by examining the corresponding change of the Fermi surface and its nesting properties.

TT 32.5 Wed 11:30 HSZ 304

Superconductivity and Magnetism in Iron-Based Superconductors: Insights from Quasiparticle Interference — •Alireza Akbari[1], Johannes Knolle[2], Ilya Eremin[1], and Roderich Moessner[2] — [1]Theoretische Physik III, Ruhr-Universität Bochum, D-44780, Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

The phase diagram of iron-based superconductors exhibits an anti ferromagnetic phase at low doping and an unconventional superconducting phase at larger carrier concentration. Some compounds are even believed to have a microscopic coexistence regime of both orders. We systematically calculate quasiparticle interference (QPI) signatures for the whole phase diagram of iron-based superconductors. Impurities inherent in the sample together with ordered phases lead to distinct features in the QPI images that are believed to be measured in spectroscopic imaging-scanning tunneling microscopy (SI-STM).

In the spin-density wave phase the rotational symmetry of the electronic structure is broken, signatures of which are also seen in the coexistence regime with both superconducting and magnetic order.

In the superconducting regime we show how the different scattering behavior for magnetic and non-magnetic impurities allows to verify the $s\pm$ symmetry of the order parameter. The effect of possible gap minima or nodes is discussed.

[1] A. Akbari, J. Knolle, I. Eremin, and R. Moessner, Phys. Rev. B, 82, (2010) (in press).
[2] J. Knolle, I. Eremin, A. Akbari, and R. Moessner, Phys. Rev. Lett. 104, 257001 (2010).

15 min. break

TT 32.6 Wed 12:00 HSZ 304

Cleavage behavior and surface states in Ferropnictides — •Klaus Koepernik[1], Alexander Lankau[1], Helmut Eschrig[1], Jeroen van den Brink[1], Sergey Borisenko[1], Erik van Heumen[2], and Mark S. Golden[2] — [1]IFW Dresden, Germany — [2]Zeeman Institute, University of Amsterdam, Netherlands

We present a density functional study of the surface electronic structure and the cleavage behavior of LiFeAs and Co-doped $BaFe_2As_2$. The results are discussed together with angle resolved photo emission (ARPES) and low energy electron diffraction (LEED) data. The two systems behave rather differently and we conclude that LiFeAs will be the ideal system for surface sensitive probes among the iron pnictide family.

TT 32.7 Wed 12:15 HSZ 304

Dichotomy between Large Local and Small Ordered Magnetic Moments in Iron-Based Superconductors — •Alessandro Toschi[1], Philipp Hansmann[1], Ryotaro Arita[2], Shiro Sakai[1], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Department of Applied Physics, University of Tokyo, Japan

We study a four-band model for iron-based superconductors within the local density approximation combined with dynamical mean-field theory (LDA + DMFT). This successfully reproduces the results of models which take As p degrees of freedom explicitly into account and has several physical advantages over the standard five d-band model. Our findings[1] reveal that the new superconductors are more strongly correlated than their single-particle properties suggest. Two-particle correlation functions unveil the dichotomy between local and ordered magnetic moments in these systems, calling for further experiments to better resolve the short time scale spin dynamics.

[1] P. Hansmann, R. Arita, AT, S. Sakai, G. Sangiovanni, K. Held, Phys. Rev. Lett. **104**, 197002 (2010)

TT 32.8 Wed 12:30 HSZ 304

Order-Parameter Anisotropies in the Pnictides - An Optimization Principle for Multi-Band Superconductivity — •Christian Platt[1], Ronny Thomale[2], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg — [2]Department of Physics, Princeton University

Using general arguments of an optimization taking place between the pair wave function and the repulsive part of the electron-electron interaction, we analyze the superconducting gap in materials with multiple Fermi-surface (FS) pockets, with application to two proto-type (P-based and As-based) ferropnictides. The main point of our work is to show that the SC state, its gap and, in particular, its anisotropy in momentum space is determined by an optimization, which balances the interplay between the attractive interaction in the sign-reversing $s_\pm$-channel and the Coulomb repulsion. This Coulomb repulsion, as discussed below, is unavoidable in a multi-band SC situation: it appears because of a kind of frustration in the $s_\pm$-channel, when more than two FS-pockets are involved in setting up the pairing interaction. On the basis of functional Renormalization Group (fRG) calculations for a wide parameter span of the bare interactions and for the different FS topologies applying to these two characteristic Fe-based superconductors, we show that the symmetry of the gap and the nodal versus nodeless behavior is driven by this optimization requirement.

TT 32.9 Wed 12:45 HSZ 304

Antiferromagnetic order in multi-band Hubbard models for iron-pnictides — •Tobias Schickling[1], Florian Gebhard[1], and Jörg Bünemann[2] — [1]Fachbereich Physik, Philipps Universität, Renthof 6, 35032 Marburg — [2]Institut für Physik, BTU Cottbus, Postfach 101344, 03013 Cottbus

In our presentation, we discuss the physics of multi-band Hubbard models for LaOFeAs which we have investigated by means of the Gutzwiller variational theory [1]. An analysis of the paramagnetic ground state shows that neither Hartree–Fock mean-field theories nor effective spin models describe these systems adequately. In contrast to Hartree–Fock-type approaches, the Gutzwiller theory predicts that antiferromagnetic order requires substantial values of the local Hund's-rule exchange interaction. For a three-band model, the antiferromagnetic moment fits experimental data for a broad range of interaction parameters. However, for the more appropriate five-band model, the iron e_g electrons polarize the t_{2g} electrons and they substantially contribute to the ordered moment. Therefore, we argue that an inclusion of the arsenic $4p$ bands is essential for a proper description of the magnetic order in LaOFeAs.

[1] T. Schickling, F. Gebhard, and J. Bünemann, arXiv:1011.6219

TT 33: CE: Metal-Insulator Transition 1

Time: Wednesday 10:30–13:00 Location: HSZ 105

TT 33.1 Wed 10:30 HSZ 105

A Microscopic View on the Mott transition in Cr-doped V_2O_3 — •Nicolaus Parragh[1], Stefano Lupi[2], Leonetta Baldassare[3], Daniele Nicoletti[4], Marino Marsi[5], Philipp Hansmann[1], Alessandro Toschi[1], Tanusri Saha-Dasgupta[6], Ole-Krogh Andersen[7], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]CNR-IOM and Universita' di Roma "La Sapienza", Italy — [3]Sincrotrone Trieste, Italy — [4]Universita' di Roma "La Sapienza" Italy — [5]Laboratoire de Physique des Solides, CNRS-UMR 8502, Orsay, France — [6]S.N.Bose Center for Basic Sciences, Kolkata, India — [7]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The metal-insulator transition in Chromium-doped Vanadium Sesquioxide has recieved much attention since its discovery in 1969. After several attempts for describing it in the framework of single-band Hubbard models some key experiments reveiled the intimate multi-band nature of this material. Here I will present the results of a recent experiment combining Infrared (IR), Scanning Photoemission Microscopy (SPEM) and X-ray Diffraction (XRD) and local density approximation + dynamical mean field theory (LDA+DMFT) calculations showing for the first time that microscopic islands characterized by bad metallic behaviour form close to the first-order transition. The bad metallicity is only partially reduced by applying pressure, pointing to a non-trivial interplay between the orbital degrees of freedom [1].

[1] Nature Communications 1, 105 (2010)

TT 33.2 Wed 10:45 HSZ 105

Symmetry of magnetite in the low-temperature phase — •Chun-Fu Chang[1], Arata Tanaka[2], Marcel Buchholz[1], Christoph Trabant[1,3], Enrico Schierle[3], Justina Schlappa[3], Detlef Schmitz[3], Marita Döhler[1], Pascal Vogt[1], Liu Hao Tjeng[1,4], and Christian Schüssler-Langeheine[1,3] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Department of Quantum Matter, ADSM, Hiroshima University, Japan — [3]Helmholtz-Zentrum Berlin, Germany — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Magnetite (Fe_3O_4) undergoes upon cooling below 123 K a first order phase transition, which is accompanied by a rise of the resistivity by two orders of magnitude: the Verwey transition. Below the transition, magnetite exhibits a complex crystal structure; structural studies so far assume a pseudo orthorhombic symmetry. We have carried out a combined experimental and theoretical analysis of the local symmetry of the divalent iron ions in octahedral environment in magnetite. Our results clearly show that the local symmetry of these iron ions cannot be described as pseudo-orthorhombic. A monoclinic distortion is not a small correction but dominant. This has important consequences for the kind of orbital order that can form in magnetite. The orbital-order models based on the pseudo-orthorhombic symmetry are hence challenged. On the other hand a model assuming a complex orbital order matches the experimental data very well. Supported by the DFG through SFB 608, by the BMBF through projects 05 S3XBA/5 and 05 KS7PK1, and by the HZB.

TT 33.3 Wed 11:00 HSZ 105

The Verwey transition ultrafast: lattice and charge/orbital order go head-to-head — •N. Pontius[1], C.-F. Chang[2], T. Kachel[1], C. Trabant[1,3], M. Beye[1], W. Schlotter[3], S. de Jong[3], F. Sorgenfrei[4], R. Kukreja[3], B. Bräuer[3], M. Döhler[2], S. Hossain[3], C. Back[3], A. Scherz[3], D. Zhu[3], J. Turner[3], W.-S. Lee[3], Y.-D. Chuang[3], O. Krupin[3], M. Buchholz[2], P. Vogt[2], W. Wurth[4], A. Föhlisch[1], H. A. Dürr[3], and C. Schüssler-Langeheine[1,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]II. Physikalisches Institut, Universität zu Köln — [3]SLAC National Accelerator Laboratory, USA — [4]Institut für Experimentalphysik, Universität Hamburg

At 120K magnetite (Fe_3O_4) undergoes a metal-to-insulator transition, the Verwey transition. It is accompanied by a transition from a charge/orbital ordered state with a monoclinic symmetry to a high temperature cubic phase without electronic order. Until today the question whether this transition is mainly driven by the lattice or by electronic degrees of freedom remains unanswered.

Here we report on a time-resolved resonant soft x-ray diffraction experiment performed at the LCLS in Stanford, USA. We studied the structural and electronic response when the insulator-to-metal transition is induced by a fs laser pulse which selectively excites the electronic subsystem. Surprisingly, the data show that both, a change of lattice symmetry and the quenching of charge/orbital order occur on a sub 200fs timescale. Moreover, the measurements suggest the formation of a new transient phase, which has not been observed in equilibrium.

TT 33.4 Wed 11:15 HSZ 105

Magnetic order in $Pr_{1-x}Ca_{1+x}MnO_4$ with x=2/3 — •H. Ulbrich[1], P. Steffens[2], O.J. Schumann[1], D. Lamago[3], Y. Sidis[3], and M. Braden[1] — [1]II. Phys. Institut, Universität zu Köln — [2]ILL, Grenoble (France) — [3]LLB, Saclay (France)

Stripe and checkerboard ordering of charges in several metal oxide compounds are thought to be linked to exotic behaviour such as high-temperature superconductivity and colossal magnetoresistivity (CMR). The coupling of charges, orbitals and spins (COS) are essential for the understanding of the CMR in the manganites. When the doping level deviates away from half-doping (x>0.5), significant controversies have arisen regarding the COS ordered structure [1,2]. Two different models have been proposed: The Bi-stripe model and the Wigner-crystal model. Investigations in $La_{0.42}Sr_{1.58}MnO_4$ exhibit an incommensurate stripe-like coupling of four order parameters: charges, orbitals and magnetic ordering of Mn^{3+} and Mn^{4+} spins [3].In order to decide between the Wigner-crystal model and the Bi-stripe model, we studied $Pr_{0.33}Ca_{1.67}MnO_4$ by elastic and inelastic neutron scattering. Our observations are in agreement with the Wigner-crystal model [4]. First studies of the magnon dispersion around the incommensurable magnetic satellites exhibit an 'hour-glass' like behaviour similar to the spin dispersion in $La_{2-x}Ba_xCuO_4$ at low doping [5].

[1] S. Mori et al., Phys. Rev. Lett. 81, 3972 (1998).
[2] P.G. Radaelli et al., Phys. Rev. B 59, 14440 (1999).
[3] H. Ulbrich et al., submitted to Phys. Rev. Lett.; arXiv: 1008.4496.
[4] H. Ulbrich et al., manuscript in preparation.
[5] J.M. Tranquada et al., Nature (London) 429, 534 (2004).

TT 33.5 Wed 11:30 HSZ 105

Charge-dynamics in Pr-doped La,Sr-bilayer manganites with 40% hole doping — •Jan Thöne, Torben Hänke, Volodymyr Zabolotnyy, Mircae Apostu, Klaus Koepernik, Sergei Borisenko, Bernd Büchner, and Jochen Geck — Leibnitz Institute for Solid State and Materials Research Dresden

To analyse the charge dynamics of La,Sr-bilayer manganites we performed angle resolved photoemission measurements on $(La_{1-x}Pr_x)_{1.2}Sr_{1.8}Mn_2O_7$ single crystals. The spectra are compared to a tight-binding Wannier model. The measured bilayer splitting is much smaller than the calculated one, indicating a strongly reduced hybridization between the bilayer-planes in the real material. Further the spectral function exhibits fingerprints of a periodic perturbation with an interaction strength of around 400 meV. A possible origin of

such a perturbation are CE-type charge-order fluctuations.

15 min. break

TT 33.6 Wed 12:00 HSZ 105

Total Energy Study of Orbital Ordering Phenomena with LDA+DMFT — •Andreas Flesch[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich — [2]German Research School for Simulation Sciences, 52425 Jülich

Orbital and magnetic ordering phenomena play a crucial role in the physics of strongly correlated transition-metal oxides. $LaMnO_3$, the parent compound of the colossal magnetoresistance manganites, is considered a textbook example of an orbitally ordered material. To determine the orbital and spin order in this system, we perform low temperature total energy [1,2] calculations based on the LDA+DMFT approach. Consequences for the origin of the cooperative Jahn-Teller distortions [3] will be discussed.

[1] B. Amadon et al., PRL **96**, 066402 (2006)
[2] I. Leonov et al., PRL **101**, 096405 (2008)
[3] E. Pavarini and E. Koch, PRL **104**, 086402 (2010)

TT 33.7 Wed 12:15 HSZ 105

LDA+DMFT study of (Sr, Ca)$_{n+1}$Ru$_n$O$_{3n+1}$ ruthenates — •Evgeny Gorelov and Eva Pavarini — IFF and IAS, Forschungszentrum Jülich, 52425 Jülich

The ruthenates of the Ruddelsen-Popper series $(Sr, Ca)_{n+1}Ru_nO_{3n+1}$ are unique among transition-metal oxides: changes in the number of RuO_2 layers, Sr/Ca content and temperature lead to a variety of different properties, ranging from Mott insulating behavior and orbital order to metallic ferro- and meta- magnetism.

In order to understand how structural changes affect the properties, we perform and LDA+DMFT calculations for material-specific Hubbard models describing the partially filled *Ru* $4d^4$ shells. Since the e_g *Ru* bands are well above the Fermi level, we consider only the t_{2g} bands. For $n = 3$ the unit cell contains two inequivalent *Ru* atoms, thus for this system we perform six-orbital LDA+cDMFT calculations.

The LDA+cDMFT scheme used is based on the ab-initio NMTO downfolding procedure and a weak-coupling CT-QMC impurity solver with full rotationally-invariant Coulomb interaction. We use a self-energy matrix in orbital space - Σ_{ij}.

We identify the main difference among the materials in a substantial rearrangement of Ru t_{2g} occupations, controlled by the interplay between Coulomb repulsion, number of RuO_2 layers n, which reflects effective dimensionality, and changes in the t_{2g} crystal field.

TT 33.8 Wed 12:30 HSZ 105

Evidence for a temperature-induced spin-state transition of Co^{3+} in La$_{2-x}$Sr$_x$CoO$_4$ — •Nils Hollmann[1], Maurits Haverkort[2], Mohammed Benomar[1], Matthias Cwik[1], Markus Braden[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

The magnetic susceptibility of mixed-valent $La_{2-x}Sr_xCoO_4$ single crystals in a doping range of $0.5 \leq x \leq 0.8$ and in a temperature range up to 1000 K is studied with the focus on the spin-state of the Co ions. The materials bear close resemblance to $LaCoO_3$, a compound well-known for a spin-state transition of its Co^{3+} ions. In $La_{2-x}Sr_xCoO_4$, the magnetism below room temperature can be described by paramagnetic Co^{2+} in the high-spin state and Co^{3+} in the non-magnetic low-spin state [1]. Above room temperature, however, an increase in susceptibility compared to the behavior expected from Co^{2+} is seen. We attribute this rise in moment to a thermally-induced spin-state transition of Co^{3+}, and analyze the experimental data by comparison to full-multiplet calculations for the thermal population of a higher-spin state of Co^{3+}. We find the energy gap between the spin states being in the order of 2000 K, which hardly changes with doping. *This work is supported by the SFB through SFB 608.*

1] N. Hollmann *et al.*, New Journal of Physics **10**, 023018 (2008).

TT 33.9 Wed 12:45 HSZ 105

Two Pressure-induced structural phase transitions in TiOCl — •Jihaan Ebad-Allah[1], Andreas Schoenleber[2], Sander van Smaalen[2], Michael Hafland[3], Mattias Klemm[1], Siegfried Horn[1], Sebastian Glawion[4], Michael Sing[4], Ralph Claessen[4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Laboratory of Crystallography, Universität Bayreuth, 95440 Bayreuth, Germany — [3]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France — [4]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (with X=Cl or Br) are low-dimensional materials which undergo an unconventional transition to a spin-Peierls state via a structural incommensurate state. With the electronic configuration $3d^1$ these compounds are Mott-Hubbard insulators with a charge gap of ≈2 eV. As a follow-up to our recent investigations on TiOX [1], we studied the crystal structure of TiOCl by powder X-ray diffraction measurements at room temperature up to high pressures of p≈25 GPa. Besides a phase transition at p_{c1}≈15 GPa from the orthorhombic Pmmn to the monoclinic $P2_1/m$ crystal structure with a 2a×2b×c superstructure, we find a pressure-induced isostructural phase transition p_{c2}≈22 GPa for the monoclinic phase with anomalies in the lattice parameters [2].

[1] C. A. Kuntscher et al., Eur. Phys. J. Special Topics **180**,29 (2010).
[2] J. Ebad-Allah et al., Phys. Rev. B **82**, 134117 (2010).

TT 34: TR: Quantum Coherence and Quantum Information Systems 2 (jointly with MA and HL)

Time: Wednesday 14:00–18:45 Location: HSZ 03

TT 34.1 Wed 14:00 HSZ 03

Multiplexing Readout of a Qubit Array via a Single Transmission Line — •Markus Jerger[1], Stefano Poletto[1], Pascal Macha[1,2], Uwe Hübner[2], Alexander Lukashenko[1], Evgeni Il'ichev[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany

A resonant circuit coupled to a qubit displays a shift of its resonance frequency depending on the quantum state of the qubit. The qubit state can be thus measured by probing the resonator near its resonance frequency. By coupling every qubit to its individual resonator of distinct frequency, one can read out the state of an array of many qubits through a single microwave line coupled to all resonators. Moreover, this readout can be performed simultaneously by using a multi-tone microwave pulse with frequency-division multiplexing. We will present measurements on an ensemble of 7 superconducting flux qubits located on one chip and each coupled to an individual transmission-line resonator. We performed spectroscopy of all qubits and determined their parameters in a single measurement run. Our latest experiments on simultaneous preparation and readout of the 7-qubit array will be presented.

TT 34.2 Wed 14:15 HSZ 03

A flux-driven Josephson parametric amplifier for experiments with propagating quantum microwaves — •Edwin P. Menzel[1], Alexander Baust[1], Frank Deppe[1], Peter Eder[1], Thomas Niemczyk[1], Elisabeth Hoffmann[1], Max Haeberlein[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-shi, Japan — [4]NEC Corporation, Tsukuba, Japan

For the detection of propagating quantum microwaves in circuit QED linear amplifiers are key ingredients. 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 often introduce a finite amount of noise. We have recently shown that, despite such a residual noise, signals on

the quantum level can be fully characterized using two amplification chains and suitable correlations [E.P. Menzel et al., PRL 105, 100401 (2010)]. In this work, we characterize a flux-driven JPA. At 5.64 GHz the maximum degenerate gain is 25.5 dB and the signal bandwidth is 1.8 MHz. Phase-insensitive measurements yield a noise temperature of 100±20 mK, which is below the standard quantum limit of 135 mK.

This work is supported by SFB 631, NIM, Basque Government IT4720-10, Spanish MICINN FIS2009-12773-C02-01, and EU project SOLID.

TT 34.3 Wed 14:30 HSZ 03

Generation of non-classical states for microwave photons in networks of circuit cavities — •Martin Leib and Michael J. Hartmann — TU München,Munich,Germany

State of the art fabrication of superconducting microwave resonators coupled to Josephson qubits provides us with an architecture where strong coherent interaction of individual microwave photons with individual two-level systems (qubits) has been realised with exceptional control over both, photons and qubits. Here we consider a network of multiple microwave resonators each equipped with a Josephson qubit and analyse the quantum states of the output photons at several ports of the network. With time independent [1] or sequential driving one can generate highly non-classical states of the microwave field in specific network nodes. We investigate the generation, propagation and dissipation of these states along branches of the network. As a signature for the non-classical nature of the microwave field we quantify the generation of entanglement between various output ports of these networks of circuit QED systems.

[1] M. Leib and M.J. Hartmann *Bose-Hubbard dynamics in a chain of circuit QED cavities* **New Journal of Physics** Vol. 12 Nr. 9 pp. 093031

TT 34.4 Wed 14:45 HSZ 03

Probing decoherence through Fano resonances — •Stefan Rotter[1], Andreas Bärnthaler[1], Florian Libisch[1], Joachim Burgdörfer[1], Stefan Gehler[2], Ulrich Kuhl[2], and Hans-Jürgen Stöckmann[2] — [1]Institute for Theoretical Physics, TU Vienna, Austria — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany

We investigate the effect of decoherence on Fano resonances in wave transmission through resonant scattering structures [1]. We show that the Fano asymmetry parameter q follows, as a function of the strength of decoherence, trajectories in the complex plane that reveal detailed information on the underlying decoherence process. Dissipation and unitary dephasing give rise to manifestly different trajectories. Our predictions are successfully tested against microwave experiments with metal cavities and against previously published data on the temperature dependence of transport through quantum dots [2].

[1] A. Bärnthaler, S. Rotter, F. Libisch et al., Phys. Rev. Lett. 105, 056801 (2010).
[2] I. G. Zacharia, D. Goldhaber-Gordon, G. Granger et al., Phys. Rev. B 64, 155311 (2001).

TT 34.5 Wed 15:00 HSZ 03

Dissipative Landau-Zener Transitions at High Temperatures — •Peter Nalbach and Michael Thorwart — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

We study Landau-Zener transitions in a dissipative environment including excitation survival probability [1,2] by a numerically exact approach. Competition between relaxation and the external driving results in nonmonotonic behaviour of the ocupation probabilities which we explain in terms of an appealing phenomenological model. We furthermore show that the nonmonotonic behaviour survives up to very high temperatures where so far monotonic behaviour due to dominant dephasing was expected.

[1] P. Nalbach and M. Thorwart, Phys. Rev. Lett. 103, 220401 (2009)
[2] P. Nalbach and M. Thorwart, Chem. Phys. 375, 234 (2010)

TT 34.6 Wed 15:15 HSZ 03

Feedback Control of a Transport Charge Qubit — •Christina Pöltl, Clive Emary, and Tobias Brandes — TU Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, D-10623 Berlin, Germany

We study a simple feedback control operation acting on a transport double quantum dot instantaneously after an electron jumps into the dot. A qubit system such as a double quantum dot is affected by decoherence once it is coupled to an environment. An electronic transport system always experiences decoherence and the projection on the qubit-state relaxes into a statistical mixture. However, we show that feedback qubit rotations enable the generation of pure states as steady states of the system.

We use a master equation jump approach in order to include the feedback which allows us to investigate the steady state as well as the full counting statistics of the transport qubit with feedback.

15 min. break

Invited Talk TT 34.7 Wed 15:45 HSZ 03

Coupled evolution and coherence of two-electron spin qubits — •Hendrik Bluhm — Harvard University, Cambridge, USA and RWTH Aachen, Germany

One of the fundamental requirements for quantum computing is to coherently couple qubits in order to generate entanglement. For semiconductor qubits, such entangling gates have yet to be demonstrated in fully operational devices. I will give a brief overview of our recent experiments on enhancing the coherence of two-electron spin qubits in GaAs double quantum dots, and then focus on current progress towards the realization of two-qubit entangling gates.

By manipulating a qubit in a way that decouples its evolution from the fluctuations of its nuclear spin bath, we extended its coherence time to more than 200 μs, two orders of magnitude longer than previously measured. Operating the qubit as a feedback loop that controls the nuclear bath enables universal single qubit control with greatly improved gate fidelities.

Using the Coulomb interaction between two adjacent double dots, we demonstrate a dependence of the coherence of one qubit on the state of the other, which results in strong correlations in a joint single shot readout of the two qubits. In this operation, the control qubit completely dephases due to low frequency electrical noise. Using a spin echo pulse, the single-qubit dephasing time can be extended by an amount that is expected to enable a fully coherent cPHASE gate, which would entangle the two qubits.

TT 34.8 Wed 16:15 HSZ 03

Dynamical switching of a driven nonlinear resonator caused by a two-level fluctuator — •Stephan André[1,2], Michael Marthaler[1,2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

In recent "circuit QED" experiments, a nonlinear resonator was used to perform a quantum non-demolition readout of a superconducting qubit with a high contrast [1,2]. A driven nonlinear resonator can show bistability; increasing the driving strength will lead to switching from a state of low amplitude to a state of high amplitude oscillations. As the switching of the resonator occurs at a driving strength which depends on the state of the qubit, the resonator can be operated at a working point where, depending on the qubit state, it will switch to high amplitude oscillations or not, which provides a digital readout of the qubit.

We theoretically study the influence of a two-level fluctuator (TLF) coupled to a driven nonlinear resonator. TLFs have frequently been observed in superconducting circuits and generally affect the dynamics of the system. We investigate how the presence of a TLF influences the switching of the driven resonator between the two dynamical states. This will lead to a change in the readout contrast when the resonator is used to measure a qubit.

[1] M. Metcalfe *et al.*, Phys. Rev. B **76**, 174516 (2007)
[2] F. Mallet *et al.*, Nature Physics **5**, 791 (2009)

TT 34.9 Wed 16:30 HSZ 03

Measuring the temperature dependence of individual two-level systems by direct coherent control — •Jürgen Lisenfeld[1,4], Clemens Müller[2,4], Jared H. Cole[3,4], Pavel Bushev[1,4], Alexandr Lukashenko[1,4], Alexander Shnirman[2,4], and Alexey V. Ustinov[1,4] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

We demonstrate a new method to directly manipulate the state of

individual two-level systems (TLSs) in phase qubits. It allows one to characterize the coherence properties of TLSs using standard microwave pulse sequences, while the qubit is used only for state readout. We apply this method to measure the temperature dependence of TLS coherence for the first time. The energy relaxation time T_1 is found to decrease quadratically with temperature for the two TLSs studied in this work, while their dephasing time measured in Ramsey and spin-echo experiments is found to be T_1 limited at all temperatures.

TT 34.10 Wed 16:45 HSZ 03

Defect models in superconducting phase qubits — •Clemens Müller[1,2], Jared H. Cole[3,2], Pavel Bushev[4,2], Grigorij J. Grabovskij[4], Jürgen Lisenfeld[4], Alexey V. Ustinov[4,2], and Alexander Shnirman[1,2] — [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

Superconducting qubits often show signatures of coherent coupling to intrinsic two-level systems (TLS), which manifest themselves as avoided level crossings in spectroscopic data. We use detailed theoretical models to determine the form of the coupling between a superconducting phase qubit and a TLS. Fitting the experimental data with our theoretical model allows us to determine all relevant system parameters. A strong qubit-defect coupling is observed, with a nearly vanishing longitudinal component. Using these estimates, we quantitatively compare several existing theoretical models for the microscopic origin of TLS.

TT 34.11 Wed 17:00 HSZ 03

Holonomic transformations with superconducting qubits — •Ingo kamleitner and Alexander Shnirman — Institut für Theorie der kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany

Holonomic transformations are known to be robust to small variations of the Hamiltonian and are therefore a promising method to achieve fault tolerant quantum gates for quantum information processing. Here we propose an experimentally feasible holonomic transformation using three superconducting qubits of the transmon type coupled to a cavity. The Hamiltonian in the one-excitation subspace is of the tripod type, which naturally has a degenrate subspace and is well suited for holonomies. The effective cavity transmon couplings are achieved via external driving of the transmons and are tunable.

TT 34.12 Wed 17:15 HSZ 03

Deterministic creation and stabilization of entanglement in circuit QED by homodyne-mediated feedback control — Zhuo Liu[2], Lülin Kuang[2], Kai Hu[2], Luting Xu[2], Suhua Wei[2], Xinqi Li[2], and •Lingzhen Guo[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Department of Physics, Beijing Normal University, Beijing 100875, China

In a solid-state circuit QED system, we demonstrate that a homodyne-current-based feedback can create and stabilize highly entangled two-qubit states in the presence of a moderate noisy environment. Particularly, we present an extended analysis for the current-based Markovian feedback, which leads to an improved feedback scheme. We show that this is essential to achieve a desirable control effect by the use of dispersive measurement.

15 min. break

TT 34.13 Wed 17:45 HSZ 03

Monitoring and Markovian Feedback Control of a Solid-state Charge Qubit — •Gerold Kiesslich, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

We investigate theoretically a charge qubit capacitively coupled to a single-electron transistor (SET). A quantum master equation approach [1] is used to address the question how it is possible to continuously monitor the qubit dynamics by SET transport observables. We further demonstrate analytically and numerically the qubit manipulation and control by instantaneous feedback of the SET current into qubit parameters. Feedback-induced qubit rotations and pure states as steady states can be generated.

[1] G. Schaller, G. Kießlich, and T. Brandes, Phys. Rev. B **80**, 245107 (2009). *ibid.* **81**, 205305 (2010). *ibid.* **82**, 041303(R) (2010).

TT 34.14 Wed 18:00 HSZ 03

Hybridization and spin decoherence in heavy-hole quantum dots — •Jan Fischer[1] and Daniel Loss[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland

We theoretically investigate the spin dynamics of a heavy hole confined to a III-V semiconductor quantum dot interacting with a narrowed nuclear-spin bath [1]. We show that band hybridization leads to an exponential decay of hole-spin superpositions due to hyperfine-mediated nuclear pair flips, and that the accordant single-hole-spin decoherence time T2 can be tuned over many orders of magnitude by changing external parameters. In particular, we show that, under experimentally accessible conditions, it is possible to suppress hyperfine-mediated nuclear-pair-flip processes so strongly that hole-spin quantum dots may be operated beyond the 'ultimate limitation' set by the hyperfine interaction which is present in other spin-qubit candidate systems.

[1] J. Fischer and D. Loss, arXiv:1009.5195 (2010).

TT 34.15 Wed 18:15 HSZ 03

Different types of integrability and their relation to decoherence in central spin models — •Bjoern Erbe and John Schliemann — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

In a large variety of nanostructures spins couple to a bath of other spin degrees of freedom. Important examples are given by semiconductor and carbon nanotube quantum dots, phosphorus donors in silicon, nitrogen vacancy centers in diamond and molecular magnets. Commonly such systems are described by so-called central spin models [1,2].

We present recent results on the relation between integrability and decoherence in central spin models with more than one central spin [3]. We show that there is a transition between integrability ensured by Bethe ansatz and integrability ensured by complete sets of commuting operators. This has a significant impact on the decoherence properties of the system, suggesting that it is not necessarily integrability or non-integrability which is related to decoherence, but rather its type or a change from integrability to non-integrability.

[1] J. Schliemann, A. Khaetskii, and D. Loss, J. Phys.: Condens. Mat. 15, R1809 (2003).
[2] W. A. Coish and J. Baugh, phys. stat. sol. B 246, 2203 (2009).
[3] B. Erbe and J. Schliemann, Phys. Rev. Lett. 105, 177602 (2010).

TT 34.16 Wed 18:30 HSZ 03

Turning a vice into a virtue: Hyperfine induced nuclear spin dynamics in double quantum dots — •Bjoern Erbe and John Schliemann — Department of Physics, University of Regensburg, 93040 Regensburg, Germany

Electron spins confined in semiconductor quantum dots with an s-type conduction band, like for example GaAs quantum dots, interact with the surrounding nuclear spins via the hyperfine interaction [1]. With respect to possible future solid state quantum computation systems utilizing the electron spin as the qubit [2], these interactions act as a source of decoherence. We demonstrate that it is possible to turn vice into virtue by using the hyperfine interaction in order to utilize nuclear baths for quantum information purposes [3].

To this end, we numerically study the hyperfine induced nuclear spin dynamics in a system of two coupled quantum dots in zero magnetic field. Each of the electron spins is considered to interact with an individual bath of nuclear spins. Through quantitative investigations of several scaling behaviors we show that it is possible to swap the nuclear ensembles and indicate that it might even be possible to fully entangle them. It turns out that the larger the baths are, the more relevant they become as a ressource of quantum information.

[1] see e.g. J. Schliemann, A. Khaetskii, and D. Loss, J. Phys.: Condens. Matter 15, R1809 (2003).
[2] D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998).
[3] B. Erbe and J. Schliemann, in preparation

TT 35: CE: Low-dimensional Systems - Materials 3

Time: Wednesday 14:00–19:45 Location: HSZ 301

TT 35.1 Wed 14:00 HSZ 301

EELS and RIXS measurements of $La_{1-x}Sr_{1+x}MnO_4$, signatures of polarons — •Roberto Kraus[1], Matthias Schrade[1], Valentina Bisogni[1], Pieter Glatzel[2], Martin Knupfer[1], Bernd Büchner[1], and Jochen Geck[1] — [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 states 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 have performed electron energy-loss spectroscopy (EELS) and resonant inelastic X-ray scattering (RIXS) at the Mn K-edge. The observed in-gap excitation shows a small positive dispersion, which is a sign of a delocalized excitation. As a function of temperature a clear positive shift for this peak was found in the half-doped sample, implying a strong coupling of charge and spin dynamics. We present a model of electronic polarons for the new in-gap states which are created around the doped holes. The finite dispersion provides further the indication of polaron-ploaron interactions.

TT 35.2 Wed 14:15 HSZ 301

Magnetic and phononic excitation spectrum of the spin dimer system $Sr_3Cr_2O_8$ — •Dirk Wulferding[1], Peter Lemmens[1], Kwang-Yong Choi[1,2], Vladimir Gnezdilov[1,3], Diana Quintero-Castro[4], Bella Lake[4], Seunghun Lee[5], Hiroaki Ueda[6], Yutaka Ueda[6], and Joachim Deisenhofer[7] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]Chung-Ang Univ., Seoul, Korea — [3]ILTPE NAS, Ukraine — [4]Helmholtz-Zentrum Berlin, Germany — [5]Dep. of Phys., Univ. of Virginia, USA — [6]ISSP, Tokyo, Japan — [7]EP V, Univ. Augsburg, Germany

We present a Raman spectroscopic investigation of $Sr_3Cr_2O_8$, a spin dimer system with appreciable interdimer interactions. At T = 275 K the system undergoes a structural phase transition from hexagonal to monoclinic together with strong Jahn-Teller induced orbital fluctuations, that persist down to 120 K. Our temperature dependent study reveals phonon anomalies in this temperature range, as well as two magnetic modes with further decrease of temperature. We compare our results to theoretical calculations and previous neutron and infrared spectroscopic studies.

Work supported by DFG, IGSM and NTH.

TT 35.3 Wed 14:30 HSZ 301

Magnons in the Quantum Dimer Antiferromagnet $Sr_3Cr_2O_8$ — •Diana Lucia Quintero-Castro[1,2], Bella Lake[1,2], Elisa Maria Wheeler[1], and Nazmul Islam[1] — [1]Helmholtz Zentrum Berlin, Berlin 14109, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

$Sr_3Cr_2O_8$ consists of a three-dimensional frustrated arrangement of antiferromagnetically coupled pairs of Cr ions or dimers. The Cr ions are in the unusual 5+ valence state resulting in one electron in the 3d shell and a spin value of 1/2 while a tetrahedral crystal field ensures that this electron occupies the doubly degenerate eg orbitals. Below room temperature $Sr_3Cr_2O_8$ undergoes a cooperative Jahn Teller distortion that lifts the orbital degeneracy so that only the $3z^2$-r^2 orbital is occupied. The low temperature structure is characterized by monoclinic crystal symmetry and antiferro-orbital ordering. The transition also gives rise to spatially anisotropic exchange paths and results in three crystal twins. We have grown single crystals of $Sr_3Cr_2O_8$ and have performed DC susceptibility measurements, high field magnetisation and powder and single crystal inelastic neutron scattering experiments. The data reveals a singlet ground state and gapped triplet excitations consisting of three modes, coming from the three crystal twins. Using a random phase approximation, we have extracted the magnetic exchange interactions within the dimer and between dimers. $Sr_3Cr_2O_8$ is a candidate for the study of the critical properties in the quantum phase transition as the magnetic field can drive a Bose Einstein condensation of magnons.

TT 35.4 Wed 14:45 HSZ 301

Evidence for strong orbital fluctuations below the Jahn-Teller transition in $Sr_3Cr_2O_8$ — •Zhe Wang[1], Michael Schmidt[1], Axel Günther[1], Sebastian Schaile[1], Nikola Pascher[1], Franz Mayr[1], Yurri Goncharov[1], Diana Quintero-Castro[2,3], A. T. M. Nazmul Islam[2], Bella Lake[2,3], Hans-Albrecht Krug von Nidda[1], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [3]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

We report on the magnetic and phononic excitation spectrum of $Sr_3Cr_2O_8$ determined by THz and infrared (IR) spectroscopy, specific heat, and electron spin resonance measurements. We identify the singlet-triplet excitations in the dimerized ground state and observe an extended temperature range 125 K < T < 285 K below the Jahn-Teller transition, where the IR active phonons change only gradually with decreasing temperature. A clear anomaly in the specific heat marks the onset of orbital ordering at 285 K, but a detailed analysis of the orbital contribution to the specific heat shows the persistence of strong fluctuations down to 125 K in agreement with the IR data. Due to these fluctuations we can observe electron spin resonance absorptions only below 125 K with a linewidth proportional to exp(-Δ/kT) indicating an Orbach-type spin relaxation via the excited orbital state of the Cr e-doublet split by Δ/k=388 K.

TT 35.5 Wed 15:00 HSZ 301

Low dimentional magnetic properties of compounds belonging to the $CrVO_4$-type structure — •Joseph M. Law[1,2] and Reinhard K. Kremer[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart — [2]Department of Physics Loughborough University, Loughborough, Leics, LE11 3TU United Kingdom

Compounds with the ABX_4 composition exhibit a range of different magnetic properties. In recent years we have concentrated on only those adopting the $CrVO_4$-type structure, where we have a magnetic atom occupying the A position and a diamagnetic only atom within the B position. The A atom is housed within a distorted octahedral environment, the AO_6 units are edge sharing and form buckled ribbon chains along the c-axis. The B atoms are contained within tetrahedral Oxygen environments which bridge the ribbon chains.

We are present first results on the magnetic properties of some selected of this series which show, multiferroic behavior, spin-Peierls transitions and conventional long-range magnetic ordering.

15 min. break

TT 35.6 Wed 15:30 HSZ 301

Magnetic phase diagram of quasi one-dimensional Ising spin-1/2 chain system $BaCo_2V_2O_8$ — •Sandra Niesen, Gerhard Kolland, Oliver Heyer, Daniel Löwen, Martin Valldor, 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. 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. Here, we present the magnetic phase diagram extracted from measurements of the magnetization, the specific heat, the thermal expansion, magnetostriction, and the thermal conductivity in magnetic fields up to 17 T. 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. Apart from this expected Ising anisotropy, we have discovered a new magnetic anisotropy for fields applied within the aa plane. For fields applied along [110] T_N is only weakly suppressed, while for magnetic fields applied along [100] T_N is completely suppressed above about 10 T. In this case the T-H-phase boundary exhibits most probably a quantum critical point.

This work is supported by the DFG through SFB 608.

TT 35.7 Wed 15:45 HSZ 301

***Ab initio* modeling of Bose-Einstein condensation in $Pb_2V_3O_9$** — •Alexander Tsirlin and Helge Rosner — Max Planck Institute CPfS, Dresden, Germany

We present the computational approach to the microscopic study of Bose-Einstein condensation (BEC) in quantum magnets. Using density functional theory band structure calculations, we establish the microscopic magnetic model of a BEC compound $Pb_2V_3O_9$, refine the model by fitting the experimental data, and further simulate the full temperature-vs-field phase diagram. In contrast to previous theoretical descriptions based on the alternating-spin-chain model, we find that $Pb_2V_3O_9$ represents an unfrustrated quasi-two-dimensional spin system of coupled spin dimers. The intradimer coupling is about 30 K, whereas the interdimer couplings are both ferro- and antiferromagnetic. The structural implementation of the model is rather non-trivial, with weaker ferromagnetic couplings along the chains of corner-sharing VO_6 octahedra and stronger antiferromagnetic couplings between the structural chains. Our model leads to remarkable agreement with the available experimental data on the BEC in $Pb_2V_3O_9$ and discloses the role of individual exchange couplings in this compound. While antiferromagnetic couplings alone lead to a one-dimensional spin system, the presence of ferromagnetic couplings and the two-dimensionality are essential for the BEC high-field ground state of $Pb_2V_3O_9$.

TT 35.8 Wed 16:00 HSZ 301

Spin orbit coupling induced phonon anomalies and relevant electronic energy scales in Sr_2IrO_4 — •Mehmet Fatih Cetin[1,2], Peter Lemmens[1,2], Vladimir Gnezdilov[1,3], Dirk Wulferding[1,2], Dirk Menzel[1], Wolfram Brenig[4,2], Tomohiro Takayama[5], Kei Ohashi[5], and Hidenori Takagi[5,6] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]NTH, Germany — [3]ILTPE NAS, Ukraine — [4]ITP, TU-BS, Braunschweig, Germany — [5]AM, University of Tokyo, Japan — [6]RIKEN Advanced Science Institute, Japan

Sr_2IrO_4 is a Mott insulator due to the interplay of strong spin orbit coupling and crystal field interactions. The strong spin orbit interaction is evident in our study via pronounced phonon anomalies and multiphonon scattering. In addition we observe broad high energy modes that are attributed to exchange scattering on a square plane with J_{eff}=1/2.

Work is supported by DFG, IGSM and NTH School for Contacts in Nanosystems.

TT 35.9 Wed 16:15 HSZ 301

Helica magnetic structure in the distorted triangular antiferromagnet α-$CaCr_2O_4$ — •Sandor Toth[1,2], Bella Lake[1,2], Nazmul Islam[1], Simon Kimber[3], Oliver Pieper[1], Dimitri Argyriou[1], Manfred Reehuis[1], and Oksana Zaharko[4] — [1]Helmholt Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [3]ESRF, 6 Rue Jules Horowitz BP 220, 38043 Grenoble Cedex 9, France — [4]Laboratory for Neutron Scattering, PSI, CH-5232 Villigen, Switzerland

α-$CaCr_2O_4$ is a distorted triangular lattice antiferromagnet. The S=3/2 magnetic Cr^{3+} ions are located on slightly distorted stacked triangular layers. The octahedral enviroment ensures that the 3 d-electrons occupy the low lying t_{2g} levels and that the orbital moment is quenched. Magnetic susceptibility suggests strong magnetic correlations below 50 K. Powder and single crystal neutron diffraction show helical magnetic ordering below T_N=42.6 K, where the ordering wave vector k$\sim$(0 1/3 0) and the angle between neighboring spins within the triangular plane is 120°. Spherical neutron polarimetry unambiguously proved that the helical plane is perpendicular to the b axis. The observed magnetic order is a characteristic of nearest neighbor Heisenberg interactions on an equilateral triangular lattice in apparent contradiction to the distorted crystal which allows for 4 inequivalent nearest neighbour exchange paths. By simulating the magnetic order of α-$CaCr_2O_4$ as a function of these 4 interactions it is found that 120° helical order is in fact stable over a large range of parameter space.

TT 35.10 Wed 16:30 HSZ 301

Imaging of the two-dimensional polarization landscape at the $LaAlO_3/SrTiO_3$ interface — •Tim Günter[1], Andrea Rubano[1], Thomas Fink[1], Domenico Paparo[2], Fabio Miletto Granozio[2], Umberto Scotti di Uccio[2], Lorenzo Marrucci[2], Jochen Mannhart[3], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]CNR-INFM Coherentia, Università Federico II, Napoli, Italy — [3]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

$LaAlO_3/SrTiO_3$ interfaces are a challenging topic in the field of perovskite oxides. A conductive two-dimensional electron liquid (2DEL) appears at the interface for a $LaAlO_3$ thickness of n$\geq$4 unit cells. However, many questions regarding the origin and characteristics of the 2 DEL have to be adressed yet. In particular, this includes the spatial homogeneity of the interface reconstruction.

Second Harmonic Generation (SHG) is an ideal tool for studying interfaces, since it is sensitive to the interfacial symmetry breaking along the stacking direction. Furthermore, the spatial degrees of freedom of optical techniques can be exploited. Here we use SHG with amplified femtosecond laser pulses for imaging the $LaAlO_3/SrTiO_3$ interface with a spatial resolution of ≈ 2 μm. For n=1 a pronounced interfacial inhomogeneity on a lengthscale of < 1 μm is observed. The lateral dimension of these inhomogeneities increases for n=2 pointing to a step-like reconstruction of the interface. At n=3, the interface becomes homogeneous which may reflect the completion of a fully reconstructed interface, though yet without the emergence of conductivity.

15 min. break

TT 35.11 Wed 17:00 HSZ 301

Evaluation of Realistic Parameters in Organics — •Andreas Dolfen and Erik Koch — German Research School For Simulation Sciences, FZ-Jülich and RWTH Aachen University, 52425 Jülich, Germany

The study of exotic correlation effects in real strongly correlated materials evidently requires realistic parameters for the model Hamiltonians. Traditionally, they have been fitted to experiment, or semi-empirically determined. This approach is, obviously, unsatisfactory. Still, for general materials these procedures are state-of-the-art as no feasible other way is known. For organic crystals, however, we devised an approach to systematically evaluate realistic, material-specific model parameters for extended Hubbard models. Starting from density-functional calculations we include the renormalization of the model parameters due to the down-folded degrees using a distributed dipole approach. We apply the method to Θ-$(BEDT\text{-}TTF)_2I_3$.

TT 35.12 Wed 17:15 HSZ 301

Vibrational control of Mottness in the organic Mott insulator ET-F2TCNQ — Stefan Kaiser[1], •Daniele Nicoletti[1], Raanan I. Tobey[2], Nicky Dean[2], Stefano Lupi[3], Hiroshi Okamoto[4], Jun'ya Tsutsumi[4], Tatsuo Hasegawa[4], and Andrea Cavalleri[1,2] — [1]Max Planck Research Department for Structural Dynamics, Center for Free Electron Laser Science & University of Hamburg, c/o DESY, Hamburg, Germany — [2]Department of Physics, Oxford University, UK — [3]Department of Physics, University of Rome La Sapienza, Italy — [4]AIST, Tsukuba, Japan

Control of on-site electronic wavefunctions is achieved in the organic conductor ET-F2TCNQ by resonant excitation of localized vibrational modes of the ET molecule. Such excitation modulates the on-site Coulomb repulsion and modifies the relative strength of electron correlations and hopping, thus controlling the Mott criterion. We performed pump-probe experiments using optical parametrical amplifiers, with a time resolution of 80 fs. Excitation was achieved with mid-IR pulses from difference frequency mixing, resonant with two different intramolecular vibrations at 10 and 6 microns. The probe was tuned over the whole IR range, in order to trace the reflectivity changes in the charge-transfer band and the possible filling of the Mott gap, thus providing a direct evidence of the control of on-site Coulomb repulsion. Through such mode-selective excitations, the Mott gap can be filled and the system is pushed forward to the less correlated and metallic side. This approach promises a new way of control for electronic and even superconducting properties in correlated electron systems.

TT 35.13 Wed 17:30 HSZ 301

Thin films and single crystals of new organic charge transfer salts — •Milan Rudloff and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main

We synthesized and characterized both, thin films and single crystals of several new organic charge transfer (CT) systems. In general these materials consist of donor and acceptor molecules that show an additional electrostatic attraction induced by Coulomb interaction between donor and acceptor. The electronic behaviour of the resulting new complex (depending on crystal structure, temperature and pressure) can be insulating, semiconducting, metallic or superconducting.

The thin films were prepared by organic molecular beam deposition (OMBD) while single crystals were grown from solution. Samples were primarily characterized by light microscopy, X-ray diffractometry and (temperature dependent) transport measurements.
We succeeded in synthesizing a series of CT salts and thus extended the material base of CT thin films. The results presented here focus on the system 4,5,9,10-Tetramethoxypyrene-9-Dicyanomethylene-2-4-7-trinitrofluorene, especially its electronic transport characteristics.

TT 35.14 Wed 17:45 HSZ 301

Spin Excitations in the Odd Homonuclear Antiferromagnetic Molecular Nanomagnet Fe_9 — •Nikolaos P. Konstantinidis, Joscha Nehrkorn, Stefan Stuiber, and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

The homonuclear ring Fe_9 has an odd number of antiferromagnetically coupled Fe^{III} spin-5/2 centers, therefore frustration plays an important role in determining its magnetic properties. Molecular wheels of odd size have been known to possess a doubly-degenerate lowest level in each total spin S sector in the absence of magnetic anisotropy. We have performed inelastic neutron scattering measurements which produced very sharp peaks that located the transitions between the energy levels very accurately. Our magnetic susceptibility data also provided an estimate for the strength of the exchange interactions, while torque magnetometry reveals the presence of weak magnetic anisotropy. Different Hamiltonians are used to find the appropriate model for the magnetic properties of Fe_9, with the energy levels characterized by the symmetry of the Hamiltonian. Exchange interactions that respect the spatial symmetry of the molecule coupled with a uniform single-site anisotropy term can not reproduce the splitting of the lowest energy levels. Especially the lowest lying $S = 3/2$ doublet is unexpectedly robust against perturbations. This particular nature of the theoretically generated low-energy spectrum will be discussed.

TT 35.15 Wed 18:00 HSZ 301

3d-4f molecular nanomagnets investigated by X-ray magnetic circular dichroism — •Jan Dreiser[1], Cinthia Piamonteze[1], Frithjof Nolting[1], Stefano Rusponi[2], Harald Brune[2], Kasper S. Pedersen[3], Jesper Bendix[3], and Hoegni Weihe[3] — [1]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI, Switzerland — [2]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [3]Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

Single-molecule magnets are exchange-coupled spin clusters showing slow relaxation of magnetization. In recent years, efforts have been intensified to increase the magnetization reversal barrier and thus enhance relaxation times by combining rare earth ions with transition-metal ions. Rare-earth ions exhibit very large magnetic anisotropies due to their strong spin-orbit coupling and their mostly unquenched orbital momentum. In this contribution we use X-ray magnetic circular dichroism to observe element-specific magnetization curves. In conjunction with SQUID magnetization and susceptibility measurements, we are able to determine the magnetic coupling between 3d and 4f ions.

15 min. break

TT 35.16 Wed 18:30 HSZ 301

Nanogranular Metals: From electronic correlations to strain-sensing applications — •Christian H. Schwalb[1,2] and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]NanoScale Systems GmbH, Robert-Bosch-Str. 7, 64293 Darmstadt, Germany

Granular metals are artificial materials in which a conducting phase made of metallic nanoparticles is (randomly) dispersed into an insulating matrix. The charge transport in such systems is dominated by tunneling between neighboring metallic nanoparticles, a process that is strongly influenced by correlation effects. These fundamental processes can be used for practical applications, since the tunnel coupling has an intrinsically exponential dependence on the inter-grain distance that is altered under strain.

In this work, we present a novel methodology for strain-sensing based on nanogranular metals using focused electron-beam-induced deposition (FEBID). The gauge factor for these nanogranular metals depends on the conductivity of the sensor element that can be altered by electron-beam irradiation leading to a distinct maximum in the sensitivity that can be attributed to a persistent change of the dielectric carbon matrix.[1] Additionally an analysis scheme is presented that draws on recent advances in the understanding of charge transport mechanisms in granular metals [2] and allows for a semi-quantitative description of the sensitivity of granular metal based strain sensors.
[1] C. H. Schwalb *et al.*, Sensors **10**, 9847 (2010)
[2] M. Huth, J. Appl. Phys. **107**, 113709 (2010)

TT 35.17 Wed 18:45 HSZ 301

Tomonaga-Luttinger Liquid Behavior in Atomic-Scale Gold Chains on a Semiconductor — •Christian Blumenstein[1], Jörg Schäfer[1], Sebastian Meyer[1], Sebastian Mietke[2], Michael Lochner[2], Rene Matzdorf[2] und Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Institut für Physik, Universität Kassel

Atomic nanowires formed by self-organization of metal adatoms on semiconductor surfaces offer a vast playground for physics in low dimensions. While effects like a charge density wave were reported there, the quest for the observation of Tomonaga-Luttinger liquid (TLL) behavior has been ongoing. Recently, Au-induced chains on Ge(001) have been prepared [1], which are structurally and electronically of exceptional one-dimensional (1D) character. Therefore they provide an opportunity to study exotic 1D physics.

The talk will address the electronic properties of these Au chains, which have been investigated by scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) over a wide temperature range. A power-law behavior in the density of states upon energy has been discovered, characteristic of a TLL. The corresponding exponent α is found independently by both STS and ARPES. Furthermore, *universal scaling* behavior is observed as a hallmark of TLL physics. This renders the Au/Ge(001) chains the first TLL system at a crystal surface, opening new possibilities to probe modified interactions from specific atomic configurations.
[1] J. Schäfer et al., Phys. Rev. Lett. 101, 236802 (2008).

TT 35.18 Wed 19:00 HSZ 301

Tuning the electrical properties of Pt-based granular metals prepared by focused electron beam induced deposition — •Roland Sachser, Fabrizio Porrati, Christian H. Schwalb, and Michael Huth — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany

We investigated granular metals which have been prepared by focused electron beam induced deposition (FEBID) using the precursor trimethyl(methylcyclopentadienyl)platinum. Microstructural changes of the matrix caused by additional electron beam irradiation after the deposition process lead to an increase of the tunnel coupling between the metallic particles and thus allow a continuous tuning from insulating to metallic behavior with increasing irradiation dose. Transport measurements in the range from 2 K to 260 K were performed on a set of samples which had been exposed to different irradiation doses. For samples with low irradiation dose Efros-Shklowski variable range hopping is observed. Longer irradiated samples show instead a logarithmic conductivity versus temperature dependence over a wide range, e. g. from about 7 K to 260 K for an irradiation dose of $4.4 \cdot 10^5 C/m^2$. Applying a recent theoretical model [1] on this specific sample gives characteristic values for the dimensionless tunnel coupling strength, which is expected close to the metal insulator transition. The observed logarithmic temperature dependence of the conductivity is also predicted by this theory. For much higher irradiation doses we observe a metallic behavior with a positive temperature coefficient of the resistance.
[1] I. S. Beloborodov et al., Rev. Mod. Phys. **79**, 469 (2007)

TT 35.19 Wed 19:15 HSZ 301

Four-leg Shastry-Sutherland tubes in a magnetic field — •Gregor Foltin[1], Salvatore Manmana[2], Frederic Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany — [2]JILA, University of Colorado at Boulder, Colorado 80309, USA — [3]CTMC, EPF Lausanne, 1015 Lausanne, Switzerland

The origin of the exotic magnetization of the highly frustrated quantum magnet $SrCu(BO_3)_2$ is currently not understood. One theoretical challenge is the fact that it is microscopically well described by the so-called two-dimensional Shastry-Sutherland model in a parameter regime close to a quantum critical point. Especially the experimentally most prominent plateau at 1/8 seems to be not stable in the Shastry-Sutherland model at least up to intermediate couplings. The latter finding is obtained by deriving an effective low-energy model using perturbative continuous unitary transformations (pCUTs) which is

then solved in the classical approximation (CA).

In this contribution, we focus on quasi-1d versions of the model where the pCUT(+CA) approach can be compared with density matrix renormalization group (DMRG). This has been already done successfully for a two-leg Shastry-Sutherland tube. Interestingly, a novel type of magnetization plateau is found at 1/5 consisting of bound states of triplons with different quantum numbers. Here we want to extend this work by studying a Shastry-Sutherland tube with four orthogonal dimer chains. To this end results from pCUT(+CA) and DMRG are compared.

TT 35.20 Wed 19:30 HSZ 301

Quantum transport in correlated nanosystems — •Malcolm Einhellinger[1], Alex Cojuhovschi[1], Eric Jeckelmann[1], Sabine Tornow[2], and Gertrud Zwicknagl[2] — [1]Leibniz Universitaet Hannover — [2]TU Braunschweig

We investigate the transient dynamics and steady-state transport properties of correlated nanowires and the charge transfer through molecular bridges contacted to donor and acceptor species. The time-evolving block decimation (TEBD) [1] and time-dependent numerical renormalization group (TD-NRG) [2] methods are used to simulate the nonequilibrium dynamics of quantum many-body fermion models. Correlated nanowires are described as interacting one-dimensional fermion chains such as the spinless fermion model and the Hubbard model. We obtain a good agreement with the predictions of the Luttinger liquid theory. To study the charge transfer through molecules we propose a model describing a complex interacting structure contacted to non-interacting leads, which generalizes the tight-binding model proposed in [3], and discuss the TEBD and TD-NRG performances and predictions for this model.

[1] G. Vidal, Phys. Rev. Lett. 91, 147902 (2002); 93, 040502 (2004)
[2] F.B. Anders and A. Schiller, Phys. Rev. Lett. 95, 196801 (2005)
[3] S.S. Skourtis et al., Phys. Rev. Lett. 101, 238103 (2008)

TT 36: SC: Fe-based Superconductors - 122 - Properties, Electronic Structure, Mechanisms

Time: Wednesday 14:00–18:30 Location: HSZ 304

TT 36.1 Wed 14:00 HSZ 304

High-resolution thermal expansion of $Ba(Fe_{1-x}Co_x)_2As_2$: evidence for quantum criticality — •Christoph Meingast[1], Frederic Hardy[1], Philipp Burger[1,2], Devang Joshi[1], Peter Adelmann[1], Doris Ernst[1], Rainer Fromknecht[1], Peter Schweiss[1], Rolf Heid[1], and Thomas Wolf[1] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Fakultät für Physik, 76128 Karlsruhe, Germany

Unconventional superconductivity is often found in the vicinity of a doping- or pressure-induced magnetic instability, or quantum phase transition (QPT). For a pressure-induced QPT, the Grüneisen parameter is expected to diverge as temperature approaches zero and is thus a very sensitive parameter for detecting a QPT. Experimentally, the Grüneisen parameter can be determined by the ratio of the thermal expansivity to the specific heat. Here we report on high-resolution thermal expansion and specific heat measurements of $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals as a function of doping. We show that the electronic Grüneisen parameter exhibits all the features expected at a QPT: 1) non-Fermi-liquid behavior, 2) sign change of the Grüneisen parameter at the spin-density-wave transition, and 3) a divergences of the Grüneisen parameters at the beginning and end points of the superconducting dome.

TT 36.2 Wed 14:15 HSZ 304

Thermodynamic investigations of the doping and pressure dependences of the electronic density of states and the superconducting gaps in the electron-doped iron pnictide $Ba(Fe_{1-x}Co_x)_2As_2$ — •Frédéric Hardy[1], Philipp Burger[1], Thomas Wolf[1], Peter Schweiss[1], Peter Adelmann[1], Doris Ernst[1], Robert A. Fisher[2], Robert Eder[1], Rolf Heid[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

Using specific-heat and high-resolution thermal-expansion measurements, we present an extensive study of the normal- and superconducting state properties of high-quality single crystals of the electron-doped iron pnictide $Ba(Fe_{1-x}Co_x)_2As_2$. We determine the evolution of the electronic density of states and superconducting gaps with Co-doping and pressure. Our measurements illustrate the competition between magnetism and superconductivity to monopolize the Fermi surface and also reveal the existence of large gapless contributions in strongly under- and over-doped conditions. These observations are discussed in terms of pair-breaking and changes of the electronic band structure, in line with recent theories.

TT 36.3 Wed 14:30 HSZ 304

Simulation of pressure effects in the 122 family of iron pnictides — •Milan Tomić, Roser Valenti, and Harald O. Jeschke — Institut für Theoretische Physik, Johan Wolfgang Goethe Universität, Frankfurt am Main, Germany

In this talk we will present first principles structural relaxations for the Family of 122 iron pnictide materials under hydrostatic and uniaxial pressure. We discuss the properties of the structures predicted at different pressure values and compare to experiment. We determine the critical pressures for the phase transitions in $CaFe_2As_2$ and $BaFe_2As_2$.

TT 36.4 Wed 14:45 HSZ 304

Doping dependent electronic anisotropies in $Ba(Fe_{1-x}Co_x)_2As_2$ — •F. Kretzschmar[1], B. Muschler[1], R. Hackl[1], J.-H. Chu[2,3], J. G. Analytis[2,3], and I. R. Fisher[2,3] — [1]Walther Meissner Institute, 85748 Garching — [2]SIMES, SLAC, Menlo Park, CA 94025, USA — [3]GLAM, Stanford University, CA 94305, USA

Superconductivity in the iron pnictides with T_c up to 56 K does probably not originate from electron-phonon coupling. The compounds have well nested hole and electron pockets with similar cross sections encircling the $(\pi, 0)$ points and the center of the (1 Fe) unit cell which can essentially be probed independently by electronic Raman scattering (ERS) in A_{1g} and B_{1g} symmetry, respectively. We present results of ERS experiments on $Ba(Fe_{1-x}Co_x)_2As_2$ measured as a function of temperature, $T > T_c$, and doping x. The data of five samples with $x = 0.045$, 0.051, 0.055, 0.061, and 0.085 with $T_c^{\max} = 24$ K at $x = 0.061$ were analyzed applying an extended Drude model. The resulting dynamical relaxation rates $\Gamma_\mu(\omega, T)$ are distinctly different in the two symmetries μ. In particular, the zero-energy extrapolation values $\Gamma_\mu(\omega \to 0, T)$ vary strongly for B_{1g} and weakly for A_{1g} symmetry indicating a band dependence of the electronic relaxation. Surprisingly, $(\Gamma_{A1g} + \Gamma_{B1g})/2$ compares well with the temperature dependence of the DC resistivity. The anisotropy resembles that in cuprates. However, in the cuprates the electronic relaxation depends on the location on a single Fermi surface rather than on the individual sheet. We conclude, that in either case only the coupling of the electrons to spin and/or charge excitations can explain these anisotropies.

TT 36.5 Wed 15:00 HSZ 304

Chemical Pressure and Physical Pressure in Phosphorous doped $BaFe_2As_2$ — •Lina Klintberg — University of Cambridge

Measurements of the superconducting transition temperature, T_c, under pressure via bulk AC susceptibility were carried out on several concentrations of phosphorous substitution in $BaFe_2As_2$. The pressure dependence of unsubstituted $BaFe_2As_2$, phosphorous concentration dependence of substituted $BaFe_2As_2$, as well as the pressure dependence of phosphorous substituted $BaFe_2As_2$ all point towards an identical maximum T_c of 31 K. This indicates that phosphorous substitution and physical pressure are similar in terms of superconductivity in this compound, and that phosphorous substitution does not induce substantial impurity scattering.

TT 36.6 Wed 15:15 HSZ 304

Tetragonal lattice collapse in $SrFe_2As_2$ - a combined experimental and theoretical study — •Miriam Schmitt[1], Deepa Kasinathan[1], Alim Omerci[1], Katrin Meier[1], Ulrich Schwarz[1], Michael Hanfland[2], Klaus Koepernik[3], Yuri Grin[1], Andreas Leithe-Jasper[1], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Ger-

many — [2]ESRF, Grenoble, France — [3]IFW, Dresden, Germany

In a joint experimental and theoretical study we investigate the crystal structure of the Fe pnictide compounds $SrFe_2As_2$ under applied hydrostatic pressure. Applying high pressure X-ray diffraction, for a critical pressure of about 10 GPa we observe a sudden collapse of the tetragonal c axis, accompanied by a small expansion of the basal plane. This results in a drastic reduction of the c/a ratio and a significant decrease of the unit cell volume. This tetragonal collapse is well described by DFT band structure calculations and can be assigned to the formation of an additional As-As bond along the tetragonal c axis.

15 min. break

TT 36.7 Wed 15:45 HSZ 304

High Pressure investigation of pressure-induced superconductivity in $CaFe_2As_2$ — •Patrick Reuvekamp[1], Reinhard Kremer[1], Renato Gonnelli[2], and Janusz Karpinski[3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Dipartimento di Fisica and CNISM, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino (TO), Italy — [3]ETH Zurich, Rämistrasse 101, 8092 Zurich, Switzerland

Since the discovery of superconductivity in iron pnictides, many compounds in this family have been heavily studied due the easily induced superconductivity using chemical doping. In the case of $CaFe_2As_2$, high pressure can be used to establish and tune superconductivity instead. In this investigation, the phase diagram and the pressure induced onset/disappearance of superconductivity were studied using ac-resistive measurements in magnetic fields up to 11 T.

TT 36.8 Wed 16:00 HSZ 304

Interplay of antiferromagnetism, ferromagnetism and superconductivity in $EuFe_2(As_{1-x}P_x)_2$ single crystals — •Hirale S. Jeevan, Jannis Maiwald, and Philip Gegenwart — I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Friedrich Hund Platz 1, 37077 Goettingen, Germany

We present a systematic study on the influence of antiferromagnetic and ferromagnetic phases of Eu^{2+} moments on the superconducting phase upon doping the As site by isovalent P, which acts as chemical pressure on $EuFe_2As_2$. In this contribution, we shall report the magnetic susceptibility, magnetization, resistivity, specific heat and thermal conductivity measurements performed on P doped $EuFe_2As_2$ single crystals. Bulk superconductivity with transition temperatures of 22 K and 28 K is observed for x = 0.16 and 0.20 samples respectively. The Eu ions order antiferromagnetically for x = 0.13, while a crossover is observed for x = 0.22 whereupon the Eu ions order ferromagnetically. We discuss in detail the coexistence of superconductivity and magnetism in a tiny region of the phase diagram and comment on the competition of ferromagnetism and superconductivity in the title compound. In collaboration with Deepa Kasinathan and H.Rosner

TT 36.9 Wed 16:15 HSZ 304

Bridging angle-resolved photoemission spectroscopy (ARPES) with other experiments in case of iron arsenides — •Daniil Evtushinsky, Volodymyr Zabolotnyy, Alexander Kordyuk, Timur Kim, Bernd Büchner, and Sergey Borisenko — IFW Dresden

The single crystals of $(Ba,K)Fe_2As_2$ and LiFeAs were measured with angle-resolved photoemission spectroscopy (ARPES). After clarification of the Fermi surface topology, we address the issue of the superconducting gap in these compounds, which was determined via fitting the distribution of the quasiparticle density to a model, incorporating finite lifetime and experimental resolution effects. Low energy electronic structure defines many macroscopic properties of a solid, which allowed us to perform the calculation of the London penetration depth and Hall coefficient purely on the basis of ARPES data.The agreement with different measurements of the superfluid density and with magnetotransport experiments was observed. Overview of the available experimental results suggests two-gap superconductivity for most of the studied iron arsenides.

TT 36.10 Wed 16:30 HSZ 304

Electronic structure studies of parent $Ba(Eu)Fe_2As_2$ and their superconducting derivatives using angle-resolved photoemission spectroscopy (ARPES) — •S. Thirupathaiah[1], E.D.L. Rienks[1], E. van Heumen[2], H.S. Jeevan[3], P. Gegenwart[3], M.S. Golden[2], and J. Fink[1,4] — [1]HZB, Berlin — [2]Uni. Amsterdam, The Netherlands — [3]Georg-August- universität-Göttingen, Germany — [4]IFW, Dresden

The advent of $LaO_{1-x}F_xFeAs$ with T_c=26 K has brought enormous interest to the high-Tc superconductor community. It is most important to study the electronic structure of these new superconductors, i.e., Fermi surfaces and band dispersions near the Fermi level at high symmetry points in order to obtain microscopic understanding of superconductivity. We have studied the electronic structure of Fe based 122 type parent compounds and their superconducting derivatives to reveal the important information on the Fermi surface nesting conditions (between hole pockets at the Brillouin zone center and electron pockets at zone corner) as a function of electron, hole doping, and isovalent substitution of P at As site in $Ba(Eu)Fe_2As_2$. Our findings show that electron doping into parent $BaFe_2As_2$ destroy the nesting conditions and superconductivity emerges, accompanied by increase in the dimensionality of electronic structure. We observe that charge carrier doping into parent compounds show a rigid-band-like behavior of electronic structure where as isovalent substitution show a non rigid-band-type nature.

TT 36.11 Wed 16:45 HSZ 304

Electronic dispersion anomalies in iron-pnictide superconductors — •Andreas Heimes[1], Roland Grein[2], and Matthias Eschrig[1] — [1]Department of Physics, Royal Holloway, University of London — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institut of Technology

Recently, experimental studies of the spin excitation spectrum revealed a strong temperature dependence in the normal state and a resonance feature in the superconducting state of several Fe-based superconductors. Based on these findings, we develop a model of electrons interacting with a temperature dependent magnetic excitation spectrum and apply it to angle resolved photoemission in Ba_{1-x} K_x Fe_2 As_2. We reproduce in quantitative agreement with experiment a renormalization of the quasiparticle dispersion both in the normal and the superconducting state, and the dependence of the quasiparticle linewidth on binding energy. We estimate the strength of the coupling between electronic and spin excitations. Our findings support a dominantly magnetic pairing mechanism.

TT 36.12 Wed 17:00 HSZ 304

Electronic structure of TM doped *Ba122* Iron Arsenide superconductors — •Anna Buling[1], Ernst Kurmaev[2], John McLeod[3], Nikolai A. Skorikov[2], Manfred Neumann[1], Alexander Moewes[3], Yuri A. Izyumov[2], Larisa D. Finkelstein[2], Ni Ni[4], Sergey L. Bud'ko[4], and Paul C. Canfield[4] — [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 S7N 5E2, Canada — [4]Ames Laboratory U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

We report on a detailed investigation of the electronic structure of undoped and $3d-metal$ doped Ba122 superconductors by means of x-ray spectroscopy.

Suprisingly it is found that in spite of the localized magnetic moments a substitution of Fe sites in $BaFe_2As_2$ with Ni and Co results in superconductivity. The characteristic changes in the electronic structure of Ba122 induced by doping are determined by XPS and RIXS measurements. DFT calculations are added to underline the influence of the doping.

The main goal of this work is to illuminate the superconductivity mechanism in this compound.

15 min. break

TT 36.13 Wed 17:30 HSZ 304

Unconventional Raman scattering in the line node superconductor $BaFe_2(As_{1-x}P_x)_2$ — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Yurii Pashkevich[3], Sergei Gnatchenko[2], Shiregu Kasahara[4], and Yuji Matsuda[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]ILTPE NAS, Ukraine — [3]DonFTI NAS, Ukraine — [4]Dep. of Phys., Kyoto University, Japan

The phase diagram of the system $BaFe_2(As_{1-x}P_x)_2$ is probed using Raman scattering. We observe a breakdown of selection rules and a pronounced effect of the folding back of the energy versus wave vector

of dispersion curves in the non-Fermi liquid regime. This behavior contrasts with the observation of quantum oscillations in magneto transport. Possible mechanisms of such unexpected behavior are discussed.

Work supported by DFG.

TT 36.14 Wed 17:45 HSZ 304

Optical Investigations of the Superconducting State in 122 Iron-Pnictides — •Dan Wu[1], Martin Dressel[1], Guanghan Cao[2], Philipp Gegenwart[3], Bernhard Holzapfel[4], Jules Carbotte[5], and Ewald Schachinger[6] — [1]1.Physikalisches Institut, Unversitat Stuttgart — [2]Zhejiang University, China — [3]Universitat Gottingen — [4]IFW, Dresden — [5]McMaster University,Canada — [6]Graz University of Technology, Austria

The new high-Tc iron pnictide superconductors have a pronounced multiband character, which complicates the electronic properties and allows for a variety of possible superconducting ground states. We have used the infrared spectroscopy–one of the most powerful tools to investigate the low-energy electrodynamic properties of superconductors–to study several pnictide families. We made a comparison between them with the aim to answer the following questions: (1) Is it possible to have more than one superconducting gap in iron pnictide? (2) Can their order parameters be distinct from each other? (3) How does the coupling between different bands influence the gap? (4) Do the gaps have a three-dimensional character? (5) Is the gap scenario universal for all the iron pnictides? We could show that the pairing condition depends sensitively on the similarity of geometry and dimension between hole and electron Fermi-surfaces.

TT 36.15 Wed 18:00 HSZ 304

Highly anisotropic energy gap in superconducting $Ba(Fe_{0.9}Co_{0.1})_2As_2$ from optical conductivity measurements — •A. V. Pronin[1], T. Fischer[1], J. Wosnitza[1], K. Iida[2], F. Kurth[2], S. Haindl[2], L. Schultz[2], B. Holzapfel[2], and E. Schachinger[3] — [1]Dresden High Magnetic Field Laboratory (HLD), FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]IFW Dresden, Institute for Metallic Materials, 01171 Dresden, Germany — [3]Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We have measured the complex dynamical conductivity, $\sigma = \sigma_1 + i\sigma_2$, of superconducting $Ba(Fe_{0.9}Co_{0.1})_2As_2$ ($T_c = 22$ K) in the terahertz and infrared ranges. The temperature dependence of σ_1 demonstrates a pronounced coherence peak at frequencies below 15 cm^{-1} (1.8 meV). The temperature dependence of the penetration depth, calculated from σ_2, shows power-law behavior at the lowest temperatures. Analysis of the conductivity data with a two-gap model, gives the smaller isotropic s-wave gap of $\Delta_A = 3$ meV, while the larger gap is highly anisotropic with possible nodes and its rms amplitude is $\Delta_0 = 8$ meV. Overall, our results are consistent with a two-band superconductor with an $s_\pm$ gap symmetry.

TT 36.16 Wed 18:15 HSZ 304

Pseudogap-like phase in $Ca(Fe_{1-x}Co_x)_2As_2$ revealed by ^{75}As NQR — •Seung-Ho Baek, Hans-Joachim Grafe, Guillaume Lang, Lumanita Harnagea, S. Singh, Sabine Wurmehl, and Bernd Buechner — IFW-Dresden, Institute for Solid State Research, PF 270116, 01171 Dresden, Germany

We report ^{75}As nuclear quadrupole resonance (NQR) measurements on single crystalline $Ca(Fe_{1-x}Co_x)_2As_2$ ($0 < x < 0.09$). The nuclear spin-lattice relaxation rate T_1^{-1} as a function of temperature T and Co dopant concentration x reveals a normal-state pseudogap-like phase below a crossover temperature T^* in the under- and optimally-doped region. The resulting x-T phase diagram shows that, after suppression of the spin-density-wave order, T^* intersects T_c falling to zero rapidly near the optimal doping regime. Possible origins of the pseudogap are discussed.

TT 37: MLT: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ...

Time: Wednesday 14:00–18:00 Location: HSZ 105

TT 37.1 Wed 14:00 HSZ 105

Stroboscopic observation of quantum many-body dynamics — •Stefan Kessler[1], Andreas Holzner[2], Ian McCulloch[3], Jan von Delft[2], and Florian Marquardt[1,4] — [1]Institute for Theoretical Physics, Friedrich-Alexander-Universiät Erlangen-Nürnberg, Erlangen, Germany — [2]Physics Department, ASC, CeNS, Ludwig-Maximilians-Universität München, München, Germany — [3]School of Physical Sciences, University of Queensland, Brisbane, Australia — [4]Max Planck Institute for the Science of Light, Erlangen, Germany

In recent experiments single-site resolved observation of cold atoms in optical lattices has been demonstrated. Thus it is possible to take a snapshot of a quantum many-body system, which opens a new way of observing its real-time dynamics. This inspired us to address the question how an interacting quantum-many body system evolves in time when the positions of the atoms are frequently observed. Using time-dependent DMRG we obtain the time evolution of the full many-body wave function, that is then periodically projected in order to simulate realizations of stroboscopic measurements. For the example of a 1-D chain of spin-polarized fermions with nearest-neighbor interaction, we find regimes for which many-particle configurations are stabilized and destabilized depending on the interaction strength and the time between observations. This model can be experimentally realized in optical latices with 2-species fermions in the insulating phase. We also discuss the possibility of observing just a single site and thus requiring only partial information about the many-body system. This leads to new effects that are not related to the usual quantum Zeno physics.

TT 37.2 Wed 14:15 HSZ 105

Breakdown of diffusion and negative absolute temperatures for ultracold atoms in optical lattices — •Stephan Mandt, Akos Rapp, David Rasch, and Achim Rosch — Institute of Theoretical Physics, University of Cologne, Germany

The last years have seen dramatic progress in the control of quantum gases in optical lattices, which allows to study out-of-equilibrium dynamics and transport properties in strongly correlated systems. We investigate the breakdown of diffusion in the transport of fermionic atoms on a lattice described by a homogeneous Hubbard model, based on an experiment by the group of Immanuel Bloch on an expanding cloud. We observe a crossover from diffusive behavior in the center of the cloud to a ballistic motion of atoms in its outer regions: While the cloud's shape remains round in the diffusive regime, it obtains a square shape when the motion becomes ballistic. Surprisingly, the system exhibits a strong feedback from the ballistic on the diffusive regions characterized by a universal loss rate of particles obeying singular diffusion equations.

In the second part we suggest and model a dynamical process in which an atomic gas with a negative absolute temperature can be created by inverting the sign of the harmonic trap. Due to the finite bandwidth of the lattice, which gives both an upper and a lower bound to the kinetic energy, the system still gets trapped even by the inverted potential, but equilibrates to a negative absolute temperature. We analyze the time scales needed to equilibrate to $T < 0$ and study the amount of heat generated by this non-equilibrium process.

TT 37.3 Wed 14:30 HSZ 105

The Quantum Kinetic Theory of Collisionless Superfluid Internal Convection — •Lukas Gilz and James Anglin — TU Kaiserslautern, Kaiserslautern, Germany

When a superfluid is heated locally, condensate and non-condensate fractions flow in opposite directions. As if to rebut the 19th century conclusion that cold is merely absence of heat, condensate flows like a flux of cold, from cooler regions to hotter. Wereas this phenomenon of "superfluid internal convection" is usually described within Landau's phenomenological two fluid model, we obtain a more fundamental picture of internal convection by extending a standard master equation formulation of quantum kinetic theory to include two reservoirs of different temperatures. We find that internal convection occurs even in collisionless regimes and that coherent scattering is essential to the observation of a condensate flow. Besides computing estimates of particle-, energy- and entropy flow, we propose an experimental approach by which this behavior can be observed in trapped ultracold Bose gases.

TT 37.4 Wed 14:45 HSZ 105

Ginzburg-Landau theory for the Jaynes-Cummings-Hubbard model — •Christian Nietner[1], Axel Pelster[2], Gernot Schaller[1], and Tobias Brandes[1] — [1]ITP, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]FB Physik, Uni Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

We develop a Ginzburg-Landau theory for the Jaynes-Cummings-Hubbard model, which describes the thermodynamics of photons evolving in an infinite lattice of cavities each filled with a two-level atom. Following Ref. [1], we calculate the effective action in first order of the hopping term. With this we reproduce at first the finite-temperature mean-field result of Refs. [2,3] for the quantum phase boundary between a Mott-insulating and a superfluid phase of polaritons. Subsequently, we investigate the excitation spectra in both the Mott phase and the superfluid phase. We find that our results for the energy gap and the effective masses of the particle and hole excitations in the superfluid phase are in good quantitative agreement with Ref. [4]. We determine the sound velocity of polaritons as a function of the detuning between the cavity mode and the two-level system. Finally, we outline how to obtain finite-size corrections to these results.

[1] B. Bradlyn, F. E. A. dos Santos, and A. Pelster, Phys. Rev. A **79**, 013615 (2009).
[2] J. Koch and K. L. Hur, Phys. Rev. A **80**, 023811 (2009).
[3] S. Schmidt and G. Blatter, Phys. Rev. Lett. **103**, 086403 (2009).
[4] S. Schmidt and G. Blatter, Phys. Rev. Lett. **104**, 216402 (2010).

TT 37.5 Wed 15:00 HSZ 105

Mott-insulator and superfluid phases in the bosonic dynamical mean-field theory with the strong coupling impurity solver — •Anna Kauch[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, PL-00-681 Warszawa, Poland

We investigate the phase diagram of correlated lattice bosons using the bosonic dynamical mean field theory (BDMFT). The BDMFT, formulated by Byczuk and Vollhardt (Phys. Rev. B 77, 235106 (2008)), is a comprehensive and thermodynamically consistent approximation in which the normal and condensed bosons are treated on equal footing. Within BDMFT the lattice bosonic problem is replaced by a single impurity coupled to two bosonic baths (corresponding to normal and condensed bosons, respectively). The resulting set of equations, the so-called "impurity problem", has to be solved self-consistently. Our approach is the strong coupling expansion within which the phase transition between the Mott-insulating superfluid phases can be described. Different thermodynamical quantities (particle density, compressibility, order parameter) as well as the bosonic density of states are investigated across the transition line.

15 min. break

TT 37.6 Wed 15:30 HSZ 105

Functional renormalization group approach to interacting bosons at zero temperature — •Andreas Sinner[1], Nils Hasselmann[2], and Peter Kopietz[3] — [1]Universität Augsburg, Germany — [2]Universidade Federal do Rio Grande do Norte, Brazil — [3]Universität Frankfurt, Germany

We investigate the single-particle spectral density of interacting bosons within the non-perturbative functional renormalization group technique. The flow equations for a Bose gas are derived and solved within a truncation scheme which allows to extract the complete frequency and momentum structure of the normal and anomalous self-energies. Both the asymptotic small momentum regime, where perturbation regime fails, as well as the perturbative regime at larger momenta are well described within a single unified approach. The self-energies do not exhibit any infrared divergences, satisfy the U(1) symmetry constraints, and are in accordance with the exact relation which states that the anomalous self-energy vanishes at zero momentum and zero frequency. From the self-energies we extract the single-particle spectral density of the two-dimensional Bose gas. The dispersion is found to be of the Bogoliubov form and shows the crossover from linear Goldstone modes to the quadratic behavior of quasi-free bosons. The damping of the quasiparticles is found to be in accordance with the standard Beliaev damping.

TT 37.7 Wed 15:45 HSZ 105

Detecting the Amplitude Mode of Strongly Interacting Lattice Bosons by Bragg Scattering — •Ulf Bissbort[1], Yongqiang Li[1], Sören Götze[2], Jannes Heinze[2], Jasper S. Krauser[2], Malte Weinberg[2], Christoph Becker[2], Klaus Sengstock[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe Universität, 60438 Frankfurt/Main — [2]Institut für Laser-Physik, Universität Hamburg, 22761 Hamburg

We report the first detection of the Higgs-type amplitude mode using Bragg spectroscopy in a strongly interacting condensate of ultracold atoms in an optical lattice. By the comparison of our experimental data with a spatially resolved, time-dependent dynamic Gutzwiller calculation, we obtain good quantitative agreement. This allows for a clear identification of the amplitude mode, showing that it can be detected with full momentum resolution by going beyond the linear response regime. A systematic shift of the sound and amplitude modes' resonance frequencies due to the finite Bragg beam intensity is observed. Within an extended Bogoliubov-de Gennes approach, an extensive quasi-particle analysis of the dynamical processes during the spectroscopic measurement is presented.

TT 37.8 Wed 16:00 HSZ 105

Bose-Einstein condensation at finite momentum and magnon condensation in thin film ferromagnets — •Johannes Hick, Francesca Sauli, Andreas Kreisel, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We use the Gross-Pitaevskii equation to determine the spatial structure of the condensate density of interacting bosons whose energy dispersion $\epsilon_{\boldsymbol{k}}$ has two degenerate minima at finite wave-vectors $\pm\boldsymbol{q}$. We show that in general the Fourier transform of the condensate density has finite amplitudes for all integer multiples of $\boldsymbol{q}$. If the interaction is such that many Fourier components contribute, the Bose condensate is localized at the sites of a one-dimensional lattice with spacing $2\pi/|\boldsymbol{q}|$; in this case Bose-Einstein condensation resembles the transition from a liquid to a crystalline solid. We use our results to investigate the spatial structure of the Bose condensate formed by magnons in thin films of yttrium-iron garnet .

TT 37.9 Wed 16:15 HSZ 105

Correlated Bosons beyond Pairwise Interactions - Dimersuperfluid in Two Dimensions — •Lars Bonnes and Stefan Wessel — Institut für Theoretische Physik III, Pfaffenwaldring 57, 70550 Stuttgart, Germany

We consider ultra-cold atoms loaded into a two-dimensional optical lattice with strong three-body losses, i.e. three bosons sharing one lattice site scatter inelastically and dissipate from the system. This process dynamically stabilizes a three-body on-site repulsion in analogy to the quantum Zeno effect. The system studied here is described by a Bose-Hubbard model on a square lattice with on-site attraction. The maximal number of particles per lattice site is restricted to two in order to take the three-body repulsion into account. Field theoretical considerations and numerical simulations using Matrix Product States in one dimension suggest the existence of a dimer superfluid phase for small tunneling rates that is effectively described by the condensation of pairs bosons and the absence of an atomic condensate. In this work we explore the ground state and finite-temperature phase diagram for our model using large-scale quantum Monte-Carlo simulations. Our main emphasis is the detection of the dimer superfluid phase and we address the issue of extrapolating our finite-temperature data to the thermodyanmic limit at T=0. We address the numerical issues i.e., fat-tailed distributions in the condensate density and demonstrate how we are able to overcome this issue by adding a term that couples lineary to the order parameter leading to a system with arbitrary long-range pair-hopping processes.

TT 37.10 Wed 16:30 HSZ 105

Dipolar bosons in coupled one-dimensional tubes — •Marianne Bauer and Meera Parish — Cavendish Laboratory, JJ Thompson Avenue, Cambridge, CB3 0HE, United Kingdom

Dipolar bosons in one-dimensional optical lattices are known to exhibit interesting phenomena. The phase diagram of such a system forms a complete devil's staircase in the classical limit of zero intersite hopping [1]. Including hopping leads to a competition of the crystalline Mott phases with a superfluid of defects [2]. However, a central question is how this behaviour survives as we perturb away from one dimension. Here, we provide an important step in this direction by considering

the case of two coupled one-dimensional tubes. We find that the coupling between tubes can affect the types of defects appearing within the Mott phases, thus changing the region in chemical potential over which each filling fraction is stable. We also investigate how the Mott lobes vary with respect to intertube distance. Finally, we discuss the implications of our results for cold-atom experiments.
[1] P. Bak and P. Bruinsma, Phys. Rev. Lett. **49**, 249 (1982)
[2] F. J. Burnell, M. M. Parish, N. R. Cooper and S. L. Sondhi, Phys. Rev. B, **80**, 174519 (2009)

15 min. break

TT 37.11 Wed 17:00 HSZ 105

Thermodynamics of the 3D Hubbard model on approach to the Néel transition — •Sebastian Fuchs[1], Emanuel Gull[2], Lode Pollet[3,4], Evgeny Burovski[5,6], Evgeny Kozik[4], Thomas Pruschke[1], and Matthias Troyer[4] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Physics, Columbia University, New York, NY 10027, USA — [3]Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA — [4]Theoretische Physik, ETH Zürich, 8093 Zürich, Switzerland — [5]LPTMS, CNRS and Université Paris-Sud, 91405 Orsay, France — [6]Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK

We study the thermodynamic properties of the 3D Hubbard model for temperatures down to the Néel temperature using cluster dynamical mean-field theory [1]. In particular we calculate the energy, entropy, density, double occupancy and nearest-neighbor spin correlations as a function of chemical potential, temperature and repulsion strength. To make contact with cold-gas experiments, we also compute properties of the system subject to an external trap in the local density approximation. We find that an entropy per particle $S/N \approx 0.65(6)$ at $U/t = 8$ is sufficient to achieve a Néel state in the center of the trap, substantially higher than the entropy required in a homogeneous system. Precursors to antiferromagnetism can clearly be observed in nearest-neighbor spin correlators [2].
[1] T. Maier *et al.*, Rev. Mod. Phys. 77, 1027 (2005)
[2] S. Fuchs *et al.*, arXiv:1009.2759v1 (2010)

TT 37.12 Wed 17:15 HSZ 105

Localization of correlated fermions in optical lattices with speckle disorder — •Denis Semmler[1], Julia Wernsdorfer[1], Ulf Bissbort[1], Krzysztof Byczuk[2,3], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

Strongly correlated fermions in three- and two-dimensional optical lattices with experimentally realistic speckle disorder are investigated. We extend and apply the statistical dynamical mean-field theory, which treats local correlations non-perturbatively, to incorporate on-site and hopping-type randomness on equal footing. Localization due to disorder is detected via the probability distribution function of the local density of states. We obtain a complete paramagnetic ground state phase diagram for experimentally realistic parameters and find a strong suppression of the correlation-induced metal insulator transition due to disorder [1]. Our results indicate that the Anderson-Mott and the Mott insulator are not continuously connected due to the specific character of speckle disorder.
[1] D. Semmler, J. Wernsdorfer, U. Bissbort, K. Byczuk, and W. Hofstetter, arXiv:1009.3438.

TT 37.13 Wed 17:30 HSZ 105

BCS-BEC crossover of a spin-imbalanced Fermi gas in one dimension — •Fabian Heidrich-Meisner[1], Adrian Feiguin[2], Ulrich Schollwöck[1], and Wilhelm Zwerger[3] — [1]LMU Munich, Germany — [2]University of Wyoming, Laramie, USA — [3]TU Munich, Germany

We present a numerical study of the one-dimensional BCS-BEC crossover of a spin-imbalanced Fermi gas [1]. The crossover is described by the Bose-Fermi resonance model in a real space representation. Our main interest is in the behavior of the s-wave pair correlations, which, in the BCS limit, are of the Fulde-Ferrell-Larkin-Ovchinnikov type, while in the BEC limit, a superfluid of diatomic molecules forms that exhibits quasi-condensation at zero momentum. We use the density matrix renormalization group method to compute the phase diagram as a function of the detuning of the molecular level and the polarization. As a main result, we show that FFLO-like correlations disappear well below full polarization close to the resonance. The critical polarization depends on both the detuning and the filling.
[1] Heidrich-Meisner, Feiguin, Schollwöck, Zwerger Phys. Rev. A 81, 023629 (2010).

TT 37.14 Wed 17:45 HSZ 105

Relaxation of fermionic quantum systems after an interaction quench — •Simone A. Hamerla and Götz S. Uhrig — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

The impressive progress on experimental side in the context of fermionic atoms in optical lattices and especially the tunability of the interaction strength has led to new interest in the dynamics of quantum systems out of equilibrium.

We study the time evolution of fermionic systems after a quench, i.e. a sudden change in the intrinsic parameters of the system. In this context interaction quenches, where the interaction between particles is suddenly turned on, are of special interest.

In this setup we do not focus on the long time behavior of the system, which determines the thermalization but on short times after the quench, the so called prethermalization. The relaxation of the system is studied by the use of a semi-analytic approach based on the Heisenberg equations of motion [1]. This higher order equation of motion approach enables us to study the momentum distribution and other quantities of the system after the quench.
[1] G.S. Uhrig Phys. Rev. A 80, 061602(R)

TT 38: Poster Session Transport

Time: Wednesday 14:00–18:00 Location: P3

TT 38.1 Wed 14:00 P3

Charge transfer statistics of double quantum dots in the Kondo regime — •David Breyel and Andreas Komnik — Institut für Theoretische Physik, Universität Heidelberg

We calculate the full counting statistics (FCS) for a system consisting of two quantum dots in the Kondo regime which are subject to different magnetic fields and are coupled to two metallic leads biased by a finite voltage. With certain restrictions on the coupling constants a transformation consisting of bosonization, rotation and refermionisation maps the Hamiltonian of the system to one of a noninteracting system as in [1,2]. We use the Schwinger-Keldysh-formalism for the Green's functions in order to derive the FCS along the lines of [3]. We concentrate on the Fano factor which can be calculated from the FCS as well as the effective transmission coefficients. We explain different features of the Fano factor depending on different system parameters. Furthermore, we succeed in linking the features of the effective transmission coefficients to individual transport processes. For instance we conclude that every transport process through the system is accompanied by a spin flip the the positions of the peaks in the transmission coefficient match the strength of the applied magnetic field. Finally, we discuss the experimental implications of the identified FCS features.
[1] V. J. Emery and S. Kivelson, Phys. Rev. B 46 (1992), 10812
[2] A. Schiller and S. Hershfield, Phys. Rev. B 58 (1998), 14978
[3] A. O. Gogolin and A. Komnik, Phys. Rev. Lett. 97 (2006), 016602

TT 38.2 Wed 14:00 P3

Magnetostrictive effects in ferromagnetic Dy break-junctions — •Marc Müller[1], Christoph Sürgers[1], Richard Montbrun[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

A characteristic property of the rare-earth metals are their large

magnetostrictive strains which are related to the magnetocrystalline anisotropy through the elastic energy. We have investigated the electrical conductance G of mechanical break-junctions of a dysprosium wire at 4.2 K where Dy is in the ferromagnetic state. In zero magnetic field we find the usual variation of the conductance G vs. electrode distance x while breaking the wire mechanically, with a sequence of steps and more or less prominent plateaus. The behavior $G(x)$ is modified in magnetic fields $\mu_0 H$ up to 1 T due to the large magnetostriction of Dy. In addition, the conductance can be changed reproducibly by variation of H. For a number of contacts we observe discrete changes in $G(H)$ in the range of several $G_0 = 2e^2/h$. The behavior of $G(H)$ and its angular dependence can be quantitatively understood by taking into account the magnetostrictive properties of Dy. This first realization of a magnetostrictive atomic switch demonstrates the possibility of reproducibly tuning the conductance of magnetic nanocontacts by a magnetic field.

Work supported by the DFG Center for Functional Nanostructures (CFN).

TT 38.3 Wed 14:00 P3

Time-domain interferometry with single quantum dots — •Alexander Croy and Ulf Saalmann — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Coherent control of nanoscale devices is one of the main topics of current research on electron transport in systems on the nanometer scale. A very successful method for the coherent manipulation of charge and spin qubits in double quantum dots consists in using nearly rectangular voltage pulses. Moreover, recent experiments demonstrate that the creation of high-frequency pulse trains is feasible, which paves the way for observing new coherent transport phenomena.
Here we present numerical and analytical results demonstrating the influence of such pulse trains on the time-averaged occupation of a single quantum dot and the currents through the system. For very high and low frequencies coherent destruction of tunneling and adiabatic transport can be observed, respectively. Additionally, we consider random voltage pulse-trains given by a random telegraph process. In this case the coherent features cannot be observed.

TT 38.4 Wed 14:00 P3

Effects of Coulomb interaction on the dynamics of an open quantum dot system — •Benjamin Baxevanis and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg

We study the effect of Coulomb interaction on the time-dependent dynamics of a quantum dot system weakly coupled to an electronic reservoir. The two systems are assumed to be initially separated and we calculate the evolution from a non-equilibrium state to equilibrium as the interaction between the systems is instantly switched on. We determine the current flow from the reservoir to the single quantum dot in the sequential tunnelling regime using a master equation. The exact eigenstates of a finite number of correlated electrons in the quantum dot are taken into account provided by the exact-diagonalization method. We discuss the significance of the few-particle states which are involved in the charging of the quantum dot. We encounter signatures of Coulomb blockade in the transient regime of the current-voltage characteristics which emerged in recent experiments [1].
[1] B. Marquardt, M. Geller, B. Baxevanis, D. Pfannkuche, A. D. Wieck, D. Reuter, A. Lorke, preprint arXiv:1007.0392

TT 38.5 Wed 14:00 P3

Different time scales in the dynamics of an interacting quantum dot — •L.Debora Contreras-Pulido[1], Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[3] — [1]RWTH-Aachen University, Aachen, Germany — [2]Victoria University of Wellington, Wellington, New Zealand — [3]Universität Duisburg-Essen and CeNIDE, Duisburg, Germany

The recent theoretical and experimental analysis of the controlled emission of charge (as well as current correlations) from a quantum capacitor, shows its potential application in quantum information, in nanoelectronics operating in Gigahertz frequencies, and also in the study of a few-particle physics, including the dynamics of nanoscale systems [1]. We extend the study presented in [2] for the time-dependent decay after a step pulse has been applied to a single-level quantum dot with Coulomb interaction and coupled to an electronic reservoir. Our results show that besides the independent decay of charge and spin, an additional time scale appears which we calculate up to second order in a perturbation expansion in the tunneling coupling. We relate the decaying quantity to deviations of the electron-hole occupation and the symmetry of the Anderson Model. Importantly, the decay rate is independent of the level position.
[1] See e.g. A. Mahé *et al.*, Phys. Rev. B **82**, 201309(R) (2010); M. Moskalets, P. Samuelsson, M. Büttiker Phys. Rev. Lett. **100**, 086601 (2008), and references therein.
[2] J. Splettstoesser, M. Governale, J. König, M. Büttiker Phys. Rev. B **81**, 165318 (2010).

TT 38.6 Wed 14:00 P3

Josephson current through interacting quantum dots — •Stephanie Droste, Janine Splettstoesser, and Sabine Andergassen — Institut für Theorie der Statistischen Physik RWTH Aachen & JARA-Fit, Germany

Motivated by recent experiments on transport through carbon nanotube double dots with superconducting leads, we study the effects of Coulomb interactions on transport through such a device. Richer physics due to the proximity effect is expected, as a consequence of the more complex level structure and differing interaction strengths between different dot levels. We extend a recent analysis [1] of Coulomb interaction effects in a single-level quantum dot to a serial double dot coupled to superconducting leads. We derive a local effective Hamiltonian including the atomic or molecular levels as well as the induced proximity effect on the quantum dot and compute the Josephson current as well as a Δ-dependent phase diagram. The effective Hamiltonian is the starting point of a detailed analysis of dissipative effects.
[1] T. Meng et al., Phys. Rev. B **79**, 224521 (2009).

TT 38.7 Wed 14:00 P3

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

The real-time renormalization group in frequency space (RTRG-FS) is a formally exact perturbative renormalization group scheme from which the kernel of the kinetic equation for the reduced density matrix can be calculated. The method is applicable for small quantum systems, such as quantum dots, in contact with several particle or heat reservoirs. Since the formalism is based on a perturbative expansion in the system-reservoir coupling quantum systems with arbitrary large interaction strength can be treated. In its original form [1] the RTRG-FS was formulated for systems coupled to normal leads only. Here we present a generalization of the method to the case where the leads may be both normal or superconducting. In the latter case transport can be provided either by quasiparticle or Andreev tunneling giving rise to a rich variety of interesting physical phenomena. When several superconducting leads at different chemical potentials are present it is important to consider the energy contribution from the Cooper pair condensate in the leads. We in particular account for this situation. Finally we discuss some applications of the method.
[1] H. Schoeller, Eur. Phys. J. Special Topics **168**, 179 (2009).

TT 38.8 Wed 14:00 P3

Superconductivity-enhanced transport through a carbon nanotube quantum dot with Nb contacts — •Thomas Geiger[1], Kicheon Kang[1,2], Dmitry Ryndyk[3], Andreas Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Department of Physics, Chonnam National University, Gwangju 500-757, Korea — [3]Institute for Theoretical Physics, University of Regensburg, Germany

We present the effect of superconductivity in high quality Nb contacts ($T_c = 8.5$K, $B_c = 4.5$T in parallel field) on transport through a SWCNT quantum dot explored by means of high resolution charging diagrams. We find clear transport spectroscopy signatures of the superconductivity in the leads: Over a wide gate range density of states (DOS)-enhanced elastic cotunneling features are observed at an energy of twice the reduced gap of 500 μeV. In some gate regions, Andreev reflection (AR) causes low energy features near the degeneracy points and the contacts' DOS peaks are reflected in inelastic cotunneling lines.

The magnetic field dependence of these features shows an expected decrease following the gradual suppression of the gap-parameter in the leads. Remarkably, the sub-gap features at certain degeneracy points emerge and show a nonmonotonic temperature dependence: With just precursors visible close to base temperature, a rich structure of the AR

features develops much more prominently at a few hundred mK.
[1] Grove-Rasmussen, K., Jørgensen, H. I., Andersen, B. M., Paaske, J., Jespersen, T. S., Nygård, J., Flensberg, K. and Lindelof, P. E.; Phys. Rev. B **79**, 134518 (2009)

TT 38.9 Wed 14:00 P3

Kondo effect in quantum dots: slave-boson Keldysh field theory — •Sergey Smirnov and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg

We consider a single impurity Anderson model, a quantum dot with a single spin degenerate level coupled to two contacts possibly at different chemical potentials. Assuming strong electron-electron interactions in the dot we restrict the dot Hilbert space to a subspace of the empty and singly occupied states at the expense of transforming to new fermions and introducing a slave-boson. Using this new fermi-bose representation we construct an effective Keldysh field theory suitable for both equilibrium and non-equilibrium situations. The conservation of the total number of the fermions and bosons leads to a constraint in the integration over the fermionic and bosonic fields. This mathematical complication, a consequence of the interacting nature of the problem, is dealt with by introducing an additional integration removing the constraint. After integrating over the fermionic fields of the dot and contacts we obtain an effective Keldysh action with respect to the dot slave-bosonic field. We further develop a saddle point analysis of this action equivalent to the mean field approach known from the imaginary time equilibrium field theories developed previously for the Kondo effect.

TT 38.10 Wed 14:00 P3

Shot-noise of tunnel current coupled to a local plasmon — •Fei Xu, Federica Haupt, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D- 78457 Konstanz, Germany

Current noise in mesoscopic conductors is an important tool to investigate quantum many-body effects in electron transport. If the noise is measured at frequencies in the quantum range, $\hbar\omega \gg k_B T$, the measurement amounts to the detection of photons produced by current fluctuations. This is important in view of recent experiments on photon-emission from tunnel junctions formed by a scanning tunneling microscope on a metallic surface [1,2]. These works showed a considerable intensity of photons emitted with a frequency larger than the applied bias voltage $\hbar\omega > eV$ [1,2]. While photons with frequency $\hbar\omega < eV$ can be readily interpreted in terms of fluctuations in single-electron transfer processes, over-bias ($\hbar\omega > eV$) photon emission is a fingerprint of electronic correlations. We address the problem of over-bias photon emission formulating it in terms of current fluctuations in a conductor interacting with an electromagnetic environment. The latter can mediate cooperative processes in which two electrons team up crossing the junction, emitting a single phonon with energy up to $2eV$ [3]. To describe the set-up of Ref. [1], we employ a minimal model consisting of a local tunnel junction coupled to an electric RLC circuit, whose dynamics mimics the local plasmon mode in the metal junction.
[1] G. Schull, *et al.* PRL 102, 057401 (2009).
[2] N. L. Schneider, *et al.* PRL 105, 026601 (2010).
[3] J. Tobiska, *et al.*, PRL. 96, 096801 (2006).

TT 38.11 Wed 14:00 P3

Laser induced electronic transport through metallic atomic-sized contacts — •Matthias Bädicker, Daniel Benner, Reimar Waitz, Johann Berres, Paul Leiderer, Johannes Boneberg, and Elke Scheer — Fachbereich Physik, Universität Konstanz

We investigate the influence of chopped laser light onto the electronic transport through a metallic point contact. It has been shown that there are several contributions to the laser induced effect like thermal expansion, plasmons and others. Here we concentrate on the thermal effects by varying the metal and the substrate material using correlation measurements of mechanical stress and optical excitation.

We use lithographically fabricated Mechanically Controllable Break-Junctions (MCBJs) operated at ambient conditions for fabricating atomic-size contacts and atomically-sharp tips of gold or platinum. The substrates we used are massive reflective and semi-transparent materials.

Detailed analysis of light-induced conductance changes has shown photo-assisted transport due to the excitation of high-energetic quasiparticles and collective effects such as surface plasmon excitation. We optimize the light-induced effects for the development of optoelectronic devices by studying systematically the effects on different metals (gold and platinum), wavelengths, position of the laser spot, and geometries (e.g. polarization of the laser light).

TT 38.12 Wed 14:00 P3

Magneto-resistance Measurements on Atomic Platinum Chains — •Christopher Espy, Florian Strigl, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Recently there have been many theoretical predictions that platinum, nonmagnetic in bulk, is indeed magnetic in nanostructures [1][2]. How and when this magnetism manifests is still a point of discussion [3]. Preliminary experiments investigating magnetic effects in nanostructures of various metals have been performed, however conclusive evidence confirming previous theoretical predictions regarding magnetism in platinum nanostructures has yet to be found [4].

In this contribution we present the study of suspended monatomic platinum nanowires, fabricated using the mechanically controllable break junction technique. Various experiments are carried out at low temperatures, T $<$ 4.2 K, and under cryogenic vacuum conditions, including the generation of conductance histograms, magneto-resistance investigations, and study of the current-voltage characteristics of the nanostructures. We find strong chain length-dependent magneto-resistive effects of considerable magnitude, up to 25%.
[1] Smogunov et al. Nat. Nanotechnol. 3 (2008) 22
[2] García-Suárez et al. Phys. Rev. B 79 (2009) 060408
[3] Thiess et al. Phys. Rev. Lett. 103 (2009) 217201
[4] Untiedt et al. Phys. Rev. B 69 (2004) 081401(R)

TT 38.13 Wed 14:00 P3

Higher-order perturbation theory applied to time-dependent electron transport processes — •Bogdan Popescu and Ulrich Kleinekathöfer — Jacobs University Bremen, Germany

In the present work, the electron transport through a quantum system, modelled as a linear chain of tight-binding sites and coupled to external fermionic leads, is investigated using a reduced density matrix formalism [1]. This model may be applied to characterize a molecular wire or consecutive quantum dots coupled in series. The dynamics of the electrons tunnelling through the system is described by a quantum master equation derived in the framework of perturbation theory. The influence of higher-order terms [2] in the coupling to the leads has been investigated, i.e., the limits of the second-order perturbation theory have been shown. The present method is suitable to accurately describe stronger system-lead coupling. Additionally, this approach is able to accurately account for time-dependent effects of an external electric or magnetic field.
[1] S. Welack, M. Schreiber and U. Kleinekathöfer, J. Chem. Phys. **124**, 044712 (2006).
[2] J. Jin, X. Zheng and Y. Yan, J. Chem. Phys. **128**, 234703 (2008).

TT 38.14 Wed 14:00 P3

Extension of the nonequilibrium Green's funtion towards systems with broken translational invariance — •Steven Achilles[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

Electronic structure calculations are nowadays an important tool for investigating and predicting physical effects of new materials on the nanometerscale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for two different types of geometries, planar junctions [3] and embedded clusters. Both implementations include the self-consistent treatment of systems under external bias using the nonequilibrium density between the chemical potentials of the left and the right lead.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for the two different types of geometries.
[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] C. Heiliger et al., J. Appl. Phys. 103, 07A709 (2008).

TT 38.15 Wed 14:00 P3

Effects of spin-orbit interaction on Andreev reflection in car-

bon nanotubes — •Anselm Schultes and Patrik Recher — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

We model transport through a carbon nanotube (CNT) in contact with a s-wave superconductor using the Dirac-Bogoliubov-de Gennes equation including spin-orbit interaction (SOI) in the CNT. For a transparent normal-superconductor (NS) interface the subgap conductance, which is dominated by Andreev reflection, is modified in the presence of SOI. Depending on the chirality of the CNT, transport can be spin-dependent. In a NSN junction the nonlocal conductance carried by crossed Andreev reflection and elastic co-tunneling is strongly influenced by SOI and can be manipulated by a gate voltage.

TT 38.16 Wed 14:00 P3

0.7 anomaly in QPC – temperature dependence of conductance in matsubara formalism — •Florian Bauer, Jan Heyder, and Jan von Delft — Arnold Sommerfeld Center, LMU München

To study the physics of the 0.7 anomaly in Quantum Point Contacts (QPCs), we calculate the conductance as a function of magnetic field and analyse the relevance of geometry. We study an extended 1D-Hubbard chain and model the QPC by a single smooth potential barrier. We use the functional renormalization group in Matsubara formalism to calculate the selfenergy and interaction vertex functions at Matsubara frequencies.

A calculation of the finite-temperature conductance for this chain model requires, in contrast to the SIAM, an analytic continuation to the real axis. We show that it is possible to avoid analytic continuation of the vertex function provided that the chain model is invariant under a L↔R parity transformation. For this case, we derive a conductance formula similar to the Meir-Wingreen formula, which expresses the conductance (including vertex contributions) purely in terms of two point correlators.

TT 38.17 Wed 14:00 P3

Geometry Dependent Spin Conductance in Quantum Dots with Spin-Orbit Interaction — •Vitalij Lutsker[1], Inanc Adagideli[2], Matthias Scheid[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Istanbul, Turkey

In a recent publication[1] it was demonstrated that the average two-terminal spin conductance of a cavity with Rashba spin-orbit interaction(SOI) depends on the orientation of the vector connecting the two terminals. This effect originates from an effect of the SOI on the electron dynamics, leading to a geometrical correlation, which survives in chaotic and diffusive dots. Here we present a systematic numerical analysis of this effect, based on a recursive Green's function approach to transport. We study statistics of the spin conductance, its dependence on the number of leads, and the role of additional linear and cubic Dresselhaus terms.

[1] I. Adagideli et al., Phys. Rev. Lett., in print (2010); arXiv:1008.4656

TT 38.18 Wed 14:00 P3

Effects of finite range exchange interactions in the RKKY spin density oscillations — •Sergey Smirnov — Institut für Theoretische Physik, Universität Regensburg

We study the impact of a finite spin distribution of a localized spin, embedded in a Fermi sea of noninteracting conduction electrons, on the induced spin density oscillations underlying the RKKY indirect exchange effect. Specifically, a one-dimensional (1D) ring at finite temperatures is considered. We show that any small but finite interaction radius always produces an essential change in the spin density oscillations if the number of electrons is large enough [1]. To understand the physical role, played by the impurity spin localization radius in the RKKY spin-density oscillations, we consider a system where those oscillations exist only if this radius is finite. The system represents a half-infinite 1D quantum wire with a magnetic ion placed at its edge. It is analytically demonstrated that the effect of the finite spin localization radius is to reduce the effective mass of the conduction electrons [2].

[1] S. Smirnov, Phys. Rev. B 79, 134403 (2009)
[2] S. Smirnov, Phys. Rev. B 81, 214425 (2010)

TT 38.19 Wed 14:00 P3

Spin-polarizing Beam Splitter Nanodevice — •Dietrich G. Rothe and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astrophysik, Würzburg, Germany

We present numerical calculations of a beam splitter device which can generate a spin-polarized current using the principle of birefringence at an interface of regions with different Rashba spin-orbit couplings. For our calculations we employ the non-equilibrium Green's function formalism, and make use of two-band as well as four-band models of the lowest subbands of the HgCdTe quantum wells. We find that the physics is governed by the interplay between Rashba and Dirac spin-orbit terms (the linear in k terms), where the latter leads to a spin polarization due to the confinement. We find that in the 4-band model, spin polarization can be measured by a helicity operator. When the interface with different Rashba SO regions is tilted at an angle well above the angle of total reflection, good spin polarization is achieved.

TT 38.20 Wed 14:00 P3

Adiabatic pumping through an interacting quantum dot with spin-orbit coupling — •Stephan Rojek[1], Jürgen König[1], and Alexander Shnirman[2] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany — [2]Institut für Theorie der Kondensierten Materie and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany

We study adiabatic pumping through a two-level quantum dot coupled to two normal leads in the presence of spin-orbit coupling. The variation of the two energy levels of the dot periodically in time leads to finite charge and spin currents. We calculate the pumped charge and spin using a diagrammatic real-time approach. Going beyond the case of noninteracting electrons on the quantum dot [1], we study the situation of finite Coulomb-interaction. For comparison, we show results for the limits of noninteracting and strongly interacting electrons. In both limits spin-orbit coupling provides the possibility for pure spin current. Furthermore, we discuss differences between the charge and spin transport characteristics.

[1] V. Brosco *et al.*, Phys. Rev. B **82**, 041309(R) (2010).

TT 38.21 Wed 14:00 P3

Probing of coherence in molecular and CNT transport — •Birgit Kiessig[1,2], Ralph Krupke[3], Regina Hoffmann[2], Dominik Stöffler[2], Kai Grube[1], Roland Schäfer[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe — [3]Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021 Karlsruhe

The advancing miniaturisation of electronic circuits has increased the scientific interest in transport properties of single molecules as the smallest available building blocks. Other promising candidates for ultrasmall electronic devices are carbon nanotubes (CNTs), which at the same time are already today far easier to handle than molecules.

We aim to probe a very special characteristic of transport through nanoscale devices, namely coherence. Its occurence in a single electronic building block leads to divergence of the behaviour of a combination of several such devices from the classical expectation.

Molecular transport measurements require the fabrication of conductive electrodes spaced only a few nm apart. To achieve such we chose a feedback controlled electromigration procedure for the preparation of our samples, which we investigated in detail.

Furthermore we also prepared and measured appropriate samples for coherence probing of transport through CNTs.

TT 38.22 Wed 14:00 P3

Inelastic transport through octane molecules and a single level model with light — •Thomas Hellmuth[1], Fabian Pauly[1], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institut of Technology (KIT) — [2]Institut für Nanotechnologie, Karlsruhe Institut of Technology (KIT)

We study the transport and vibrational modes of single-molecule junctions containing octandeamine and octanedithiol. For this we use a scheme based on density functional theory. We compare our results to experiments and map the calculated vibrational modes to the measured IETS [1]. We show the substantially different behavior for the different terminal groups, namely the pulling of gold chains for dithiols, while they are absent for the dimanines. In addition to these studies, we explore the inelastic rectification current of a light irradiated single level contact.

[1] Y. Kim, T. Hellmuth, F. Pauly, and E. Scheer (in preparation)

TT 38.23 Wed 14:00 P3

Ab-initio description of transport through biphenyl-based molecular junctions — •Marius Bürkle[1], Fabian Pauly[1], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology

Biphenyl molecules serve as prototype systems for transport through single molecule junctions. In combination with experiments, we study the electric and thermoelectric transport properties by means of density functional theory. We explore the effects of molecular conformation and anchoring groups on the electric transport in biphenyl dithiols, dinitriles, and diamines [1,2,3]. In addition, we show that they have also a strong influence on the thermoelectric properties. Namely, increasing torsion angle generally decreases the thermopower and, through doping via the anchoring groups, HOMO transport for dithiol and diamine linked molecules changes to LUMO transport for dinitriles.

[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. 10, 156 (2010)
[2] A. Mishchenko, L. A. Zotti, D. Vonlanthen, M. Bürkle, F. Pauly, J. C. Cuevas, M. Mayor, and T. Wandlowski J. Am. Chem. Soc. (2010), accepted
[3] L. Venkataraman, J. E. Klare, C. Nuckolls, M. S. Hybertsen and M. L. Steigerwald, Nature 442, 904-907 (2006).

TT 38.24 Wed 14:00 P3

Optical Control of Single-Molecule Conductance — •Yaroslav Zelinskyy[1,2] and Volkhard May[2] — [1]Bogolyubov Institute for theoretical physics, National Academy of Science of Ukraine, 14-b Metrologichna str. UA-03680, Kiev, Ukraine — [2]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489, Berlin, Germany

A kinetic model is established for current formation through a single molecule embedded in between two metallic electrodes and irradiated by an external laser pulse. Focusing on the particular case of a molecule which can be moved in its excited electronic state if it became singly charged, an analytical expression for the steady-state current is presented. A detailed analysis of the current-voltage as well as conductance-voltage characteristics at the different wavelength of the applied laser light is carried out. Based on such computations a photo-switching effect between molecular states of low and height conductivity can be proposed. In the case of weak molecule-lead coupling a voltage region showing negative differential resistance is found. Its suppression due to laser pulse excitation is indicated.

TT 38.25 Wed 14:00 P3

Electrical Characterization of Short DNA Fragments — •Matthias Wieser[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhuo Tang[2], Andreas Marx[2], Elke Scheer[2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — [2]Universität Konstanz, D-78457 Konstanz

The electrical transport properties of DNA molecules are important for future molecular electronics applications. We characterized the electrical conductance of single DNA fragments in ambient condition and in buffer solution using a Mechanically Controllable Break Junction (MCBJ) setup which allows us binding molecules between two gold electrodes. We analyzed the electrical conductance of double stranded DNA and G-quadruplex molecules. G-quadruplex molecules consist of four guanine bases arranged in the shape of a square and a cation in the center. The electrical characterization is done by investigating the I-V curves characteristics of the molecules in different conditions.

TT 38.26 Wed 14:00 P3

Electronic transport through switchable molecules — •Bernd Briechle[1], Nikola Treska[1], Dima Sysoiev[2], Jannic Wolf[2], Youngsang Kim[1], Johannes Boneberg[1], Thomas Huhn[2], Ulrich Groth[2], Ulrich Steiner[2], Artur Erbe[3], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Chemistry, University of Konstanz, Germany — [3]Forschungszentrum Dresden-Rossendorf, Dresden, Germany

We investigate transport properties of molecules in liquid solvent at room temperature. For that purpose we use lithographically fabricated Mechanically Controllable Break Junctions (MCBJs) to generate atomic-size contacts and atomically sharp tips to contact the molecules. We study molecular switches for which reversible switching from an opened to a closed conjugated backbone via light irradiation is expected. The molecular switches feature thiol- or nitrogen-based endgroups for a strong bond to the metal. Analysis is based on statistics of conductance traces recorded during opening and closing the junction, and on current-voltage characteristics taken at constant electrode distance. It has been shown that the latter can be described by a simple transport model involving a single broadened molecular orbital. Fitting the experimental current-voltage characteristics to this model, we can extract the strength of the molecule-metal bond as well as the energy of the molecular orbital next to the Fermi level. This analysis enables us to determine promising combinations of metal and molecule endgroup for stable and reproducible contacting which is a crucial requirement for our transport studies.

TT 38.27 Wed 14:00 P3

Time-dependent transport through a molecular level coupled to a nanomagnet — •Milena Filipovic, Federica Haupt, and Wolfgang Belzig — University of Konstanz, Konstanz, Germany

We study the transport through a single level quantum dot coupled to two leads in the presence of a magnetic field. The magnetic field is coupled to the quantum dot and the leads are treated as noninteracting. We use the Keldysh nonequilibrium Green function technique to derive and analyze the properties of the spin-dependent tunneling current and its linear response to the applied time-dependent magnetic field. We further analyze the transport through the single level quantum dot coupled to a precessing molecular nanomagnet.

TT 38.28 Wed 14:00 P3

Quantum Interference and Dephasing Due to Vibronic Coupling in a Single-Molecule Junction — •Michael Butzin, Rainer Härtle, and Michael Thoss — Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

We study quantum interference and dephasing effects in a biphenylacetylene-dithiolate molecular junction. To this end, we analyze the molecular orbitals relevant for charge transport through this junction and show that destructive interference effects suppress coherent transport processes. The coupling of the electronic degrees of freedom to the large number of vibrational modes of the junction strongly influences the respective current-voltage characteristics and induces a dephasing mechanism that counteracts the suppression of the current due to destructive interference. To analyze these phenomena we discuss generic model systems using a nonequilibrium Green's function approach [1]. Moreover, for a molecular junction that exhibits quantum interference effects, we identify the constructive and destructive parts of the corresponding transmission function [2]. Interestingly, in the presence of electron-electron interactions, such destructive interference effects provide a testbed for the elastic co-tunneling approximation [1], which we study employing the exact method of Gurvitz et al. [3].

[1] R. Härtle *et al.*, Phys. Rev. Lett. 102, 146801 (2009).
[2] G. C. Solomon *et al.*, Nano Lett. 6, 2431 (2006).
[3] S. A. Gurvitz, Phys. Rev. B 57, 6602 (1998).

TT 38.29 Wed 14:00 P3

Time-dependent approach to mesoscopic transport — •Tobias Kramer — Institute for Theoretical Physics, Uni Regensburg

Transport and scattering phenomena in open quantum-systems with a continuous energy spectrum are conveniently solved using the time-dependent Schrodinger equation [1]. In the time-dependent picture, the evolution of an initially localized wave-packet reveals the eigenstates and eigenvalues of the system under consideration. We discuss applications of the wave-packet method to mesoscopic systems and point out specific advantages of the time-dependent approach. In connection with the familiar initial value formulation of classical mechanics, an intuitive interpretation of transport emerges. For interacting many-particle systems, we discuss the efficient calculation of the self-consistent classical transport in the presence of a magnetic field.

[1] T. Kramer, Time dependent approach to transport and scattering in atomic and mesoscopic systems, arXiv:1011.3194
[2] T. Kramer, V. Krueckl, E. Heller, and R. Parrott: Self-consistent calculation of electric potentials in Hall devices, Phys. Rev. B, 81, 205306 (2010)

TT 38.30 Wed 14:00 P3

Diagrammatic approach to noise in adiabatically time-dependent systems — •Roman-Pascal Riwar[1], Janine Splettstoesser[1], and Jürgen König[2] — [1]Institut für Theorie

der Statistischen Physik, RWTH Aachen University, D-52056 Aachen, Germany and JARA-Fundamentals of Future Information Technology — [2]Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

Noise is an important feature in quantum electron transport. Current-current correlations carry information about the system which is not accessible via a current measurement only. Here, we are interested in the noise of interacting quantum dot systems, which are subject to time-dependent fields, as e.g. adiabatic quantum pumps. We investigate the zero-frequency noise of such systems, taking into account Coulomb interaction. For this purpose, a real-time diagrammatic approach for the treatment of adiabatic time dependence [1] is extended to the calculation of current noise (performed for the stationary case in Ref. [2]), within a perturbative expansion in the tunnel coupling.
[1] J. Splettstoesser *et al.*, Phys. Rev. B **74**, 085305 (2006)
[2] A. Thielmann *et al.*, Phys. Rev. Lett. **95**, 146806 (2005)

TT 38.31 Wed 14:00 P3

Effective two-spin models for measurement based quantum computing — •Daniel Klagges and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The cluster state is an universal resource for measurement based quantum computation. One might consider to prepare a cluster state by cooling a suitable chosen Hamiltonian into its ground state. Unfortunately there is no Hamiltonian only containing (realistic) two-spin interactions with the cluster state as its only ground state. But there exist microscopic models consisting solely of two-spin interactions for which the ground state is approximately the cluster state. Here we present high order series expansions of such Hamiltonians, in order to investigate their usability in the context of measurement based quantum computation.

TT 38.32 Wed 14:00 P3

Influence of adsorbate clustering on transport in graphene nanoribbons — •Sarah Stahl, Georgo Metalidis, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, D-76128 Karlsruhe

Until now no consensus has been reached on the dominant scattering mechanism in graphene. Several experiments have observed the adsorption of different atoms and molecules on a free-standing graphene surface and imaged the formation of clusters of such adsorbates. Clustering of adsorbates might have a major influence on the transport properties of graphene. In particular, single adsorbates form short-range scattering centers and will thus induce scattering between the two valleys in the graphene Brillouin zone breaking chirality. When they cluster together their scattering is of a longer-range and inter-valley scattering will be absent (conserving chirality). We investigate the influence of clustering with a numerical Green's function technique to study the crossover between these two regimes. In particular, we determine the mean free path as a function of the cluster size, ribbon dimensions and disorder strength.

TT 38.33 Wed 14:00 P3

Spin and Vibrations in Carbon Nanotubes — •Christoph Ohm[1], Janine Splettstoesser[1], Christoph Stampfer[1,2], and Maarten R. Wegewijs[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, and JARA - Fundamentals of Future Information Technology, Germany — [2]Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, Germany

Carbon nanotubes are ideal systems to probe the interplay of quantized degrees of freedom. We theoretically study the influence of vibrations on the spin dynamics in carbon nanotube quantum dots. We consider various types of spin-phonon coupling mechanisms and their influence on transport.

TT 38.34 Wed 14:00 P3

Transport studies of microsoldered Graphene — •Nils Freitag[1], Marcus Liebmann[1], Viktor Geringer[1], Alexander Georgi[1], Bart Szafranek[2], Daniel Neumeier[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumethal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

We present transport measurements on microsoldered Graphene using a 300 mK/ 10 T He^3-bath cryostat. These are complementary to our previous scanning tunneling microscopy studies [1]. Amongst the determination of the mobility of the samples, a distinct half-integer Quantum-Hall effect appears at high fields, whereas the low-field regime is dominated by the weak localisation and antilocalisation features which are analysed in detail. Interestingly, the mobility of graphene exhibits a sudden change at the critical field of the superconducting In-contacts.
[1] V. Geringer, D. Subramaniam, A. K. Michel, B. Szafranek, D. Schall, A. Georgi, T. Mashoff, D. Neumaier, M. Liebmann, M. Morgenstern, Appl. Phys. Lett. **96**, 082114 (2010).

TT 38.35 Wed 14:00 P3

Four-wave mixing to detect wave-packet revivals on graphene — •Viktor Krueckl, Tobias Kramer, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

By applying a perpendicular magnetic field the quasi-relativistic electrons of graphene are quantized into non-equidistantly spaced Landau levels. Consequently the time-evolution of an excited wave-packet undergoes collapses and revivals similar to the dynamics of highly excited Rydberg states [1]. We investigate the detection of graphene revivals by means of four-wave mixing. A few cycle laser pulse is used to generate an excited state, which is probed by a second time-delayed pulse. We apply a non-pertubative wave-packet scheme which allows for the calculation of the complete angle resolved polarization. The resulting integrated signals show a clear correspondence between the time-delay of the probe pulse and the wave-packet revival time.
[1] Viktor Krueckl and Tobias Kramer, New J. Phys. **11** 093010 (2009)

TT 38.36 Wed 14:00 P3

Superlattice Effects on Graphene Nanoribbons — •Fedor Tkatschenko, Jan Bundesmann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We study how an additional, spatially modulated electric field affects the electronic properties of graphene nanoribbons. Previous efforts [1, 2] investigated peculiar effects on the electronic structure of bulk graphene such as the emergence of new Dirac points in the energy spectrum and an anisotropic velocity renormalization. These new characteristics are also reflected in the density of states and the conductivity. Insted of the bulk we will here consider the influence of a periodic modulation, oriented along the direction of a graphene nanoribbon, on its bandstructure and transport properties. To this end we employ a numerical Green function method based on the tight binding graphene Hamiltonian.
[1] M. Barbier, P. Vasilopoulos, and F. M. Peeters, Phys. Rev. B **79** 115427 (2010)
[2] Li-Gang Wang, and Shi-Yao Zhu, Phys. Rev. B **81** 205444 (2010)

TT 38.37 Wed 14:00 P3

A route to strong p-doping of epitaxial graphene on SiC — •Udo Schwingenschlögl and Yingchun Cheng — PSE Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effects of Au intercalation on the electronic properties of epitaxial graphene grown on SiC0001 substrates are studied using first principles calculations. A graphene monolayer on SiC0001 restores the shape of the pristine graphene dispersion, where doping levels between strongly n-doped and weakly p-doped can be achieved by altering the Au coverage. We predict that Au intercalation between the two C layers of bilayer graphene grown on SiC0001 makes it possible to achieve a strongly p-doped graphene state, where the p-doping level can be controlled by means of the Au coverage [1].
[1] Appl. Phys. Lett. 97, 193304 (2010)

TT 38.38 Wed 14:00 P3

Surface quantum criticality in topological insulators — •Matthias Sitte, Lars Fritz, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The discovery of graphene has allowed to experimentally study a (2+1)-dimensional variant of quantum electrodynamics. It is known that a phase transition to a gapped phase with broken chiral symmetry can in principle be driven by varying the fine structure constant α. However, in graphene the tunability of α is quite limited. Recently, the surfaces of 3D topological insulators have shown to host states that are also described by massless relativistic Dirac fermions in

2+1 dimensions. In this work we study the tunability of α in materials such as HgTe and CdTe by driving the bulk towards its quantum critical point. We investigate under which conditions chiral symmetry breaking on the surface can be expected.

TT 38.39 Wed 14:00 P3

Charge-spin duality in non-equilibrium transport of helical liquids — •Jan Carl Budich, Chao-xing Liu, Patrik Recher, and Björn Trauzettel — Institute for theoretical physics and astrophysics, Wuerzburg, Germany

Non-equilibrium transport properties of charge and spin sector of two edges of a quantum spin Hall insulator are investigated theoretically in a four-terminal configuration. A simple duality relation between charge and spin sector is found for two helical Tomonaga Luttinger liquids (hTLLs) connected to non-interacting electron reservoirs. If the hTLLs on opposite edges are coupled locally or non-locally, the mixing between them yields interesting physics where spin information can be easily detected by a charge measurement and vice versa. Particularly, we show how a pure spin density in the absence of charge current can be generated in a setup that contains two hTLL and one spinful Tomonaga Luttinger liquid in between.

TT 38.40 Wed 14:00 P3

Edge transport and backscattering in a two-dimensional topological insulator in strong magnetic fields — •G. Tkachov and E. M. Hankiewicz — Würzburg University, Germany

Unlike ordinary band insulators, a recently identified class of materials - topological insulators - exhibit unusual conducting states on sample boundaries. Recently, a large body of experimental and theoretical work has been devoted to detection and characterization of such states in topological insulators (see, e.g. Refs. [1,2]). In this work we discuss how the edge states in a two-dimensional topological insulator can be probed by means of quasiballistic transport in strong magnetic fields. We find in particular that defects, which cause edge-state backscattering, can generate strong energy and magnetic- field dependences of the longitudinal conductance [3].

[1] M. König, H. Buhmann, L. W. Molenkamp, T. Hughes, C.-X. Liu, X.-L. Qi, and S.-C. Zhang, J. Phys. Soc. Jpn. **77**, 031007 (2008).
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[3] G. Tkachov and E. M. Hankiewicz, Phys. Rev. Lett. **104**, 166803 (2010).

TT 38.41 Wed 14:00 P3

Spin Transport in HgTe Quantum Wells — •Rolf W. Reinthaler, Dietrich G. Rothe, and Ewelina M. Hankiewicz — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We study the spin transport in the topological insulators HgTe quantum wells which are described within an effective four band model (conduction/heavy hole bands) including space inversion breaking terms [1]. In the ballistic regime, we find that the spin transport is governed by the Rashba term, i.e. the spin signal precesses with the electric field perpendicular to the plane of the quantum well. However, the precession length is modified due to the Dirac-like structure of the Hamiltonian. In particular, we find a large background signal near the topological insulator state as well as an enhanced spin rotation. We attribute these effects to the properties of the Hamiltonian and the confinement potential of the two-dimensional topological insulator.

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

[1] D. G. Rothe, R. W. Reinthaler, C.-X. Liu, L. W. Molenkamp, S.-C. Zhang, and E. M. Hankiewicz, New Journal of Physics 12 065012 (2010).

TT 39: Spin Structures/ Skyrmions (jointly with MA)

Time: Wednesday 14:00–16:30 Location: HSZ 04

Invited Talk TT 39.1 Wed 14:00 HSZ 04

Skyrmion crystals and topological transport phenomena — •Yoshinori Tokura — Department of Applied Physics, University of Tokyo, Tokyo, Japan

A class of helimagnet is derived from the Dzyaloshinskii-Moriya(DM) interaction on a non-centrosymmetric crystal; prototypical examples are the B20 type (FeSi type) transition-metal silicide and germanide families. Recently, the Skrymion lattice was confirmed to form in a narrow temperature(T) -magnetic field(B) region near the hlimagnetic to paramagnetic transition boundary. By contrast, thin films of B20 type MSi (M=Mn or Fe1-xCox) or MGe (M=Mn, Fe), whose thickness is smaller than the helical spin modulation period (=10-100nm), ubiquitously form the two-dimensional (2D) Skyrmion crystal with magnetic fields (B) applied normal to the film plane over a wide T-B region. The implication of such a 2D Skyrmion crystal in the magneto-transport properties is discussed, such as the spin-chirality- induced topological Hall effect.

This work was done in collaboration with X.Z. Yu, N. Kanazawa, Y. Onose, Y. Shiomi, Y. Matsui, N. Nagaosa, J.H. Park, J.H. Han, K. Kimoto, W.Z. Zhang, T. Arima, S. Wakimoto, K. Ohoyama, and K. Kakurai

Invited Talk TT 39.2 Wed 14:30 HSZ 04

Discovery of an atomic-scale skyrmion lattice in an ultrathin magnet: Fe/Ir(111) — •S. Heinze[1], K. von Bergmann[2], M. Menzel[2], J. Brede[2], A. Kubetzka[2], R. Wiesendanger[2], G. Bihlmayer[3], and S. Blügel[3] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel — [2]Institute of Applied Physics, University of Hamburg — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA

Skyrmions are topologically protected field configurations with particle-like properties that play an important role in various fields of science. They have been predicted to exist also in bulk magnets and in recent experiments it was shown that they can be induced by a magnetic field. A key ingredient for their occurrence is the Dzyaloshinskii-Moriya interaction (DMI) which was found to be strong also in ultrathin magnetic films on substrates with large spin-orbit coupling [1]. In these systems the DMI stabilizes spin-spirals with a unique rotational sense propagating along one direction of the surface [1,2]. Here, we go a step beyond and present an atomic-scale skyrmion lattice as the magnetic ground state of a hexagonal Fe monolayer on Ir(111). We develop a spin-model based on density functional theory that explains the interplay of Heisenberg exchange, DMI and the four-spin exchange as the microscopic origin of this intriguing magnetic state. Experiments using spin-polarized scanning tunneling microscopy confirm the skyrmion lattice which is incommensurate with the underlying atomic lattice. [1] M. Bode et al., Nature 447, 190 (2007). [2] P. Ferriani et al., Phys. Rev. Lett. 101, 027201 (2008).

Invited Talk TT 39.3 Wed 15:00 HSZ 04

Skyrmion states in noncentrosymmetric magnets — •Alexei N. Bogdanov, Andrei A. Leonov, and Ulrich K. Rössler — IFW Dresden

Axisymmetric magnetic strings with a fixed sense of rotation and nanometer sizes (chiral magnetic vortices or Skyrmions) have been predicted to exist in a large group of noncentrosymmetric crystals more than two decades ago [1]. Recently these extraordinary magnetic states have been directly observed in thin layers of cubic helimagnet (Fe,Co)Si [2]. In this report we apply our earlier theoretical findings and recent results [3] to review main properties of chiral Skyrmions, to elucidate their physical nature, and to analyse these recent experimental results on magnetic-field-driven evolution of Skyrmions and helicoids in chiral helimagnets. Concentrating on the physical side of the problem rather than on mathematical details we give an elementary introduction into the properties of chiral Skyrmions in magnetism. [1] A. N. Bogdanov, A. D. Yablonsky Sov. Phys. JETP 68 (1989) 101. [2] X. Z. Yu et al. Nature 465 (2010) 901. [3] U. K. Rößler et al., Nature 442 (2006) 797; arXiv:1009.4849; A. A. Leonov et al., arXiv:1001.1992v2.

Invited Talk TT 39.4 Wed 15:30 HSZ 04

Complex Magnetic Phase Diagram of the cubic Helimagnet FeGe — •Heribert Wilhelm — Diamond Light Source Ltd., Chilton, Didcot, OX11 0DE, United Kingdom

Cubic FeGe (B20 structure type) shows helical order below T_c =

278.3 K. Depending on temperature and magnetic field a complex sequence of cross-overs and phase transitions in the vicinity of T_c has been observed in magnetization and ac-susceptibility measurements in fields parallel to the [100] direction. In a narrow temperature range below T_c several magnetic phases have been found before the field-polarized state occurs. Of particular interest is the so-called A-phase. It splits in at least two distinct areas, A_1 and A_2. This has been confirmed by small-angle neutron scattering data. These data also yield a hexagonal scattering pattern, the fingerprint of a Skyrmion lattice, within the A_1 and A_2 regions. Precursor phenomena found above T_c display a complex succession of temperature-driven cross-overs and phase transitions before the paramagnetic phase is reached at T_0. The low-field state for $T_c < T < T_0$ is probably characterized by some kind of magnetic correlations concluded from nuclear forward scattering data. They revealed that this phase exists up to about 27 GPa, although the helical order is already suppressed at 19 GPa. No signatures of magnetic order have been observed above 30 GPa. Within a phenomenological model for chiral ferromagnets, which includes magnetic anisotropy, Skyrmionic phases and 'confined' chiral modulations were obtained. The observed precursor phenomena are then a general effect related to the confinement of localized Skyrmionic excitations.

Invited Talk TT 39.5 Wed 16:00 HSZ 04

Magnetoelectric effects in non-collinear magnets — •Maxim Mostovoy — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

The coupling of the electric field to the spin degrees of freedom in Mott insulators leads to a variety of spectacular phenomena in multiferroic materials, such as the magnetic field control of electric polarization in spiral magnets, the clamping between the ferroelectric and (anti)ferromagnetic domain walls in orthorhombic and hexagonal manganites and the excitation of magnons by the electric component of light (electromagnon peaks). The microscopic mechanisms of magnetoelectric coupling also allow for the electric field control of non-collinear spin structures in conventional magnets, which may find applications in spintronics. I will discuss the relevance of unusual magnetic multipoles, such as the monopole and toroidal moments, for the linear magnetoelectric effect and electromagnon excitation. I will also discuss the new dynamic magnetoelectric interaction, which can be used to move non-collinear spin textures in ferromagnets with an applied electric field. The effect of this coupling is dramatically enhanced for non-coplanar topological magnetic defects, such as magnetic vortices and Skyrmions.

TT 40: Topological Insulators (jointly with HL, MA)

Time: Wednesday 16:45–19:15 Location: HSZ 04

TT 40.1 Wed 16:45 HSZ 04

Complex spin structure of the topological insulator $Bi_2Te_3(0001)$ — •Jürgen Henk[1], Arthur Ernst[1], Sergey V. Eremeev[2], and Evgueni V. Chulkov[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Donostia International Physics Center, San Sebastian, Spain

Topological insulators — like $Bi_2Te_3(0001)$ — show a unique surface electronic structure. A model Hamiltonian [1] describes well the anisotropic dispersion of the Dirac state, as is evident from agreement with photoemission experiments (e. g. [2]). The spin of the Dirac state shows a circular arrangement in the momentum distribution, even in the presence of warping.

We prove by relativistic first-principles calculations that the spin structure of the Dirac state in $Bi_2Te_3(0001)$ is much more complicated than that derived from model calculations. First, all three spin components at the top Te layer are reversed with respect to those in the subsurface layers, and, second, the circular spin structure is destroyed at the cusps of warped momentum distributions, showing a vortex-like structure. Our findings are explained by hybridization of p orbitals in the topmost quintuple layer and may have implications for spintronic applications.

[1] L. Fu, Phys. Rev. Lett. **103** (2009) 266801.
[2] D. Hsieh et al, Phys. Rev. Lett. **103** (2009) 146401.

TT 40.2 Wed 17:00 HSZ 04

Thermal and structural stability of the topological state on Bi_2Se_3 — •Dandan Guan[1,2], M. Bianchi[1], R. C. Hatch[1], S. Bao[2], J. Mi[3], B. B. Iversen[3], and Ph. Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Department of Physics, Zhejiang University, Hangzhou, China — [3]Department of Chemistry, Aarhus University, Denmark

Topological insulator surfaces have recently attracted considerable attention, not least because they are predicted to play host to many novel physical phenomena. The topological states are also thought to have possible applications in (spin) transport, since they are not only protected from back-scattering, their very existence can be viewed as a bulk property. This implies that minor surface modifications can change the detailed dispersion of the topological state, but not remove it altogether.

We investigate the thermal and structural stability of the topological state on Bi_2Se_3 using angle resolved photoemission spectroscopy. The electron-phonon coupling strength is obtained through measurements of the temperature-dependent self-energy and the resulting λ value is compared to the bulk and to other surface-localized states. The structural stability is tested by surface modifications through noble gas ion bombardment.

TT 40.3 Wed 17:15 HSZ 04

Does magnetism destroy the Dirac state in a topological insulator? — Arthur Ernst[1], •Jürgen Henk[1], Evgueni V. Chulkov[2], Igor V. Maznichenko[3], and Ingrid Mertig[3] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Martin Luther University Halle-Wittenberg, Halle, Germany

A striking feature of topological insulators is that the Dirac states are protected by topology. However, how robust are these surface states against perturbations really? Given the prescribed spin structure of the Dirac state, one may ask whether magnetism destroys this state or — at least — modifies its spin-resolved dispersion.

To answer the above question we have investigated theoretically the topological insulator $Bi_2Te_3(0001)$ by means of relativistic *ab initio* calculations. The Bi atoms in the topmost quintuple layer form a substitutional alloy with Mn (i. e. $Bi_{1-c}Mn_c$) that is described within the coherent potential approximation. We find significant modificiations of the Dirac state in dependence of the Mn concentraction c and on the orientation of the Mn magnetic moments.

TT 40.4 Wed 17:30 HSZ 04

Surface electronic structure and surface state topology of Sb(110). — •Marco Bianchi[1], D. Guan[1,2], A. Strozecka[3], C.H. Voetmann[1], J. I. Pasqual[3], S. Bao[2], and Ph. Hofmann[1] — [1]Inst. Fysik og Astronomi Aarhus Universitet, Aarhus, Denmark — [2]Dep. of Physics, Zheijang University, Hangzhou, China — [3]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

Topological insulators are a recently discovered class of materials where the bulk is insulating while fundamental topological considerations require the surfaces to be metallic. The first experimentally confirmed topological insulator was the intermetallic alloy $Bi_{1-x}Sb_x$ ($0.09 < x < 0.18$). This topological insulator phase owes its existence to important changes in the band structure as the two semimetals are alloyed. Theoretical predictions based on the topological character of the bulk electronic structure agree with measurements on the alloy and also predict pure Sb to be a strong topological insulator. On the other hand, the electronic structure of the Bi surfaces, while being very similar to that of the alloy, appears to be consistent with that of a topologically trivial material.

We report on an experimental investigation of the Sb(110) electronic structure combining scanning tunnelling microscopy with angle-resolved photoemission. The topological character of the surface states can be inferred from the number of Fermi level crossings between time-reversal invariant momenta in the surface Brillouin zone. This surface topology is compared to that of Bi(110), Sb(111) and the theoretical predictions.

TT 40.5 Wed 17:45 HSZ 04

Topological insulators in ternary compounds with a hon-

eycomb lattice — •Stanislav Chadov[1], Jürgen Kübler[2], and Claudia Felser[1] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universtität, 55099 Mainz — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt

Based on electronic structure calculations we propose the certain extension to the class of the topological insulators which provide the convenient material base to realize the phenomenon of quantum spin Hall effect intensively studied nowadays. These new candidates (e. g. LiAuSe, KHgSb) are ternary semiconductors with a weakly coupled honeycomb layers (e. g. Au-Se, Hg-Sb) analogical to a weakly graphite sheets. It makes them very similar to graphene which is a single layer of graphite: their band structures exhibit the so-called linearly dispersive Dirac cone centered at the Fermi energy. However, in contrast to graphene with two Dirac cones at K and K' points, these materials exhibit the surface states formed by only a single Dirac cone at the Γ point, allowing for the non-vanishing quantum spin Hall effect. The additional stuffing" elements (Li, K, etc.) extend the material multifunctionality, i. e. give more possibilities for tuning and coupling of their properties. In contrast to other topologically non-trivial systems, as e. g. recently proposed half-Heuslers, the honeycomb compounds possess the non-zero band gap in the bulk, i. e. provide the "natural" 3D topological materials.

TT 40.6 Wed 18:00 HSZ 04

Thallium-based topological insulators from first principles — •Gustav Bihlmayer[1], Sergey V. Eremeev[2], Stefan Blügel[1], and Eugene V. Chulkov[3] — [1]Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Institute of Strength Physics and Materials Science, Tomsk, Russia — [3]Donostia International Physics Center (DIPC), San Sebastián, Spain

Currently, there is a substantial interest in topological insulators, which show protected edge-states carrying dissipationless spin currents. Among the new classes of these materials the Tl-based compounds $TlAB_2$ (A=Bi,Sb; B=Se,Te) have attracted considerable interest both on the experimental and theoretical side. We present density functional theory calculations of the bulk materials and their (111) surfaces, displaying protected Dirac-cone shaped surface states together with "trivial" surface states. In contrast to layered materials like Bi_2Te_3, these compounds are of more three-dimensional character. From the bulk calculations we observe a strong sensitivity of the topological properties on the structural details, that have to be described very accurately. In the surface calculations deeply penetrating Dirac-cone states are observed, calling for careful convergence of the calculations with respect to the film thickness. Similar materials, e.g. the sulfides and $InAB_2$ compounds will be discussed for comparison.

TT 40.7 Wed 18:15 HSZ 04

Electronic structure of the topological semiconductors PtYSb, PtLaBi, and PtGdBi explored by hard X-ray photoelectron spectroscopy. — •Siham Ouardi[1], Shekar Shandra[1], Gerhard H. Fecher[1], S. Chadov[1], X. Kozina[1], G. Stryganyuk[1], C. Felser[1], S. Ueda[2], and K. Kobayashi[2] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universtität, 55099 Mainz — [2]National Institute for Materials Science, SPring-8, Hyogo, Japan

One of the recent topics in spintronics is the realization of the so-called topological insulators, that are insulators in the bulk and gapless semiconductors at the surface. Besides the well-known wide range of properties of the Heusler family it was recently shown that many of the heavy Heusler semiconductors with 1:1:1 composition and $C1_b$ structure are zero band-gap insulators and exhibit a inverted band structure. The density of states of several compounds was investigated by bulk sensitive hard X-ray photoelectron spectroscopy. First experimental results on PtYSb, PtLaBi, and PtGdBi give clear evidence for the zero band-gap state. Their structural, spectral and transport characteristics will be compared to calculations.

TT 40.8 Wed 18:30 HSZ 04

Tolerance of topological surface state towards adsorbed magnetic moments: Fe on Bi_2Te_3 — •Markus Scholz[1], Dmitry Marchenko[1], Jaime Sanchez-Barriga[1], Andrei Varykhalov[1], Andrei Volykhov[2], Lada Yashina[2], and Oliver Rader[1] — [1]Helmholtz-Zentrum für Materialien und Energie, Berlin, Deutschland — [2]Moscow State University, Moskau, Russland

Topological surface states on Bi_2Se_3 and Bi_2Te_3 are protected by time reversal symmetry [1]. Magnetic fields break time-reversal symmetry, and they have been used in two-dimensional spin quantum-Hall systems to destroy the topological edge states [2]. Another possibility is to introduce magnetic moments. This has been done by substitution of Mn and Fe into the bulk [3][4]. For Fe a small gap of 44meV was created, however, at very large amounts (12%). In this work, we deposit Fe directly onto the surface where the topological surface state is localized. We show for coverages of 0.25 and 1 ML Fe that the Dirac point remains intact and no gap appears. Core level spectroscopy of Bi and Te states gives insight into the interaction between substrate and adatoms. In addition, extra surface states appear at the Fermi energy which show a large Rashba-type spin-orbit splitting. The orientation of the spin of both, the topological as well as the Rashba-type split surface states is analysed. [1] Kane and Mele, Phy. Rev. Lett 95, 146802 (2005); Liang Fu et al., Phys. Rev. Lett. 98, 106803 (2007) [2] König et al.,Science 318, 5851 (2007) [3] Hsieh et al., Phys. Rev. Lett. 103, 146401 (2009) [4] Chen et al., Science 329, 5992 (2010)

TT 40.9 Wed 18:45 HSZ 04

Rashba-type surface emission observed on W(110) — •Juergen Braun[1], Jan Minar[1], Akio Kimura[2], Koji Miyamoto[2], Markus Donath[3], and Hubert Ebert[1] — [1]Department Chemie, LMU München, Germany — [2]Graduate School of Science, Hiroshima University, Higashi-Hiroshima, Japan — [3]Physikalisches Institut, Universität Münster, Germany

In this contribution we discuss surface related spectral features of bcc W(110) by means of angle- and spin-resolved photoemission. For more than thirty years Tungsten serves as a prototypical material for studying spin-orbit effects in simple metals. Also, it is used for a quite long time in electron polarimeters [1]. Nevertheless, there still remain some pecularities in its electronic structure concerning surface emission. It is known that a surface resonance exists on W(110) dispersing around $\overline{\Gamma}$ in the vicinity of the Fermi level [2]. But not much is understood concerning surface emission for higher binding energies. From our investigation we found that surface emission dominates the $E(\mathbf{k}_{\|})$ intensity distribution measured along $\overline{\Gamma N}$. The spin analysis reveals a Rashba-like behavior for features related to the spin-orbit induced symmetry gap existing at $\overline{\Gamma}$. The theoretical analysis has been performed in the framework of the fully relativistic version of the one-step model of photoemission [3].

1. J. Kirschner, Polarized electrons at surfaces, Springer, Berlin (1985). 2. R. H. Gaylord et al., PRL 62, 2036 (1989). 3. H. Ebert et al., The Munich SPR-KKR package, version 5.4, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2010).

TT 40.10 Wed 19:00 HSZ 04

Wave-packet transport in HgTe — •Viktor Krueckl and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Recent experiments have shown the Quantum Spin Hall State in mercury telluride quantum wells and the associated edge channel transport at zero external magnetic field [1]. We employ a four band model to investigate the propagation of such topological edge state wave-packets in the gap, as well as bulk states in the conducting region. Our recently developed algorithm is able to solve the time-dependent scattering problem for arbitrary scattering potentials and gives revealing insight into the occurring edge phenomena. The obtained time evolution of the wavefunction is used to calculate the complete energy dependent scattering matrix for a time-independent Hamiltonian. With this we investigate the transport in different mesoscopic setups and are particularly interested in the scattering of edge states at constrictions. [1] A. Roth, C. Brüne, H. Buhmann, L. W. Molenkamp, J. Maciejko, X.-L. Qi and S.-C. Zhang, Science **325**, 294 (2009)

TT 41: CE: Spin Systems and Itinerant Magnets 1

Time: Wednesday 18:15–19:30 Location: HSZ 105

TT 41.1 Wed 18:15 HSZ 105

Orbital fluctuations versus classical orbital order in RVO_3 studied via optical spectral weight — •Julia Küppersbusch[1], Agung Nugroho[2], Thomas Palstra[2], and Markus Grüninger[1] — [1]Universtität zu Köln — [2]Rijksuniversiteit Groningen

Spin and orbital degrees of freedom play a decisive role in the low-energy physics of strongly correlated transition-metal oxides. Whereas the spin is a true low-energy degree of freedom with propagating low-energy excitations, it is still questionable if the same holds true for the orbital degree of freedom. In a typical situation the orbitals are strongly coupled to the lattice, which makes it sufficient to consider classical orbitals with rigid orbital order. However, different groups have pointed out that orbital fluctuations may be strong in the $3d^2$ Mott-Hubbard insulators RVO_3 (R = rare earth ion or Y).
Optical spectroscopy offers an efficient method to study the nature of the orbital degree of freedom, because the spectral weight of excitations across the Mott-Hubbard gap depends sensitively on nearest-neighbor orbital-orbital correlations. We study the temperature dependence of the optical spectral weight by means of ellipsometry in the frequency range 0.75 - 5.5 eV. By comparing our experimental results for R = Y, Gd, and Ce with a theory which calculates the temperature dependence of the optical spectral weight based on a low-energy spin-orbital superexchange Hamiltonian [1,2], we draw a conclusion about the nature of the orbital degree of freedom in RVO_3.
[1] G. Khaliullin, P. Horsch, and A.M. Oles, Phys. Rev. B 70, 195103 (2004)
[2] A. M. Oles et al. Phys. Rev. B 72, 214431 (2005)

TT 41.2 Wed 18:30 HSZ 105

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], A. Agung Nugroho[4,5], Thomas T. M. Palstra[4], Pasquale Marra[6], Krzysztof Wohlfeld[6], Jeroen van den Brink[6], Maurits Haverkort[2], Thorsten Schmitt[7], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung — [6]IFW Dresden — [7]PSI Villigen

In an orbitally ordered state, exchange interactions between orbitals on neighbouring sites could give rise to a significant dispersion of the orbital excitations. These orbitons are analogous to spin waves. Here, we report on the observation of orbital excitations in YVO_3 and $GdVO_3$ by means of high-resolution RIXS across the V $L_{3,2}$ and O K edges with the new SAXES beamline at the PSI, Villigen. Due to the excellent resolution of 60 meV, we are able to resolve the different intra-t_{2g} excitations. Our data show 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]. For $GdVO_3$ the one-orbiton energy shows a shift of up to 40 meV as a function of momentum. This shift could be related to dispersive orbitons or, alternatively, to two different intra-t_{2g} excitations and a transfer of spectral weight between them. To figure this out we compare our data with recent calculations.
[1] E. Benckiser *et al.*, New J. Phys. **10**, 053027 (2008).

TT 41.3 Wed 18:45 HSZ 105

Charge dynamics in $CuGeO_3$: a combined RIXS and EELS study — •Valentina Bisogni[1], Claude Monney[2], Roberto Kraus[1], Kejin Zhou[2], Vladimir Strocov[2], Stefan-Ludwig Drechsler[1], Jeroen van den Brink[1], Thorsten Schmitt[2], and Jochen Geck[1] — [1]IFW, Dresden, Germany — [2]Paul Scherrer Institut, Villigen PSI, Switzerland

Model compounds of the high temperature superconductors (HTCS) are considered of big interest for the understanding of superconductivity but also for their fascinating, tuneable magnetic and electronic properties. Thanks to the low dimensionality, these model systems allow for a thorough theoretical analysis enabling to achieve a good understanding of the interactions at work. $CuGeO_3$ is a well known realization of one-dimensional antiferromagnetic S=1/2 spin chain, made of edge-sharing CuO_4- plaquettes, and undergoing a Spin-Peierls transition at T ≈14 K. Recently, thanks to the improved energy resolution, soft x-ray resonant inelastic scattering (RIXS) has demonstrated to be a suitable tool for the study of the HTCS. We performed RIXS experiments on $CuGeO_3$ at the ADRESS beamline of the Swiss Light Source. *dd*-excitations can be clearly observed at the Cu-L edge, while Cu-O charge transfer processes are enhanced at the O-K edge. Temperature and momentum dependent studies unambiguously identify the Zhang-Rice singlet in $CuGeO_3$, showing the importance of the magnetic configuration at the ground state and the Cu-O-Cu bond geometry. Complementary data measured with high resolution electron energy loss spectroscopy (EELS) are discussed in comparison with RIXS.

TT 41.4 Wed 19:00 HSZ 105

Spin Transfer Torques in MnSi at Ultra-low Current Densities — •F. Jonietz[1], S. Mühlbauer[1,2], C. Pfleiderer[1], A. Neubauer[1], W. Münzer[1], A. Bauer[1], T. Adams[1], T. Schulz[1], M. Wagner[1], R. Georgii[1,2], P. Böni[1], R. A. Duine[3], K. Everschor[4], M. Garst[4], and A. Rosch[4] — [1]Physik-Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, D-85748 Garching, Germany — [3]Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands — [4]Institute of Theoretical Physics, University of Cologne, D-50937 Cologne, Germany

Spin manipulation using electric currents is one of the most promising directions in the field of spintronics. We used neutron scattering to observe the influence of an electric current on the magnetic structure in a bulk material. In the skyrmion lattice of MnSi, where the spins form a lattice of magnetic vortices similar to the vortex lattice in type II superconductors [1], we observe the rotation of the diffraction pattern in response to currents [2] which are over five orders of magnitude smaller than those typically applied in experimental studies on current-driven magnetization dynamics in nanostructures. We attribute our observations to an extremely efficient coupling of inhomogeneous spin currents to topologically stable knots in spin structures.
[1] S. Mühlbauer, et al. Science 323, 5916 (2009)
[2] F. Jonietz, et al. Science, in press (2010)

TT 41.5 Wed 19:15 HSZ 105

Higher-order scattering in the Skyrmion lattice in MnSi — •Tim Adams[1], Sebastian Mühlbauer[1,2], Christian Pfleiderer[1], Peter Böni[1], and Achim Rosch[3] — [1]Physik-Department E21, TU München, 85748 Garching, Germany — [2]ETH Zürich, Institut für Festkörperphysik, Zürich, Switzerland — [3]ITP, Universität zu Köln, Köln, Germany

Recent small angle neutron scattering (SANS) experiments suggest the existence of a skyrmion lattice in the A-phase of the archetypal helical magnet MnSi, where the skyrmion lattice is stabilized by thermal Gaussian fluctuations [1]. Such a skyrmion lattice represents a hexagonal spin crystal composed of topologically stable knots of the spin structure. The observation of a topological Hall effect thereby provided stringent evidence of the topological nature of the spin structure [2]. However, in the first neutron scattering studies only first order Bragg peaks were observed. We report a very careful SANS search for higher order scattering in the A-phase to establish the particle-like nature of the skyrmions forming a lattice. So-called Renninger scans thereby allowed us to clearly distinguish double scattering from higher order scattering. We find clear evidence of second order Bragg peaks. Thus the A-phase in MnSi is indeed a lattice of particle-like knots in the spin structure.
[1] S. Mühlbauer, et al., Science 323, 5916 (2009)
[2] A. Neubauer et al., Phys. Rev. Lett. 102, 186602 (2009)
[3] M. Renninger, Z. Physik, 106, 141-176 (1937)

TT 42: SC: Fe-based Superconductors - Fe(Se,Te)

Time: Wednesday 18:45–20:00 Location: HSZ 304

TT 42.1 Wed 18:45 HSZ 304

Physical properties of $FeSe_{0.5}Te_{0.5}$ single crystals — •Vladimir Tsurkan[1,2], Joachim Deisenhofer[1], Axel Günther[1], Christian Kant[1], Florian Schrettle[1], Hans-Albrecht Krug von Nidda[1], and Alois Loidl[1] — [1]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chişinău, Republic of Moldova

We report on structural, magnetic, conductivity, and thermodynamic studies of $FeSe_{0.5}Te_{0.5}$ single crystals grown by self-flux and Bridgman methods. The lowest values of the susceptibility in the normal state, the highest transition temperature T_c of 14.5 K, and the largest heat-capacity anomaly at T_c were obtained for pure (oxygen-free) samples. The upper critical field H_{c2} of $\sim$ 500 kOe is estimated from the resistivity study in magnetic fields parallel to the c-axis. The anisotropy of the upper critical field $\gamma_{H_{c2}} = H_{c2}^{ab}/H_{c2}^{c}$ reaches a value $\sim$ 6 at $T \longrightarrow T_c$. Extremely low values of the residual Sommerfeld coefficient for pure samples indicate a high volume fraction of the superconducting phase (up to 97 %). The electronic contribution to the specific heat in the superconducting state is well described within a single-band BCS model with a temperature dependent gap $\Delta_0 = 27(1)$ K. A broad cusp-like anomaly in the electronic specific heat of samples with suppressed bulk superconductivity is ascribed to a splitting of the ground state of the Fe^{2+} ions at 2c sites. This contribution is fully suppressed in the ordered state in samples with bulk superconductivity.

TT 42.2 Wed 19:00 HSZ 304

Superconducting $FeSe_{0.5}Te_{0.5}$ under high pressure: Susceptibility, XRD and Mössbauer studies. — •Vadim Ksenofontov[1], Leslie Schoop[1], Sergey Medvedev[2], Michail Eremets[2], Vladimir Tsurkan[3], Joachim Deisenhofer[3], Alois Loidl[3], Gerhard Wortmann[4], and Claudia Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]Max-Planck-Institute for Chemistry, Mainz, Germany — [3]Institute of Physics, University of Augsburg, Augsburg, Germany — [4]Department of Physics, University of Paderborn, Paderborn, Germany

High-pressure magnetic, structural and Mössbauer studies were performed on single-crystalline samples of superconducting (sc) $FeSe_{0.5}Te_{0.5}$ with T_c = 14.5 K [1]. Susceptibility data up to 1.5 GPa revealed a strong increase of Tc up to 25 K, followed by a plateau in T_c up to 6.0 GPa. Further increase of pressure leads to a disappearance of sc state around 7.0 GPa. Structural and Mössbauer studies explain this fact by a structural phase transition of the sc PbO to the non-sc NiAs structure. We discuss the fact of an almost pressure-independent T_c, between 1.5 and 6.0 GPa by the respective variation of the lattice constants and hyperfine parameters in FeSe [2]. We conclude that the strong increase of T_c in $FeSe_{0.5}Te_{0.5}$ with pressure up to 1.5 GPa can not be attributed to a change in the phonon-DOS [3].

[1] V. Tsurkan et al., arXiv:1006.4453.
[2] S. Medvedev et al., Nature Mater. 87, 630 (2009).
[3] V. Ksenovontov et al., Phys. Rev. B 81, 184510 (2010).

TT 42.3 Wed 19:15 HSZ 304

^{57}Fe NIS studies of phonon DOS in superconducting $FeSe_{0.5}Te_{0.5}$ single crystals — •Gerhard Wortmann[1], Vadim Ksenofontov[2], Teuta Gasi[2], Aleksandr Chumakov[3], Vladimir Tsurkan[4], Joachim Deisenhofer[4], Alois Loidl[4], and Claudia Felser[2] — [1]Department of Physics, University of Paderborn, Paderborn, Germany — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Institute of Physics, University of Augsburg, Augsburg, Germany

FeSe and isostructural $FeSe_{0.5}Te_{0.5}$ could provide valuable information for the understanding of the principal mechanisms of superconductivity (SC) in the novel Fe-based superconductors. Using ^{57}Fe nuclear inelastic scattering (NIS) we have measured the phonon-DOS in single-crystalline samples of $FeSe_{0.5}Te_{0.5}$ [1] parallel and perpendicular to the c-axis. A study of the phonon-DOS as function of temperature revealed a very similar temperature dependence as observed in FeSe [2], also no changes of the phonon-DOS above and below T_c = 14.5 K. Together with results of conventional ^{57}Fe-Mössbauer studies, we can exclude any phonon softening connected with the observed SC [3]. Based on these results and previous studies of FeSe [2,4], we discuss the role of phonons in the mechanisms for SC in the Fe-based systems.

[1] V. Tsurkan et al., arXiv:1006.4453.
[2] V. Ksenovontov et al., Phys. Rev. B 81, 184510 (2010).
[3] J. Lindén et al., arXiv:1008.1680.
[4] S. Medvedev et al., Nature Mater. 87, 630 (2009).

TT 42.4 Wed 19:30 HSZ 304

Tunnelling spectroscopy (SI-STM) study of Fe(Se,Te) — •Seth Cullen White, Udai Raj Singh, Yong Liu, Chengtian Lin, and Peter Wahl — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

We use spectroscopic imaging scanning tunnelling microscopy (SI-STM) to investigate the local electronic structure of iron-based superconductors. Fe(Se,Te) has the simplest structure of these superconductors, consisting of planar iron layers with chalcogen anions above and below. The crystal structure provides a well defined cleavage plane between chalcogenide layers. In this study we map spatially the local density of states on a $Fe_{1.08}Se_{0.28}Te_{0.72}$ sample, which is superconducting below 14 K, revealing spectral features associated with defects. We investigate further the spectral features associated with excess Fe impurities, which are predicted to have a magnetic moment leading to local suppression of superconductivity.

TT 42.5 Wed 19:45 HSZ 304

Quasiparticle interference in an iron-based superconductor — •Steffen Sykora[1,2] and Piers Coleman[2] — [1]IFW Dresden, Institute for Theoretical Solid State Physics, P.O. Box 270116, D-01171 Dresden, Germany — [2]Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA

We develop a model for the effect of a magnetic field on quasiparticle interference in an iron-based superconductor. Recently, scanning tunneling experiments have been performed on Fe(Se,Te) to determine the relative sign of the superconducting gap from the magnetic-field dependence of quasi-particle scattering amplitudes. Using a simple two-band BCS model we study three different cases of scattering in a spin-split spectrum. The dominant effect of a magnetic field in iron-based superconductors is caused by the Pauli limiting of conduction electrons. Thereby time reversal odd scattering is induced which enhances the sign-preserving and depresses the sign-reversing peaks in the quasiparticle interference patterns.

TT 43: TR: Nanoelectronics II - Spintronics and Magnetotransport 2 (jointly with HL and MA)

Time: Wednesday 19:00–20:15 Location: HSZ 03

TT 43.1 Wed 19:00 HSZ 03

Spin polarized transport in metallic magnetic single electron transistors — •Stephan Lindebaum and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

We study the electronic transport through a ferromagnetic single electron transistor (fmSET), realized by a metallic island weakly coupled to two ferromagnetic leads. The polarization directions of the ferromagnets enclose a noncollinear angle. In the considered system, charging and spin effects play an important role. For example the accumulated spin on the island precesses due to a many-body exchange field, which arises as a consequence of virtual tunneling processes from the metallic island to the magnetic leads in presence of strong Coulomb interaction on the central electrode.

To analyze the system we perform a perturbative analysis of the transport properties up to first order in the tunnel-coupling strength, but without doing any approximation for the Coulomb charging energy. A diagrammatic real-time transport theory enables us to derive kinetic equations for the island charge and spin degrees of freedom.

The theory covers both the linear and nonlinear transport regimes. The electric current through the fmSET and its conductance are analyzed in detail, while we explicitly investigate the influence of the exchange field on the transport parameters.

TT 43.2 Wed 19:15 HSZ 03

Adiabatic pumping through an interacting quantum dot 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 and MacDiarmid Institute for Advanced Materials and Nanotechnology · Victoria University of Wellington · New Zealand

We investigate adiabatic charge and spin transport through a system composed of a quantum dot with Coulomb interaction, weakly tunnel coupled to one normal and one ferromagnetic lead with time-dependent magnetisation. Adiabatic pumping is typically studied in systems in which the properties of the scattering region are changed, e.g. gate voltages to vary the tunnel couplings and the level position of the quantum dot. In general, it is also possible to generate a current by varying in time the lead properties, e.g. the direction of the magnetisation solely [1]. We study the adiabatically pumped charge and spin current up to second order in the tunnel-coupling strength when pumping by varying the direction of the lead magnetisation periodically in time. To this aim, we extend a diagrammatic real-time approach for adiabatic pumping through quantum dots with ferromagnetic leads [2,3] to allow for time-dependent magnetisations. We perform a systematic expansion in both frequency and tunnel-coupling strength, treating the on-site Coulomb interaction on the quantum dot exactly.

[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 43.3 Wed 19:30 HSZ 03

Rectification effects in spin chains — •Kevin van Hoogdalem and Daniel Loss — Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We study spin transport in non-itinerant one-dimensional quantum systems. Inspired by possible applications in spintronics, we consider rectification effects in both ferromagnetic (FM) and antiferromagnetic (AF) spin chains. We find that the crucial ingredients in designing a system that displays a non-zero rectification current are an anisotropy in the exchange interaction of the spin chain combined with an offset magnetic field. For both FM and AF systems we can exploit the gap in the excitation spectrum that is created by a bulk anisotropy to obtain a measureble rectification effect at realistic magnetic fields. For AF systems we also find we can achieve a similar effect by considering a specific sort of impurity, obtained by altering two neighboring bonds in the Heisenberg Hamiltonian.

TT 43.4 Wed 19:45 HSZ 03

Relaxation mechanisms of the Persistent Spin Helix — •Matthias C. Lüffe[1], Janik Kailasvuori[2], and Tamara S. Nunner[1] — [1]Fachbereich Physik & Dahlem Center for Complex Quantum Systems, FU Berlin, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany

The Persistent Spin Helix has been predicted and recently observed as an unusually long-lived helical texture of spin polarization in a semiconductor quantum well where the Rashba- and linear Dresselhaus spin-orbit couplings are of equal strengths. In order to understand the decay in time of this object, we derive and solve semiclassical spin diffusion equations which take spin-dependent impurity scattering, cubic Dresselhaus spin-orbit coupling and, in particular, electron–electron interactions into account. We find that for reported experimental parameters the temperature-dependent lifetime of the persistent spin helix is largely determined by the interplay of cubic Dresselhaus spin-orbit coupling and electron–electron interactions. On the basis of this insight we propose for an experimental starting point a spatially damped spin profile which then evolves towards a truly persistent spin helix even in the—to some extent unavoidable—presence of cubic Dresselhaus spin-orbit interactions.

TT 43.5 Wed 20:00 HSZ 03

Design of nanostructures with maximal magnetoresistance using genetic algorithms — •Daungruthai Jarukanont — University of Kassel, Kassel, Germany

We present a theoretical study of spin-dependent electron transport through organic spin-valves, modeled by an organic molecule sandwich between two ferromagnetic electrodes. The calculations of spin-currents are based on the non-equilibrium Green's function and the Keldysh formalism at low bias. The electrodes are described by tight binding model of 3D semi-infinite leads, while molecules are method independent. We examine the influence of molecular details to spin-currents, and magnetoresistance(MR). The genetic algorithm is perform as an optimization to find the electronics structure of molecules with high values of MR. Example of molecular choices such as alkanethiols, 1,4-benzenedithiol with different molecule-electrode interactions are analyzed.

TT 44: Poster Session Correlated Electrons

Time: Thursday 10:00–13:00 Location: P1

TT 44.1 Thu 10:00 P1

NRG calculations of the magnetization of Kondo impurities in an external field — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld, Germany

The deposition of magnetic molecules on suitable substrates represents one possibility to solve the problem of addressing individual molecules so that they might be used for information storage or quantum computing purposes. However, the magnetic properties of the molecules, which for example determine the dependence of magnetization on temperature and applied field and which are crucial for such applications, will in general be influenced by the interaction with the substrate. The goal of our ongoing investigations is to better understand the form and extent of this effect.

In an attempt to theoretically approach the problem, we study single-impurity Kondo models in an external magnetic field whose impurity consists of several exchange-coupled spins and is supposed to represent a magnetic molecule. We then focus on the impurity magnetization and compare the behavior of the free and deposited molecule (the impurity) for each model.

In order to obtain reliable approximations for the thermodynamic limit of interest, i.e. the infinitely extended substrate, we carry out the calculations using Wilson's Numerical Renormalization Group (NRG). NRG is by now a well established method and has been significantly improved in the last five years. As an additional benefit, it allows us to study the impurity magnetization both as function of temperature and magnetic field.

TT 44.2 Thu 10:00 P1

Real-space Kondo correlations — •Michael Becker, Andrew Mitchell, and Ralf Bulla — Universität zu Köln

We investigate real-space Kondo correlations in various impurity models. Any physical quantity in real space can be calculated from purely local impurity correlators. In the simplest (but most revealing) example of the Anderson model, the density variation around the impurity is related to the impurity Green function, which we calculate accurately via the numerical renormalization group technique. Signatures of the 'free orbital', 'local moment' and 'strong coupling' fixed points are evident in real space, with characteristic length scales R_{FO} and R_{LM} being associated with each at $T = 0$. The 'local moment cloud' is an exponentially extended object with $R_{LM} \sim 1/T_K$; Kondo screening itself occurring for $r \gg R_{LM}$. As the temperature is increased, the Kondo effect is destroyed, as manifest in real space by the divergence of R_{LM}, implying that the uncompensated moment due to the impurity becomes infinitely extended. The familiar RG picture known for other classic models is similarly apparent in real space. In particular, the phase transition in the pseudogap Anderson model (realised here for an impurity in graphene) is associated with a diverging length scale;

and the existence of both 'local moment' and 'overscreening' clouds are demonstrated in the two-channel Kondo model.

TT 44.3 Thu 10:00 P1

Coupled Spins in a Dissipative Environment — •Etienne Gärtner, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zülpicherstr. 77 50937 Cologne, Germany

One of the fascinating consequences of quantum mechanics is that different coupled subsystems can become entangled. A classic example is a quantum impurity coupled to a dissipative environment (the standard spin-boson model). Here we consider the natural extension of this scenario, studying the entanglement generated between two impurities which are coupled to a common bosonic bath. This two-spin-boson model is analysed in detail using the bosonic numerical renormalization group (NRG) technique, with the Von Neumann entropies and phase diagram extracted directly. Recently the question has been posed as to whether a common bath could also generate entanglement between spatially separated spins. To address the question of the lenghtscale for such entanglement, we couple the spins to 1 or 2 dimensional bosonic host lattices, and calculate the dependence of physical properties on impurity separation. To this end, we extend the bosonic NRG to deal with the two-bath effective model that results.

TT 44.4 Thu 10:00 P1

Kondo physics with variational matrix-product states — •Andrej Schwabe and Michael Potthoff — I. Institut Theoretische Physik, Universität Hamburg, Hamburg, Deutschland

The screening of an impurity spin by conduction band electrons, known as the Kondo effect, is a typical many-particle phenomenon which still raises basic questions. We apply our variational matrix-product states code (VMPS [1,2]) which is based on the implementation of the corrected one-site algorithm [3] and exploits $U(1)$ symmetries. We present calculations for an impurity coupled locally to a finite, but long uncorrelated nano chain as well as calculations for an inhomogeneous two-leg Hubbard-type model with site and leg dependent Hubbard-U.
Our study focuses on the spin correlation functions, which show the emergence of the Kondo screening cloud, and comprises the investigation of its dependence on the position of the impurity, the Kondo coupling, and the length of the chain. The results are compared to previous studies [4,5]. We discuss the interference of the Kondo clouds of several impurities coupled to the chain, and the competition with the magnetic exchange coupling between the impurities (RKKY).
[1] U. Schollwoeck, arXiv:1008.3477v1 (2010)
[2] F. Verstraete et al., Advances in Phys. **57**, 143 (2008)
[3] S. R. White, Phys. Rev. B **72**, 180403 (2005)
[4] T. Hand et al., Phys. Rev. Lett. **97**, 136604 (2006)
[5] A. Holzner et al., Phys. Rev. B **80**, 205114 (2009)

TT 44.5 Thu 10:00 P1

Kondo effect in single wall carbon nanotubes with ferromagnetic contacts — Markus Gaass[1], •Daniel Steininger[1], Andreas K. Hüttel[1], Kicheon Kang[1,3], Ireneusz Weymann[2,4], Jan von Delft[2], and Christoph Strunk[1] — [1]Universität Regensburg, Germany — [2]Ludwig-Maximilians-Universität München, Germany — [3]Chonnam National University, Gwangju 500-757, Korea — [4]Adam Mickiewicz University, 61-614 Poznań, Poland

We investigate the influence of ferromagnetic contacts on the Kondo effect in quantum dots formed in SWCNTs. For this purpose we use $Pd_{0.3}Ni_{0.7}$, a ferromagnetic alloy known for providing sufficiently transparent interfaces to CNTs [1,2]. Transport spectroscopy shows a conductance anomaly around zero bias in every second Coulomb diamond. The ferromagnetic contacts cause two peaks at finite bias which can be rejoined by a finite magnetic field. The size and sign of the splitting as well as its dependence on gate voltage can be explained by spin-dependent renormalization processes of the quantum dot level that include two contributions. One, independent of gate voltage, arises from the macroscopic magnetization of the leads. The other contribution, showing a gate dependence, stems from the polarization of the spins at the Fermi energy. The data are compared to numerical renormalization group calculations. In addition, we observe a fine structure in the spectra indicating a complex level structure which may result from curvature-induced spin-orbit interaction.
[1] J.R. Hauptmann, et al., Nature Phys. **4**, 373 (2008)
[2] L. Hofstetter, et al., Phys. Rev. Lett. **104**, 246804 (2010)

TT 44.6 Thu 10:00 P1

Superconductivity in the Kondo lattice model — •Oliver Bodensiek[1], Rok Žitko[1,2], and Thomas Pruschke[1] — [1]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

We study the Kondo lattice model with an additional attractive interaction among the conduction-band electrons by means of dynamical mean-field theory in combination with the numerical renormalization group method. In the normal phase we observe a strong dependency of the low-energy scale on the attractive interaction. Thus, there exists a delicate interplay between the attractive interaction and the antiferromagnetic Kondo exchange, which results in a critical interaction, above of which the Fermi surface collapses because the spins become effectively decoupled from the conduction electrons. Additionally, we allow for a s-wave superconducting phase, which appears to be split at the point of the underlying Fermi surface collapse. We discuss the interplay between attractive interaction an Kondo exchange and its pertinence to phonons in heavy fermion physics.

TT 44.7 Thu 10:00 P1

Magnetic phase transitions in CePdAl — •S. Woitschach[1], O. Stockert[1], V. Fritsch[2], N. Bagrets[2], H. v. Löhneysen[2], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

The heavy fermion system CePdAl in its hexagonal modification shows antiferromagnetic order below $T_N = 2.7$ K and is located close to quantum criticality. By applying hydrostatic pressure or by concentration tuning via alloying Ni on the Pd site, T_N decreases continuously and finally a quantum critical point is approached. In this system geometrical frustration is present, as inferred from neutron scattering, and might play a role in tuning the groundstate. Several magnetically ordered phases have been observed in CePdAl, but so far no detailed measurements of the B-T phase diagram and the magnetic anisotropy have been performed. Here, we report on measurements of the heat capacity of a Czochralski-grown CePdAl single crystal to determine the B-T phase diagram. Especially we focus on the anisotropy for magnetic fields applied along the c-axis or in the basal plane.

TT 44.8 Thu 10:00 P1

Investigating the large degeneracy Kondo lattice metamagnet CeTiGe: Crystal growth and doping studies — •T. Gruner[1], N. Caroca-Canales[1], J. Sereni[2], M. Deppe[1], and C. Geibel[1] — [1]MPI für Chemische Physik fester Stoffe, 01187, Dresden, Germany — [2]Centro Atomico Bariloche, 8400, S. C. de Bariloche, Argentina

CeTiGe is a paramagnetic Kondo lattice system with a large orbital degeneracy involved in the formation of the heavy Fermion ground state. Recently we discovered that this compound presents a huge metamagnetic transition at $B_{MMT} \approx 13$ T, with much larger anomalies in magnetization, magnetoresistance and magnetostriction than in the archetypical Kondo lattice metamagnet $CeRu_2Si_2$. Since CeTiGe forms in a pronounced peritectic reaction the growth of single crystals is difficult. We therefore studied the Ce-Ti-Ge ternary metallographic phase diagram to get a sound basis for future crystal growth attempts. Preliminary results of growth experiments based on these studies are promising and shall be discussed. Furthermore, Ti-rich CeTiGe was recently reported to present a high temperature phase crystallizing in the closely related CeScSi structure type. In order to study this structural instability and the effect on the physical properties, we studied the effect of substituting Sc for Ti, since pure CeScGe crystallizes in the CeScSi structure type. In well annealed samples we observed a two phase region in the range 10 % - 25 %-Sc-substitution. Preliminary investigations of the $CeSc_xTi_{1-x}Ge$ alloy suggest it is a promising candidate for the observation of a ferromagnetic quantum critical point in a large degeneracy Kondo lattice system.

TT 44.9 Thu 10:00 P1

CeCo(As/P)O pnictides: complex interplay of 4f and 3d magnetism as seen from NMR (^{31}P, ^{59}Co and ^{75}As). — •Michael Baenitz[1], Rajib Sarkar[1], Eva Brüning[1], Asok Poddar[2], Chandan Majumdar[2], Anton Jesche[1], Cornelius Krellner[1], Cristoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]ECMP Division, Saha Institute of Nuclear Physics, Kolkata, India

The coupling of the magnetic sub-systems of Co-3d and Ce-4f ions in the compounds CeCoAsO and CeCoPO is studied by using the lo-

cal NMR probe. The magnetic order in such 3d-4f systems is rather complex depending on the inter-3d, inter-4f ion exchange coupling and the intra 3d-4f - ion coupling (polarization). Sometimes two separated transitions could be found (for example CeFeAsO). For CeCo(P/As)O only a single ferromagnetic transition is found at about 75 K [1, 2]. Here CeCoPO is of special interest because strong correlations (Kondo interaction) became evident at low temperatures [2]. Furthermore, recent low field magnetization results indicate a more complex type of magnetic order. One scenario is a crossover from a canted or antiferromagnetic type at low fields to a field polarized ferromagnetic type of order at higher fields.

[1] Phys. Rev. B 82, 054423 (2010)
[2] Physica B, 404 (2009) 3206.

TT 44.10 Thu 10:00 P1

Magnetic properties of CeTPO (T = Co,Ru,Os) phosphides studied by muon spin relaxation — •Johannes Spehling[1], Cornelius Krellner[2], Hubertus Luetkens[3], Til Dellmann[1], Anton Jesche[2], Christoph Geibel[2], and Hans-Henning Klauss[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232, Villingen, Switzerland — [3]Max-Planck-Institut für Chemische Physik fester Stoffe Dresden

We have investigated the magnetic ground state properties in the pnictide systems CeTPO with T = Co,Ru,Os by means of zero field (ZF) and weak transverse field muon spin relaxation (muSR). For CeCoPO, magnetic order of the Co-3d moments below 75 K is found as evidenced by the observation of a spontaneous muon spin precession frequency. A second muon frequency below 45 K suggests a spin reorientation transition. No clear indication for Ce-4f magnetic ordering is found. In contrast, for CeRuPO and CeOsPO ZF-muSR shows Ce-4f magnetic order below 15 K and 4.5 K, respectively. Here, no magnetic order of the d electronic moments is observed. This is consistent with macroscopic results [1-3]. For all systems, the temperature dependence of the magnetic order parameter (muon precession frequency) suggests a peculiar interplay between the transition metal d and rare earth Ce-4f electronic subsystems.

[1] Phys. Rev. B 76, 104418 (2007)
[2] Phys. Rev. Lett. 100, 066401 (2008)
[3] Physica B 404, 3206 (2009).

TT 44.11 Thu 10:00 P1

^{27}Al NMR/NQR study on RRu$_2$Al$_{10}$ (R: La, Ce) and RFe$_2$Al$_{10}$ (R: Y, Yb). — •Panchanana Khuntia[1], Michael Baenitz[1], Rajib Sarkar[1], André Strydom[2], and Frank Steglich[1] — [1]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Physics Department APK, University of Johannesburg, P.O. Box 524, Auckland Park 2006, South Africa

Ternary orthorhombic aluminides of RT$_2$Al$_{10}$ type (R:Ce, Yb, T: Fe, Ru, Os) are currently attracting much interest because of a number of exotic properties such as anomalously high magnetic ordering temperatures in CeRu$_2$Al$_{10}$ [1] and CeOs$_2$Al$_{10}$, and strongly hybridized Kondo insulating state in CeFe$_2$Al$_{10}$. The Fe-Al systems are of special interest because YFe$_2$Al$_{10}$ is claimed being located close to a Fe-based ferromagnetic instability at very low temperature [2]. Here pronounced non Fermi liquid (NFL) phenomena are observed. For YbRh$_2$Si$_2$ this NFL behaviour is associated to strong ferromagnetic fluctuations (see ^{29}Si NMR in [3]). Our spin relaxation study on YFe$_2$Al$_{10}$ gives strong evidence for Fe based ferromagnetic fluctuations evolving towards low temperature in small fields. YbFe$_2$Al$_{10}$ is a weak Kondo coupled heavy fermion system where no traces of Fe-magnetism could be found [2].

[1] Physica B, 404(2009)2981
[2] Phys. Stat. Solidi 4, No. 12, 356-358(2010)
[3] PRL 89, 107202(2010)

TT 44.12 Thu 10:00 P1

Exotic Heavy-Fermion Behaviour of the Filled Skutterudite SmPt$_4$Ge$_{12}$ — •Roman Gumeniuk[1], Walter Schnelle[1], Michael Nicklas[1], Helge Rosner[1], Michael Schöneich[2], and Andreas Leithe-Jasper[1] — [1]MPI Chemische Physik fester Stoffe, Dresden — [2]Anorganische Chemie, TU Dresden

Samarium-filled platinum-germanium skutterudite SmPt$_4$Ge$_{12}$ was prepared at high pressure and temperature (5.0 GPa, 1070 K). The compound is isotypic with LaFe$_4$P$_{12}$ (cubic, space group $Im\bar{3}$, a = 8.6069(4) Å). X-ray absorption spectroscopy measurements show that samarium in SmPt$_4$Ge$_{12}$ has a temperature-independent intermediate valence ($\nu = 2.90 \pm 0.03$). Van-Vleck paramagnetism is observed above ∼50 K. The low-temperature specific heat displays a broad anomaly around at 2.9 K and a large linear coefficient $\gamma' = 450$ mJ mol^{-1}K^{-2} suggesting heavy-fermion behaviour. Electrical resistivity shows a temperature dependence reminiscent of the Kondo effect. Density functional calculations result in an electronic structure that is, apart from the Sm 4f contributions, very similar to LaPt$_4$Ge$_{12}$.

TT 44.13 Thu 10:00 P1

Tuning the magnetism in YbRh$_2$Si$_2$ via isoelectronic transition metal (Co, Ir) substitutions: a ^{59}Co- and ^{29}Si-NMR study — •Michael Baenitz, Cornelius Krellner, Panchanana Khuntia, Christoph Geibel, and Frank Steglich — Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

YbRh$_2$Si$_2$ is unique among heavy fermion systems because of its proximity to a quantum critical point (QCP) in the Doniach-type phase diagram. Pronounced non-Fermi-liquid (NFL) behavior was observed. ESR as well as the ^{29}Si-NMR spin-lattice relaxation (SLR) gave strong evidence that the NFL behavior is closely related to the presence of strong ferromagnetic fluctuations competing with antiferromagnetic ones [1,2]. Here we present a ^{59}Co- and ^{29}Si-NMR study on the $x = 0, 0.07, 0.12$ and 1 samples of the Yb(Rh$_{1-x}$Co$_x$)$_2$Si$_2$ alloy together with ^{29}Si-NMR results on the pure YbIr$_2$Si$_2$.The isoelectronic substitution of the smaller Co ion on the Rh site promotes the AF order whereas the substitution of the larger Ir ion strengthen the Kondo interaction. As a consequence the SLRs $^{29}(1/T_1)$ as well as the spin-spin relaxation rates $^{29}(1/T_2)$ are damped for the YbIr$_2$Si$_2$ system, which allows to study the ^{29}Si-NMR in great detail up to room temperature.

[1] Phys. Rev. Lett. 91, 156401 (2003)
[2] Phys. Rev. Lett. 89, 1072021 (2002)

TT 44.14 Thu 10:00 P1

Magnetism and valence fluctuations in Eu(Rh$_{1-x}$Ir$_x$)$_2$Si$_2$ single crystals — •Silvia Seiro and Christoph Geibel — MPI-CPfS, Nöthnitzer Strasse 40, 01187 Dresden, Germany

Valence instabilities and intermediate valence in rare earth intermetallics RT$_2$Si$_2$, R being a rare earth element with instable 4f-shell like Ce, Eu and Yb, and T a transition metal, have been focus of research for the last three decades. In particular, much attention has been drawn by the suppression of the magnetic order of the localized f moments and the associated transition from a small to a large Fermi surface, which can be induced in Ce and Yb compounds by varying some external parameter such as pressure, composition or magnetic field. Due to the unavailability of high quality single crystals, however, the properties of homologue Eu compounds remain comparatively unexplored. We report the synthesis of Eu(Rh$_{1-x}$Ir$_x$)$_2$Si$_2$ single crystals and their physical properties as they evolve from divalent Eu antiferromagnetism for $x = 0$ to intermediate valence behavior for $x = 1$.

TT 44.15 Thu 10:00 P1

Magnetic excitations in YbCo$_2$Si$_2$ — •O. Stockert[1], A. Haase[1], K. Schmalzl[2], C. Krellner[1], N. Mufti[1], and C. Geibel[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France

Quantum phase transitions and their origin are still open issues of current research in condensed matter physics. Although YbRh$_2$Si$_2$ is a model system to study quantum criticality, microscopic studies by neutron scattering are prevented because of the large absorption of Rh for neutrons, the small ordered moment and the small available samples. Instead, we investigated YbCo$_2$Si$_2$ being isoelectronic and isostructural to YbRh$_2$Si$_2$. YbCo$_2$Si$_2$ orders antiferromagnetically below $T_N \approx 1.7$ K in an incommensurate structure and changes to a commensurate structure below $T_L \approx 0.9$ K. Using inelastic neutron scattering we studied in detail the spin excitations in the low temperature commensurate phase. Well-defined spin excitations exhibiting distinct dispersion have been detected. The results contribute to the general understanding of the magnetic interactions in YbCo$_2$Si$_2$.

TT 44.16 Thu 10:00 P1

Phase diagram of CePt$_3$B$_{1-x}$Si$_x$ — •Daniela Rauch[1], Matthias Bleckmann[1], Stefan Süllow[1], Moo Sung Kim[2], Meigan Aronson[2,3], and Ernst Bauer[4] — [1]TU Braunschweig, Institute for Physics of Condensed Matter, Braunschweig, Germany — [2]Brookhaven National Laboratory, Condensed Matter Physics and Materials Science Department, New York, USA — [3]Stony Brook University, Department of Physics and Astronomy, New York, USA —

[4]TU Vienna, Institute of Solid State Physics, Vienna, Austria

The non-centro symmetric system $CePt_3Si$ shows an unconventional heavy-fermion superconducting ground state ($T_c = 0.75$ K), in coexistence with an antiferromagnetic phase below $T_N = 2.2$ K. In contrast, $CePt_3B$ exhibits a complex magnetically ordered state at low temperatures, with an antiferromagnetic phase below $T_N = 8$ K and a second weakly ferromagnetic transition below $T_C \approx 5$ K.

Here we report a study of the magnetic phase diagram of the alloying series $CePt_3B_{1-x}Si_x$. From our investigation we find the antiferromagnetism of $CePt_3B$ to transform into the analagous phase of $CePt_3Si$. In contrast, we observe a supression of the ferromagnetically ordered phase above a critical Si concentration $x_c \approx 0.5$. We discuss the relationship of superconductivity and magnetism of the alloying series.

TT 44.17 Thu 10:00 P1

Exotic field induced phases in UPt_2Si_2 — •D. Schulze Grachtrup[1], M. Bleckmann[1], B. Willenberg[1], H. Rakoto[2], I. Sheikin[3], Y. Skourski[4], M. Bartkowiak[4], J.A. Mydosh[5], and S. Süllow[1] — [1]IPKM, TU Braunschweig, Germany — [2]LNCMI, Toulouse, France — [3]LNCMI, Grenoble, France — [4]HLD, Dresden, Germany — [5]LION, Leiden University, Netherlands

Tetragonal UPt_2Si_2 has been characterized as a moderately mass enhanced antiferromagnetic compound ($T_N = 32$ K), which in low magnetic fields resembles other materials such as URu_2Si_2 [1-3]. Here,we present an extensive study of resistivity and magnetization of single crystalline UPt_2Si_2 in high magnetic fields up to 50 T. Initially we find the phase transition at $T_N = 32$ K in zero field to shift down to lower temperatures with increasing field for both crystallographic axes. Below $\sim$ 15 K and for $B//a$ we see this transition to split up and become hysteretic, forming a new and distinct high field phase between $\sim$38T and $\sim$45T. Similarly, with $B//c$ we also find a splitting resulting in a new high field phase between $\sim$24 T and $\sim$31 T. Moreover, below 5K our measurements along the c axis show even more structure, indicating at least one more high field phase between $\sim$29 T and $\sim$33 T. Altogether, our data reveal a rich magnetic high field phase diagram, which resembles some observations made for URu_2Si_2 [4].

[1] S. Süllow *et al.*, J. Phys. Soc. Jpn. **77** (2008) 024708
[2] N. Johannsen *et al.*, Phys. Rev. B **78** (2008) 121103(R)
[3] R. A. Steeman *et al.*, J. Phys.: Condens. Matter **2** (1990) 4059
[4] K. H. Kim *et al.*, Phys. Rev. Lett. **91** (2003) 256401

TT 44.18 Thu 10:00 P1

Dynamics of the Periodic Anderson Model: exhaustion effects and the interplay of scales — •Lucas Hollender, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zülpicherstr. 77 50937 Cologne, Germany

We are investigating the paramagnetic periodic Anderson model within the framework of dynamical mean field theory, using Wilson's numerical renormalization group approach to obtain the self energy of the effective impurity model. We examine the exhaustion scenario where the conduction band is progressively emptied. Here our main interest lies in the existence of the Kondo scale and its connection to the coherence scale. We also consider a bipartite system (with two sublattices comprising inequivalent impurity sites), and study the interplay of Kondo and lattice coherence scales. Furthermore we increase the distance of the impurities to simulate dilute impurity systems, trying to find the crossover from the lattice system to the dilute impurity system.

TT 44.19 Thu 10:00 P1

Quantum Phase Transition between Semimetal and Superfluid in a Dirac Cone Model — •Benjamin Obert[1], Philipp Strack[1], So Takei[2] und Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart Germany — [2]University of Maryland, USA

We analyse a two-dimensional Dirac cone model which undergoes a quantum phase transition between a semimetal and a superfluid. We compute fluctuation effects by using flow equations derived within the functional renormalization group (fRG) framework [1]. Near the quantum critical point (QCP) fluctuations lead to non Fermi liquid behaviour. The superfluid correlation length is infinite not only at the quantum critical point, but everywhere in the semimetallic phase.

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

TT 44.20 Thu 10:00 P1

Quantum critical dynamics in the one-dimensional spin chain systems CuPzN and $(phzH)_2CuCl_4$ — •H. Kühne[1,3], M. Günther[1], H.-H. Klauss[1], A.A. Zvyagin[2], J. Litterst[3], S. Grossjohann[4], W. Brenig[4], A.P. Reyes[5], P.L. Kuhns[5], C.P. Landee[6], and M.M. Turnbull[6] — [1]IFP,TU Dresden — [2]ILTPE,Kharkov,Ukraine — [3]IPKM,TU Braunschweig — [4]IThP,TU Braunschweig — [5]NHMFL,Tallahassee,USA — [6]DoP,Worcester,USA

We present a comprehensive NMR study of the field-driven quantum phase transitions in the spin=1/2 chain systems CuPzN and $(phzH)_2CuCl_4$. The static and dynamic experimental NMR properties are compared with both quantum Monte Carlo calculations and Luttinger liquid theory. CuPzN is known to be one of the best realizations of the antiferromagnetic S=1/2 Heisenberg chain (AFHC) model with a low coupling constant J. The zero temperature saturation field B_c = 14.6 T corresponds to a quantum critical point, where the system is driven from a Luttinger liquid state to ferromagnetic polarization. In the vicinity of this point in the corresponding B- and T- parameter space, a divergent behavior of the nuclear ^{1}3C-spin-lattice relaxation rate is observed and in good agreement with theory. $(phzH)_2CuCl_4$ is a recently synthesized spin chain system. ^{1}H- and ^{3}5Cl-NMR experiments yield a field- and temperature dependent behavior of $1/T_1$ similar to that of CuPzN. But, in contrast, a pronounced second maximum is observed at about 3/4 of the saturation field B_c = 12.2 T. This effect is not found in the local or macroscopic magnetization, suggesting a more complicated magnetic interaction scheme.

TT 44.21 Thu 10:00 P1

Accurate Determination of the Gauss-Transition in the Anisotropic Spin-One Chain — •Shijie Hu[1,2], Bruce Normand[2], and Xiaoqun Wang[2] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Department of Physics, Renmin University of China

We have investigated ground-state properties and thermodynamic properties of the uniaxial anisotropic spin-one Heisenberg chain using the density matrix renormalization group method and the transfer matrix renormalization group method. We found that the gap depending on D around the Ising critical point $D_{c1} = -0.3145(1)$ is well described by a linear function. By contrast, the critical point $D_{c2} = 0.9684(2)$ cannot easily be obtained by any physical quantities except for the entanglement entropy. Simultaneously x-axis string order parameter which is used to define the Haldane phase with an incomplete $Z_2 \times Z_2$ symmetry and the scaling behavior of the spin susceptibility at low temperature are also exhibited.

TT 44.22 Thu 10:00 P1

Relation between crystal structure, magnetism and electronic properties in layered ruthenates — •Johanna Brand[1], Anna Silex[1], Karsten Binder[1], Yvan Sidis[2], Arsen Gukasov[2], Beatrice Gillon[2], Satoru Nakatsuji[3], Naoki Kikugawa[4], Andrew Mackenzie[4], Fumihiko Nakamura[5], and Markus Braden[1] — [1]II. Physik, Uni Köln — [2]LLB, Saclay — [3]ISSP, Tokio — [4]Univ. of St. Andrews — [5]ADSM, Hiroshima

Layered ruthenates exhibit a close coupling between crystal structure and magnetic and electronic properties, which strengthens the interest in these materials arising from the superconductivity in Sr_2RuO_4 and Ca_2RuO_4. By substituting Sr through isovalent Ca in Ca_2RuO_4 one tunes the system from the superconductor into a highly anomalous metal with heavy-fermion like properties and finally into an antiferromagnetic Mott insulator. The MIT in Ca_2RuO_4 can not only be induced by Sr-doping, heating and pressure but also by the application of an electric field. A part of the sample transforms into the metallic phase under the application of moderate electric fields, this phase is characterized by a longer c-lattice parameter and it can be cooled far below room temperature when a finite current density is maintained. At low temperature there is coexistence of the metallic phase and the insulating phase. Doping $Ca_3Ru_2O_7$ with Ti significantly stabilizes a weakly non-metallic phase as seen both in the transition temperature and in the resistivity jump. This effect is especially prominent at a substitution of 10

TT 44.23 Thu 10:00 P1

Low-frequency optics on $Sr_{1-x}Ca_xRuO_3$ — •Diana Geiger[1], Marc Scheffler[1], Martin Dressel[1], Melanie Schneider[2], and Philipp Gegenwart[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

The pseudo-cubic perovskite ruthenates $SrRuO_3$ and $CaRuO_3$ have attracted interest due to their unconventional electronic properties. For both materials, non-Fermi liquid behavior has been reported in previous optical studies. In addition to these compounds, the doping series $Sr_{1-x}Ca_xRuO_3$ offers a rich phase diagram: going from the itinerant ferromagnet $SrRuO_3$ to the paramagnet $CaRuO_3$, a quantum phase transition is expected at $x \approx 0.8$.

Using different approaches of optical spectroscopy, we studied thin-film samples of the $Sr_{1-x}Ca_xRuO_3$ system, which were prepared by metalorganic aerosol deposition. In order to be sensitive to the low energy scales expected close to the quantum phase transition, we address the THz and GHz frequency ranges at temperatures down to 2K. We present optical data, in particular the frequency-dependent conductivity, and discuss it in the framework of the extended Drude model and possible non-Fermi liquid behavior.

TT 44.24 Thu 10:00 P1

Ferromagnetic quantum phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider, Vasile Mosneaga, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August Universität Göttingen,Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The series $Sr_{1-x}Ca_xRuO_3$ shows a continuous evolution from itinerant electron ferromagnetism with $T_C \approx 160$ K (x = 0) towards a paramagnetic metallic state at x = 1. For thin films, which have been grown epitaxially on $SrTiO_3$ and $NdGaO_3$ substrates by metalorganic aerosol deposition technique, we present electrical transport measurements extended to mK temperatures and in applied magnetic fields. We also investigated nonlinear transport at high current densities in the non-Fermi liquid regime for microstructured thin films. Work supported by DFG through SFB 602, TP A19."

TT 44.25 Thu 10:00 P1

Quantum criticality in $Sr_3Ru_2O_7$ studied by measurements of the magnetocaloric effect — •Manuel Mchalwat[1], Yoshi Tokiwa[1], R.S. Perry[2,3], Y. Maeno[3], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Scottish Universities Physics Alliance, School of Physics, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, Scotland — [3]International Innovation Center and Department of Physics, Kyoto University, Kyoto 606-8501, Japan

The tetragonal ruthenate $Sr_3Ru_2O_7$ displays itinerant electron metamagnetism and the formation of a novel phase close to a presumed quantum critical point (QCP). Here, we address quantum criticality by measurements of the adiabatic magnetocaloric effect, determined using an alternating field method. Our results indicate universal scaling behavior over several decades in temperature over magnetic field in agreement with the predictions of the Hertz-Millis scenario for an itinerant two-dimensional metamagnetic ($z = 3$) QCP.

Work supported by the DFG through SFB 602 and research unit 960 (Quantum phase transitions).

TT 44.26 Thu 10:00 P1

Low-temperature electrical resistivity of $Yb(Rh_{0.95}Fe_{0.05})_2Si_2$ — •Maik Schubert, H.S. Jeevan, Yoshi Tokiwa, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

We report measurements of the electrical resistivity $\rho(T, B)$ on a single crystal of $Yb(Rh_{0.95}Fe_{0.05})_2Si_2$ at temperatures down to 15 mK and in magnetic fields up to 2 T. The Fe-doping has a threefold effect: (i) an increase of the residual resistivity similar as found for respective Co or Ir doping, (ii) a decrease of the Kondo temperature due to the chemical pressure effect, like it has been found for the respective Co doping, and (iii) a slight shift of the Fermi energy corresponding to the doping of 0.1 holes per unit cell. This latter effect suppresses the antiferromagnetic ordering despite the expected increase of T_N due to chemical pressure. Furthermore, we observe a moderate shift of the energy scale $T^*(B)$ with $B^*(T \to 0) = 0.03$ T. At lowest temperatures, the electrical resistivity follows Fermi liquid behavior $\Delta\rho = A(B)T^2$ both above and below 0.03 T with a divergence of the coefficient A upon approaching the critical field from both sides.

Work supported by the DFG through SFB 602 and research unit 960 (Quantum phase transitions).

TT 44.27 Thu 10:00 P1

Structural and magnetic transitions in YbPd — •Stefanie Grünheit[1], Hirale S. Jeevan[1], Devashibhai T. Adroja[2], Yoshifumi Tokiwa[1], Christian Stingl[1], Aziz Daoud-Aladine[2], and Philipp Gegenwart[1] — [1]1. Physikalisches Institut, Georg-August-Universität Göttingen — [2]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OXII, 0QX, United Kingdom

The cubic YbPd is a unique strongly-correlated electron system which shows structural and magnetic transitions upon cooling to low temperatures [1]. However, the nature of the magnetic and the atomic structure at low T has not been solved yet. We synthesized YbPd polycrystals and investigated their physical properties by electrical resistivity, magnetic susceptibility, specific heat and thermal expansion measurements. Furthermore, neutron scattering experiments were performed down to 20 mK in order to obtain microscopic information on the different phase transitions. At low temperatures, the Sommerfeld coefficient of YbPd is of the order of 200 mJ/(mol K^2) suggesting that YbPd is a moderately heavy fermion system. A reduced entropy of about one quarter of $R \log 2$ at 1.9 K is found. Remarkably this value is consistent with a structure with only half of the Yb-Ions contributing to the magnetic entropy.

Work supported by DFG through research unit 960 (Quantum phase transitions).

[1] P. Bonville et al., Phys. Rev. Lett. 57 (1986) 2733.

TT 44.28 Thu 10:00 P1

^{31}P NMR study on $Eu(Ni_{1-x}Fe_x)_2P_2$: from valence fluctuations to ferromagnetic order — •Michael Baenitz[1], Ramesh Nath[2], Rajib Sarkar[1], Hirale Jeevan[3], Philipp Gegenwart[3], Zarkir Hossain[4], Nubia Caroca-Canales[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI-CPfS , 01187 Dresden, Germany. — [2]IISER-TVM, Trivandrum-695016, India. — [3]1. Phys. Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany. — [4]Dept. of Physics, Indian Institute of Technology, Kanpur 208016 India.

Among unstable f shell sytems the magnetic phase diagram of Eu systems differs from that of Ce, Yb or U systems. In contrast to these systems the Eu valence mostly could not be tuned (by substitutions or external pressure) continuously between the magnetic ($Eu^{+2}, J = 7/2$) and the non magnetic ($Eu^{+3}, J = 0$) state. Instead of that, first order valence transitions (like in $EuNi_2(Si/Ge)_2$) or an unstable, fluctuating valence (VF) at high temperatures (like in $EuCu_2Si_2$) are rather common. For $EuCu_2Si_2$ we have shown that upon Ge substitution the VF are suppressed and a small Kondo regime exist in the phase diagram before entering the antiferromagnetic ordered state on the Ge rich side. For the valence fluctuator $EuNi_2P_2$ the question arises whether a Kondo regime exists upon Fe substitution. In contrast to the $EuCu_2(Si/Ge)_2$ series the end point of the study here, $EuFe_2P_2$, is ferromagnetically ordered. This brings up the question of competition and/or coexistence of ferromagnetic and Kondo type of interactions in this new series. ^{31}P NMR measurements are carried out on $Eu(Ni_{1-x}Fe_x)_2P_2$ samples with $x = 0, 0.15, 0.5$ and 1.

TT 44.29 Thu 10:00 P1

Grüneisen ratios at the magnetic-field-induced quantum phase transition in $NiCl_2$-4SC$(NH_2)_2$ — •Manuel Brando[1], Robert Kuechler[1], Luis Pedrero[1], Alexander Steppke[1], Armando Paduan-Filho[2], Christian Batista[3], Franziska Weickert[3], Vivien Zapf[3], Marcelo Jaime[3], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil — [3]Los Alamos National Laboratory, Los Alamos, USA

The tetragonal organic system $NiCl_2$-4SC$(NH_2)_2$ (known as DTN) is a quantum paramagnet where the Ni atoms form $S = 1$ dimers which are weakly coupled along the crystallographic c axis. The Ni^{2+} single ion anisotropy $D = 8.9$ K opens an energy gap between the $S_z = 0$ ground state and the $S_z = \pm 1$ first excited state. When a magnetic field H is applied along c, it closes the gap and induces a transition into an XY-antiferromagnetic ordered state at low temperatures. For $T = 0$ the critical field $Hc_1 \approx 2$ T. Such a quantum critical point belongs to the $d = 3$ and $z = 2$ universality class and the following theoretical laws are predicted: The magnetization $M \propto T^{d/z}$, the phase boundary line $(H - Hc_1) \propto T_c^{d/z}$, the thermal and magnetic Grüneisen ratios, Γ and Γ_H, are expected to follow T^{-1}. We present measurements of the magnetization, specific heat and thermal expansion in the temperature range $0.05 \leq T \leq 5$ K across Hc_1 and analyse the critical behavior of Γ and Γ_H at Hc_1.

TT 44.30 Thu 10:00 P1

Field and concentration dependent scaling behavior of the thermal expansion near the quantum critical point of $CeCu_{6-x}Au_x$ — •Sebastian Zaum[1,2], Kai Grube[1], Roland Schäfer[1], Veronika Fritsch[2], Thomas Wolf[1], Peter Schweiss[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe, Germany

The heavy-fermion system $CeCu_{6-x}Au_x$ exhibits long-range antiferromagnetic order at $x > 0.1$. The order can be suppressed by hydrostatic or chemical pressure, through the variation of the Au content, as well as by the application of a magnetic field. The quantum critical point at the onset of antiferromagnetism leads to non-Fermi liquid behavior visible in thermodynamic and transport properties. Among these, the thermal expansion offers a particularly sensitive probe to study the quantum critical scaling behavior due to the strong pressure dependence of the Kondo effect in heavy-fermion materials. To shed light on the difference between the two control parameters, pressure and magnetic field, we studied the scaling behavior of the thermal expansion on $CeCu_{6-x}Au_x$ single crystals with varying Au content as a function of the magnetic field in the temperature range between 40 mK and 10 K.

TT 44.31 Thu 10:00 P1

Thermal expansion and magnetostriction of $Yb_2Fe_{12}P_7$ single crystals — •Kai Grube[1], Sebastian Zaum[1,2], Roland Schäfer[1], Peter Schweiss[1], R. E. Baumbach[3], M. B. Maple[3], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe, Germany — [3]Department of Physics, University of California, San Diego, La Jolla, California 92093, USA

The noncentrosymmetric heavy-fermion compound $Yb_2Fe_{12}P_7$ exhibits a magnetic transition at ≈ 1 K. Recent resistivity measurements [1] reveal non-Fermi-liquid behavior in an extended temperature and field range. From the unusual low-temperature behavior it was concluded that $Yb_2Fe_{12}P_7$ belongs to the growing class of compounds in which the non-Fermi-liquid behavior does not conform to the standard QCP scenario which can be described by the Hertz-Millis-Moriya theory. We report on thermal expansion and magnetostriction measurements in a temperature range of $40\,\mathrm{mK} < T < 10\,\mathrm{K}$ and magnetic fields of up to 14 T parallel and perpendicular to the hexagonal c axis. From the data we construct (T, B) phase diagrams for both field directions. The Grüneisen ratio calculated from our measurements is comparatively small and does not diverge for $T \to 0$. It gives, therefore, no evidence for a nearby pressure-induced quantum critical point.
[1] R. E. Baumbach et al., Phys. Rev. Lett. 105, 106403 (2010).

TT 44.32 Thu 10:00 P1

flow equations approach to one dimensional quantum Ising model — •Amin Kiani[1], Farhad Shahbazi[2], and Seyed Akbar Jafari[3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of physics, Isfahan University of Technology, Isfahan, Iran — [3]Department of physics, Sharif University of Technology, Tehran, Iran

One dimensional quantum Ising model with nearest neighbor interaction in transverse magnetic field is one of the simplest spin models which undergoes quantum phase transition. This model has been solved with different methods exactly. In this paper, we solve this model in uniform magnetic field $-Jg\sigma_n^x$ exactly with new method called Continuous Unitary Transformations (CUT) or Flow equations and obtain the expectation values of $\langle\sigma_n^x\rangle$, $\langle\sigma_n^z\rangle$ and $\langle\sigma_n^x\sigma_{n+j}^x\rangle$. Then we apply this method on one dimensional Quantum Ising model in staggered magnetic field $(-1)^n Jg\sigma_n^x$. We observed that both models have the same critical properties as we expected. Moreover we observe that the spontaneous symmetry breaking cannot be derived from CUT.

TT 44.33 Thu 10:00 P1

Broadband dielectric spectroscopy on multiferroic compounds — •Daniel Niermann, Max Schalenbach, Christoph Grams, Florian Waschkowski, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Deutschland

Studying the dynamic dielectric response of given materials provides extensive insight in charge-carrier properties and involved relaxation processes. It was recently shown on the example of the perovskite rare-earth manganites that the occurrence of the multiferroic phase transition is often coupled to characteristic changes of relaxation dynamics [1]. We studied the frequency dependent dielectric properties of the multiferroic compounds $LuFe_2O_4$ and $MnWO_4$. To cover a wide frequency range from mHz to several GHz different setups for low-frequency impedance analysis and microwave spectroscopy were used. For the microwave regime we show transmission-measurements using a new microstrip-sampleholder, which allows a high measuring sensitivity for high-impedance samples. The measurements are performed at cryogenic temperatures down to 1.8K and high magnetic fields up to 14T. This work was supported by the DFG through SFB 608.
[1] F. Schrettle et al., *Phys. Rev. Lett.*, **102** (2009) 207208

TT 44.34 Thu 10:00 P1

Phase diagram of $NaFe(WO_4)_2$ — •Yvonne Sanders[1], Stephanie Orbe[1], Oliver Heyer[1], Sven Jodlauk[2], Sebastian Albiez[2], Petra Becker[2], Ladislav Bohatý[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Institut für Kristallographie, University of Cologne, Germany

Multiferroic materials show simultaneous ferroelectric and magnetic order, which are strongly coupled to each other. A well-known model system is $MnWO_4$ with only one kind of magnetic ions and three magnetically ordered phases below ∼13 K. Here, the multiferroic behavior of one of these phases arises from an incommensurate spin spiral structure. Much less is known about the double tungstate $NaFe(WO_4)_2$, which has a structure closely related to $MnWO_4$. While in $MnWO_4$ sheets || (100) of MnO_6 zig-zag chains alternate with similar sheets of WO_6, in $NaFe(WO_4)_2$ an alternating sheet sequence FeO_6-WO_6-NaO_6-WO_6 - is found. Consequently, the a lattice parameter is doubled and the magnetic subsystem is diluted. The ordering temperature in $NaFe(WO_4)_2$ is reduced to $T_N \approx 4$K. The magnetic structure in zero magnetic field is reported to be collinear antiferromagnetic, but the H-T phase diagram has not been published so far. Here, we present a detailed study of this phase diagram obtained by high-resolution thermal expansion and magnetostriction measurements. We find pronounced hysteresis effects, which resemble those observed in other multiferroic materials.

Supported by the DFG through SFB 608.

TT 44.35 Thu 10:00 P1

Evidence for local lattice distortions in giant magnetocapacitive $CdCr_2S_4$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[2], Yurii Pashkevich[3], Alois Loidl[4], and Vladimir Tsurkan[4,5] — [1]ILTPE NAS, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]DonFTI NAS, Ukraine — [4]EP V, Univ. Augsburg, Germany — [5]IAP AS, Moldova

Pronounced anomalies in intensity, frequency, and width of optical phonon modes were observed in the $CdCr_2S_4$ spinel. To explain the colossal magnetocapacitive effects in $CdCr_2S_4$ we developed a scenario based on hybridization effects to be in accordance with the observed enhanced polarizabilities of certain Cr-S displacements and evidence for symmetry reduction.

Work supported by DFG.

TT 44.36 Thu 10:00 P1

Tunnel-spectroscopy of tunable granular metals prepared by focused electron beam induced deposition — •Dirk Klingenberger, Fabrizio Porrati, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, D-60438 Frankfurt am Main

For the fabrication of platinum containing granular metals we used a focused electron beam and the precursor trimethyl-methylcyclopentadienyl-platinum injected into a vacuum chamber nearby the focal area of the beam. The granular metals are composed of platinum nanocrystallites, embedded in a carbonaceous matrix. Post-growth electron irradiation manipulates the surrounding matrix and allows us - via the radiation dose - to fine tune the sample's conductivity from the insulating to the metallic regime. The deposits were written onto oxidized aluminum contacts to create planar tunnel junctions. Differential conductance measurements have been performed at different temperatures utilizing a He4 cryostat to investigate the sample's density of states. So the current theory of granular metals can be tested. Especially, the behavior of the Coulomb blockade was analyzed for the different conductivity regimes.

TT 44.37 Thu 10:00 P1

Exploring the doping dependence of the Mott transition on X-ray irradiated crystals of κ-$(ET)_2Cu[N(CN)_2]Cl$ —

•Sebastian Köhler[1], 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-$(ET)_2Cu[N(CN)_2]Cl$ exhibits a rich pressure vs. temperature phase diagram, including Mott-insulating and metallic phases separated by a first order transition line. By applying moderate pressures of ~ 30 MPa (300 bar), the ratio of the kinetic energy to the onsite Coulomb repulsion t/U can be changed sufficiently to cross this phase transition line. Our objective is to study the effect of carrier doping and the accompanying changes of the first-order transition line and its second-order critical endpoint. We used X-ray irradiation [1] to introduce charge carriers into the material, doping it away from half filling. We will present resistivity data for the temperature range $5K < T < 60K$ and for pressures up to 50 MPa for κ-$(ET)_2Cu[N(CN)_2]Cl$ crystals at various doping levels and discuss the accompanied changes in the p-T-phase diagram.

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

TT 44.38 Thu 10:00 P1

Correlated heterostructures with dynamical mean field theory — •Christoph Schütte and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The interfaces between different materials in a three-dimensional nanostructures give rise to interesting electronic phenomena such as metallic or even superconducting layers between insulators. We calculate the electrical resistivity and the Hall coefficient for different heterostructures as a function of temperature. The interactions in the structure may be described by the Hubbard model with an additional self-consistent treatment of long-range Coulomb interactions in a Hartree approximation. Inhomogeneous Dynamical Mean Field Theory (DMFT) is employed to calculate the electronic structure of such a multilayered device in 3 spatial dimensions. The subsequent single impurity Anderson model (SIAM) is solved with the numerical renormalisation group (NRG), a non-perturbative method which yields the accurate low-temperature properties.

TT 44.39 Thu 10:00 P1

Stripline-based resonant microwave spectroscopy to study interacting electron systems — •Christian Fella, Marc Scheffler, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

While conventional optical spectroscopy is well suited to study solids on energy scales dominated by band structure, it cannot access many correlated electron states. For such compounds relevant energies are often of the order of 0.1 meV or below, corresponding to frequencies of 30 GHz and below. To study the frequency-dependent conductivity of such materials, microwave experiments have to be carried out at several frequencies and at low temperatures. Here we present an experimental approach for cryogenic microwave spectroscopy on metals which is based on a 1D stripline resonator. Since the sample under study acts as ground plane, the only requirement for the geometry of the sample is a flat surface of sufficient size. To address both the frequency and temperature dependence of the sample, we measure several modes of the resonator at frequencies from 2 to 20 GHz and between room temperature and ^{4}He temperatures. We present different resonator designs (based on commercial high-frequency laminates as well as on vapor-deposition of metals onto sapphire substrates), discuss their sensitivity and range of applicability for different samples, and compare them to other experimental techniques for microwave studies on metals at low temperatures.

TT 44.40 Thu 10:00 P1

Infrared properties of magnetite under pressure — •Jihaan Ebad-Allah[1], Leonetta Baldassarre[1], Michael Sing[2], Ralph Claessen[2], Vic Brabers[3], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [3]Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, the Netherlands

Magnetite (Fe_3O_4) crystallizes in the inverse cubic spinel structure and undergoes a Verwey transition at $T_v \approx 120$ K at ambient pressure. By applying pressure, T_v decreases with increasing pressure according to the phase diagram proposed in [1]. In addition, it was recently suggested that at room temperature (RT) magnetite undergoes a pressure-induced phase transition from the inverse spinel to the normal spinel structure above 6 GPa, without a change in the lattice symmetry. This proposal is, however, controversially discussed [2].

We studied the electronic and vibrational properties of magnetite by infrared reflectance measurements. First, in order to verify the conduction mechanism via polaron hopping and to search for possible signatures of the phase transition at around 6 GPa, we measured the RT reflectance as a function of pressure. Secondly, we carried out the low-temperature reflectance measurements under pressure in the far-infrared range to check the effect of high pressure on T_v and the splitting of the phonon modes.

[1] G. Kh. Rozenberg et al., Phys. Rev. Lett. **96**, 045705 (2006).
[2] S. V Ovsyannikov et al., J. Phys.: Condens. Matter **20**, 172201 (2008).

TT 44.41 Thu 10:00 P1

On the development of orbital order domains across the Verwey transition in magnetite — •M. Döhler[1], C. F. Chang[1], M. Buchholz[1], C. Trabant[1,2], T. Kachel[2], N. Pontius[2], M. Beye[2,3], F. Sorgenfrei[4], W. Schlotter[3], S. de Jong[3], R. Kukreja[3], B. Bräuer[3], S. Hossain[3], C. Back[3], A. Scherz[3], D. Zhu[3], J. Turner[3], W.-S. Lee[3], Y.-D. Chuang[3], O. Krupin[3], P. Vogt[1], W. Wurth[4], A. Föhlisch[2], J. B. Goedkoop[5], H. A. Dürr[3], and C. Schüssler-Langeheine[2,1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Helmholtz-Zentrum Berlin — [3]SLAC RSXS collaboration, USA — [4]Universität Hamburg and CFEL — [5]Van der Waals-Zeeman Institute, Universiteit van Amsterdam

The Verwey transition in magnetite (Fe_3O_4) involves a symmetry reduction from cubic to monoclinic and the formation of orbital order at low temperatures. In the low-temperature phase orbital-order domains form. We used resonant soft x-ray diffraction to study how this orbital-order domain pattern changes in the vicinity of the Verwey transition. We found that very close to the transition the domains become mobile, which we assign to fluctuations between the high- and the low-temperature phase. In order to understand how the domain pattern changes when the transition is driven by a fs-infrared-laser pulse, we carried out a time-resolved resonant soft x-ray diffraction experiment at the LCLS. We find that the IR-pulse affects mainly the peak intensity and much less the correlation length of orbital order. Supported by the DFG through SFB 608 and by the BMBF project 05K10PK2.

TT 44.42 Thu 10:00 P1

Orbital occupation and magnetic moments of tetrahedrally coordinated iron in $CaBaFe_4O_7$ — •Nils Hollmann[1], Zhiwei Hu[1,2], Hua Wu[1], Martin Valldor[1], Navid Qureshi[1], Thomas Willers[1], Yi-Ying Chin[1], Julio Criginski Cezar[3], Arata Tanaka[4], Nicholas Brookes[3], and Liu Hao Tjeng[1,2] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany — [3]European Synchrotron Radiation Facility, Boîte Postale 220, 38043 Grenoble Cédex, France — [4]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

$CaBaFe_4O_7$ is a mixed-valent transition metal oxide having both Fe^{2+} and Fe^{3+} ions in tetrahedral coordination. Here we characterize its magnetic properties by magnetization measurements and investigate its local electronic structure using soft x-ray absorption spectroscopy at the Fe $L_{2,3}$ edges, in combination with multiplet cluster calculations. We discuss the x-ray linear dichroism, finding that the Fe^{2+} ion in the unusual tetrahedral coordination is Jahn-Teller active with the high-spin $e^2_\uparrow t^3_{2\uparrow} e^1_\downarrow$ configuration having a $x^2 - y^2$-like electron for the minority spin. With x-ray magnetic circular dichroism it is deduced that there is an appreciable orbital moment of about $L_z = 0.36$ caused by multiplet interactions, thereby explaining the observed magnetic anisotropy. $CaBaFe_4O_7$ might offer new opportunities to explore charge, orbital and spin physics in tetrahedrally coordinated transition metal ions. *This work is supported by the SFB through SFB 608.*

TT 44.43 Thu 10:00 P1

Charge, orbital and spin ordering in 214- manganites, nickelates and cuprates investigated by neutron and x-ray scattering — •A. Bielefeld[1], H. Ulbrich[1], D. Senff[1], A. C. Komarek[1], P. Steffens[2], Y. Sidis[3], and M. Braden[1] — [1]II. Phys. Institut, Universität zu Köln — [2]ILL, Grenoble (France) — [3]LLB, Saclay (France)

The coupling of charges and magnetic moments in numerous transition-metal compounds leads to a complex ordering with checkerboard or stripe like patterns. For nickelates and cuprates stripe states has been intensively studied particularly due to the possible implications for high T_c superconductivity. We have studied the mixed order of electronic, orbital and magnetic degrees of freedom in the planar compounds $La_{2-x}Sr_xReO_4$ (Re = Mn, Ni, Cu). For the manganites we have examined half (x=0.5), electron-doped (x<0.5) and overdoped (x>0.5) systems. For x=0.5, the equal amount of Mn^{3+} and Mn^{4+} ions leads to a checkerboard ordering of charges. The spins of the Mn^{3+} and Mn^{4+} order in an antiferromagnetic CE-type structure following the orbital order [1-3]. For the overdoped-system we find an incommensurate stripe-like coupling of four order parameters: charges, orbitals and magnetic ordering of Mn^{3+} and Mn^{4+} [4]. The formation of stripes in overdoped manganites is similar to stripe phases in nickelates. In 214-cuprates, incommensurate magnetic ordering leads to the forming of diagonal stripes.

[1] J.B. Goodenough, Phys. Rev. 100, 564 (1955).
[2] D. Senff et al., Phys. Rev. Lett. 96, 257201 (2006).
[3] D. Senff et al., Phys. Rev. B 77, 184413 (2008).
[4] H. Ulbrich et al., arXiv: 1008.4496

TT 44.44 Thu 10:00 P1

Temperature-dependent near-edge x-ray absorption fine structure of $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ — •Stephan Uebe[1,2], Andrea Assmann[1,2], Michael Merz[1], Markus Wissinger[1,2], Hilbert von Löhneysen[1,3], Sebastian Hühn[4], Vasily Moshnyaga[4], Peter Nagel[1], and Stefan Schuppler[1] — [1]KIT, Institut für Festkörperphysik, Karlsruhe — [2]KIT, Fakultät für Physik, Karlsruhe — [3]KIT, Physikalisches Institut, Karlsruhe — [4]Universität Göttingen, Physikalisches Institut, Göttingen

All members of the $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ (LPCMO) doping series are strongly correlated electron systems where the electron-electron interaction gives rise to the macroscopic feature of colossal magnetoresistance (CMR). Changing the La/Pr ratio allows for tuning the electron-phonon coupling and thereby T_C.

Thin films of LPCMO were grown on MgO by the Metalorganic Aerosol Deposition technique. The temperature-dependent near-edge x-ray absorption fine structure of the samples was recorded with special emphasis on a double-peak structure that emerges when cooling below T_C.

This feature is known to be specific for CMR manganites and different scenarios have been suggested in literature to explain this change in the electronic structure, being obviously concomitant with the MI phase transition.

Based upon our experimental findings, we will discuss the various scenarios and their respective implications.

TT 44.45 Thu 10:00 P1

On the coupling of spin and charge order in the stripe phase of layered nickelates — •Pascal Vogt[1], Christoph Trabant[1,2], Marcel Buchholz[1], Chun-Fu Chang[1], Niko Pontius[2], Marita Döhler[1], Enrico Schierle[2], Justina Schlappa[1,2], Agung Nugroho[3], Mohamed Benomar[1], Alexander Komarek[1], Ralf Feyerherm[2], Liu Hao Tjeng[1,4], Markus Braden[1], and Christian Schüssler-Langeheine[1,2] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Instiut Teknologi Bandung, Indonesia — [4]MPI for Chemical Physics of Solids, Dresden, Germany

Stripe order is a complex pattern of spins and charge in the CuO_2-planes of doped layered cuprates and NiO_2 planes of the isostructural nickelates. Neutron diffraction finds that spin order decays at about 40 K lower temperatures than charge order, while stripe-like magnetic correlations can be found up to higher temperatures. In resonant soft x-ray diffraction this difference between the two orders is less pronounced, but an intriguing loss of spatial coherence at low temperatures is found for both orders, which is not seen by neutron diffraction. In order to understand the interplay between spin and charge order better, we carried out a comparative study of the temperature dependence of both signals as well of their non-equilibrium behaviour upon pumping with a ps-IR-laser pulse. Preliminary results show that both degrees of freedom behave in a similar way. Supported by the DFG through SFB 608, by the BMBF through projects 05 S3XBA/5 and 05 KS7PK1, and by the HZB.

TT 44.46 Thu 10:00 P1

Investigation of the Electronic Structure and the Role of Cationic Disorder in $LaAlO_3$ - $SrTiO_3$ Heterointerfaces by Soft X-ray Spectroscopy — •Andreas Koitzsch[1], Johannes Ocker[1], Martin Knupfer[1], Martina Dekker[1], Kathrin Dörr[1], Bernd Büchner[1], and Patrick Hoffmann[2] — [1]IFW Dresden, P. O. Box 270116, 01171 Dresden, Germany — [2]Hemlholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The structure of $LaAlO_3$ / $SrTiO_3$ interfaces is under intense discussion due to the appearance of metallic conductivity, magnetism and superconductivity. The most important phenomena supposed to be crucial for the observed effects are the polar catastrophe, the formation of oxygen vacancies and the intermixing of La and Sr at the interface. However, at present there is no consensus about the driving force of the unusual properties. Here we apply on and off resonant photoemission to differently prepared $LaAlO_3$ / $SrTiO_3$ interfaces. In particular we study the behavior of the valence band, the Ti 2p, Sr 3d and La 4d lines. Significant differences are found as a function of sample treatment and photon energy. A model of the interface structure is developed.

TT 44.47 Thu 10:00 P1

Design and realization of a torque magnetometer for magnetization studies on $LaAlO_3$-$SrTiO_3$ interfaces — •Matthias Brasse, Marc A. Wilde, and Dirk Grundler — Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str.1, D-85747 Garching b. München, Germany

Two-dimensional electron systems (2-DESs) have been found to form at the interface between the otherwise insulating oxides $LaAlO_3$ and $SrTiO_3$. The strongly correlated electron system show metallic and superconducting phases. The magnetic properties of the 2-DESs interface are under debate. We intend to use highly sensitive micromechanical torque magnetometry to measure the magnetization of correlated electron states in the 2-DESs formed at the interface between $SrTiO_3$ and $LaAlO_3$. This will allow us to address different phenomena such as the de Haas-van Alphen effect, dia- and paramagnetism in superconducting states, spontaneous magnetization in case of correlated magnetism as well as magnetic hysteresis and anisotropy. Methods and results of ongoing measurements will be presented. We thank S. Thiel and the group of J. Mannhart from the University of Augsburg for sample preparation. This work is supported by the DFG via TRR 80.

TT 44.48 Thu 10:00 P1

Thermal conductivity of $BaCo_2V_2O_8$ — •Gerhard Kolland, Sandra Niesen, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

$BaCo_2V_2O_8$ is a quasi one-dimensional antiferromagnetic Ising-like spin-chain. The chain can be described by an effective S=1/2 1D XXZ model with coupling constant $J \simeq 65\,\mathrm{K}$ and anisotropy parameter $\epsilon = 0.46$. Parallel to the c axis the magnetization saturates at $H_{s||} \simeq 23\,\mathrm{T}$ and perpendicular to the c axis at $H_{s\perp} \simeq 41\,\mathrm{T}$. At zero field, the system orders at $T_N = 5.4\,\mathrm{K}$. The Néel order is suppressed by a magnet field with very different rates depending on the direction of the applied field. We measured the thermal conductivity parallel ($\kappa_{||}$) and perpendicular ($\kappa_\perp$) to the chains in the temperature range from room temperature down to 250 mK. For both directions, we observe a sharp anomaly at T_N and two maxima, one in the ordered phase and one above. In the ordered phase, the thermal conductivity is isotropic ($\kappa_{||} = \kappa_\perp$), while above T_N, $\kappa_{||}$ is significantly higher than $\kappa_\perp$. As this may suggest an additional magnetic contribution to $\kappa_{||}$ in the disordered phase, we compare our data to numerical calculations of the anisotropic κ using the 1D XXZ model Hamiltonian. Moreover, we analyze the field dependence of κ for different directions of the applied magnetic field. *Supported by the DFG through SFB 608.*

TT 44.49 Thu 10:00 P1

Synthesis and characterization of low dimensional magnetic spin systems — •Johanna Frielingsdorf, Ralf Müller, Simon Scharffe, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

The physics of low-dimensinal spin systems is fundamentally controlled by quantum fluctuations and therefore a hot topic. Thus, the preparation of materials with suitable magnetic subsystems, that experimentally realize various theoretical model hamiltonians, is highly desireable. The synthesis and characterization of spin-chain systems such as $BaCo_2V_2O_8$, $BaMn_2V_2O_8$, $SrMn_2V_2O_8$, $CoNb_2O_6$, and Cs_2CoCl_4 is subject of this poster. These compounds provide transition-metal

oxides with partly filled 3d shells and hence are suitable to study spin systems from S=1/2 to 5/2. $BaCo_2V_2O_8$, as a quasi one-dimensional S=1/2 Ising system, belongs to the alkaline earth (A)- transition metal(M)- vanadates $AM_2V_2O_8$. $BaMn_2V_2O_8$ on the other hand is an S=5/2 nearly isotropic Heisenberg system. $CoNb_2O_6$, known as columbite, is a quasi one-dimensional Ising ferromagnet and shows a complex interplay of quantum criticality and geometrical frustration. A quasi one-dimensional frustrated XY antiferromagnet is represented by Cs_2CoCl_4, where a spin-liquid ground state can be reached by applying magnetic fields.

This work is supported by the DFG through SFB 608.

TT 44.50 Thu 10:00 P1

Thermodynamic properties of the XY-spin-$\frac{1}{2}$ chain system Cs_2CoCl_4 — •Oliver Breunig, Daniel Löwen, Ralf Müller, Oliver Heyer, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

Cs_2CoCl_4 contains $CoCl_4$ tetrahedrons, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split up by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The lowest doublet is separated from the second by approximately 14 K, such that at low enough temperatures the system can be described by the one-dimensional spin-$\frac{1}{2}$ XY model. The intra-chain exchange constant being much stronger than the coupling between the chains suppresses the antiferromagnetic order to $T_N \simeq 220$ mK. Here, we present measurements of specific heat and magnetization in a temperature range from about 0.3 to 20 K. The one-dimensional magnetism is reflected by a pronounced maximum in c_p around 1 K. The zero-field data are well described by numerical calculations yielding an intra-chain exchange constant $J/k_B \simeq 2.5$ K. In magnetic fields the specific heat changes drastically, as the system undergoes a quantum phase transition to a fully polarized state at fields of about 2 T. We compare our experimental data for different field directions to numerical calculations.

This work was supported by the DFG through SFB 608.

TT 44.51 Thu 10:00 P1

Strong Electron Correlations in a Two-Dimensional Electron System on a Surface — •Philipp Höpfner[1], Jörg Schäfer[1], Thomas Schramm[1], Max Herpich[1], Gang Li[2], Werner Hanke[2], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Institut für Theoretische Physik und Astronomie, Universität Würzburg

A truly two-dimensional system with strong electron-electron correlation effects can be generated in dilute atomic adlayers on surfaces. An intriguing experimental realization is the Sn/Si(111)-($\sqrt{3} \times \sqrt{3}$) system. Interestingly, this triangular lattice naturally implies spin frustration. Contrary to the naive expectation of a metallic system, there have been recent indications that it is a Mott insulator at low temperature, based on scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) [1]. However, spectral weight and temperature-dependent changes are largely not understood yet.

Here, we present new data on this system from both STS and ARPES. We find that Sn/Si(111) shows an apparent low-temperature band gap of order 1 eV. It is retained even at room temperature, yet accompanied by changes in the spectral weight. ARPES reveals a surface state of rather narrow band width, which may be attributed to the lower Hubbard band. In comparison to recent advances in theoretical treatments of the triangular lattice, e.g., by dynamical mean field theory, the general trend of the findings can be reproduced, and implications for potential antiferromagnetic order at the surface are discussed.

[1] S. Modesti *et al.*, Phys. Rev. Lett. **98**, 126401 (2007).

TT 44.52 Thu 10:00 P1

Thermal expansion under pressure - test measurements on Azurite $[Cu_3(CO_3)_2(OH)_2]$ — •Rudra Sekhar Manna and Michael Lang — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany

Thermal expansion measurements provide a sensitive tool for exploring a material's thermodynamic properties. Particularly strong effects in the expansivity are expected in cases where the Grüneisen parameter is large or even diverges. The latter situation is encountered upon approaching a quantum phase transition [1] or a finite-temperature critical end point [2], by, *e.g.*, the application of hydrostatic pressure. Here we report on the realization of a dilatometer designed for measurements under Helium-gas pressure p $\leq$ 2.5 kbar. For test measurements, a single crystal of Azurite $[Cu_3(CO_3)_2(OH)_2]$ - a realization of a one-dimensional distorted Heisenberg chain - has been used, where significant pressure effects are expected.

[1] L. Zhu *et al.*, Phys. Rev. Lett. **91**, 066404 (2003).
[2] L. Bartosch *et al.*, Phys. Rev. Lett. **104**, 245701 (2010).

TT 44.53 Thu 10:00 P1

Investigatons of modified interlayer coupling in the anisotropic antiferromangnet $[Cu(pyz)_2(HF_2)]SbF_6$ — •R. Beyer[1], J.L. Manson[2], J.A. Schlueter[3], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor (HLD), Forschungszentrum Dresden-Rossendorf (FZD), Dresden, Germany — [2]Department of Chemistry and Biochemistry, EasternWashington Univ., Cheney, USA — [3]Materials Science Division, Argonne National Laboratory, Argonne, USA

In recent years, many synthetic strategies have emerged with regard to the crystal engineering of functional magnetic materials. The group of J.L. Manson *et al.* were able to grow single crystals of a quasi-2D antiferromagnet $[Cu(pyz)_2(HF_2)]SbF_6$ and a defective polymorphic pendant $[Cu_2(pyz)_4F(HF)(HF_2)](SbF_6)_2$ where 50% of the HF_2^- links are broken, leading to two crystallographically unique Cu^{2+} sites. The chemical composition remains unchanged, the structural configuration indicates a minor Jahn-Teller distortion. We studied the two branches of this compound by means of magnetization and specific heat measurements, in order to get a better understanding of the importance of H-F hydrogen bonds for establishing long-range magnetic ordering in polymeric quantum magnets. Part of this work has been supported by EuroMagNET II.

TT 44.54 Thu 10:00 P1

Doping dependence of collective spin states in $LaCoO_3$ — •A. Alfonsov[1], E. Vavilova[1,2], V. Kataev[1], A. Podlesnyak[3], E. Pomjakushina[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]ETH Zurich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

We have shown recently that a small Sr doping of $LaCoO_3$ yields the spin-state polaron with a big spin value and substantial spin orbital coupling [1]. The Sr for La substitution provides the hole doping due to different valency of Sr and La. In addition, it gives rise to a distortion of the crystal field around the doped ion due to the mismatch of ionic radii. The present work is aimed to discriminate between the effect of the charge (hole- or electron) doping and the effect of structural distortion. For that we have carried out a comparative high field electron spin- (ESR), nuclear magnetic resonance (NMR) and static magnetization study of lightly doped samples of $La_{0.998}A_{0.002}CoO_3$ (A = Sr, Ca, Y, Sn, Ce). We will discuss the role of the heterovalent hole- (Sr^{2+}, Ca^{2+}) and electron doping (Sn^{4+}, Ce^{4+}) as well as the homovalent doping with Y^{3+} ($r^{ion}_{Y^{3+}} \ll r^{ion}_{La^{3+}}$) for the formation of the spin-state polaron in $LaCoO_3$.

[1] A. Podlesnyak et al., Phys. Rev. Lett. **101**, 247603 (2008)

TT 44.55 Thu 10:00 P1

On the influence of inter-chain couplings on the magnetic properties of the strongly frustrated chain cuprate Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R.O. Kuzian[2], S. Nishimoto[1], S. Petit[3], Y. Skourski[4], N. Wizent[1], R. Klingeler[5], and B. Büchner[1] — [1]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Inst. f. Problems of Materials Science, Kiev, Ukraine — [3]Laboratoire Léon Brillouin, Saclay, France — [4]Hochfeld-Magnetlabor Dresden(HLD), FZ-Dresden-Rossendorf, Dresden, Germany — [5]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany

We report on detailed experimental and theoretical studies on the magnetic properties of Li_2CuO_2. This compound serves as a simple, but representative model system for an interesting class of spin-chain materials. Their magnetic properties are determined by strong nearest-neighbor ferromagnetic interactions in the chain which are frustrated by an antiferromagnetic (afm) coupling to next-nearest-neighbors. The competition of interactions can induce incommensurate correlations in the chain. On the example of Li_2CuO_2 we illustrate on the basis of our thermodynamical and inelastic neutron scattering data, how relatively weak inter-chain couplings can prevent incommensurate long-range order and determine solely the saturation field [1,2]. In particular, we discuss the influence of the inter-chain couplings onto the magnetic phase transitions.

[1] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).
[2] S. Nishimoto *et al.*, arXiv:1004.3300v2 (2010).

TT 44.56 Thu 10:00 P1

Magnetic and Thermal properties of a Honeycomb lattice system Li_2IrO_3 — •Soham Manni, Yogesh Singh, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Recently Ir based oxides have come into prominence because the interplay between spin-orbit and electronic correlations can lead to a novel Mott insulating state. Sr_2IrO_4 and Na_2IrO_3 are two such examples.

Na_2IrO_3 is an insulator which shows frustrated magnetic interactions which lead to an antiferromagnetic ordering below T_N = 15K even though the magnetic interactions are relatively strong as seen by the Weiss temperature of θ = - 120 K.

Applying pressure is one way to tune an insulator to a metallic state. We have synthesized Li_2IrO_3 in an attempt to apply chemical pressure to Na_2IrO_3. We present results of our transport, magnetic, and thermal property measurement with emphasis on how the magnetic and transport properties change when compared to Na_2IrO_3.

TT 44.57 Thu 10:00 P1

Quasi-1D Transport Measurements on $(TMTTF)_2X$ under Hydrostatic Pressure — •Karl Schrem, Eva Rose, Gabi Untereiner, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

The charge transfer salts $(TMTTF)_2X$ and $(TMTSF)_2X$ are model compounds for low-dimensional strongly correlated electron systems where the interplay of electronic, spin and lattice degrees of freedom together with changes of dimensionality result in a rich temperature-pressure phase diagram. All $(TMTTF)_2X$ compounds are located on the quasi-one dimensional part of the phase diagram and develop a charge-ordered phase at different temperatures T_{CO}, except $(TMTTF)_2ClO_4$ and $(TMTTF)_2Br$. In the group with non-centrosymmetric anions (X=ClO_4, BF_4, ReO_4) one can observe anion ordering for $T < T_{AO}$, resulting in a doubling of the unit cell. The different phases can easily be tuned both by chemical and hydrostatic pressure. We investigated several non-centrosymmetic compounds by carrying out electrical transport measurements under hydrostatic pressure up to 12 kbar and down to 4.2 K along different crystal axis. Our measurements show the changes in band width and dimensionality by pressure and its consequences on correlation effects, such as charge order. The shift of T_{AO} and the modification of the related transport characteristics stress the importance of the coupling between electronic system and the lattice.

TT 44.58 Thu 10:00 P1

Doping effects on the non-linear transport in blue bronze — •Ali Al-Hadeethi[1], Duminik Grund[1], Song Yue[2], Martin Dressel[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

When low-dimensional metals are cooled, they often undergo a phase transition to an insulating state exhibiting a new type of order. A famous example is the blue bronze $K_{0.3}MoO_3$, which undergoes a Peierls transition at $T_P \approx 180$ K to a charge-density-wave (CDW) state. In this work, the temperature dependence of the dc resistivity and the non-linear transport properties in pure, Rb-doped, and W-doped blue bronze single crystals is presented. Our measurements show that substituting K by Rb and Mo by W shifts T_P to lower values and smears out the metal-insulator transition. At temperatures below T_P nonlinear conductivity due to charge transport by the CDW is observed, when the applied electric field exceeds the so-called first threshold field. The temperature dependence of the first threshold field is presented for all studied samples. Furthermore, the temperature dependence of the second threshold field, which is usually attributed to the onset of coherent CDW sliding, is discussed.

TT 44.59 Thu 10:00 P1

Quantitative measurement of low temperature magnetisation by a caloric technique — •Hanjo Ryll[1,2], Klaus Kiefer[1], Christian Rüegg[3], Simon Ward[3], Karl Krämer[4], and Tobias Müller[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Technische Universität Berlin, Germany — [3]London Centre for Nanotechnology and Department of Physics and Astronomy, Great Britain — [4]Universität Bern, Switzerland — [5]Universität Kassel, Germany

Measurements of absolute magnetisation at very low temperatures and in high magnetic fields are notoriously difficult. The magnetocaloric effect (MCE) offers an alternative approach, which is applicable down to the mK temperature range. A quantitative MCE measurement is performed by precisely determining the temperature difference between sample and thermal bath with a well known thermal resistivity between bath and calorimeter. This allows for the measurement of the heat (δQ) generated or absorbed by the sample for a changing field (δB). Using Maxwell's relations, the MCE yields the derivative of magnetisation with respect to temperature: $(\delta Q/\delta B)/T = -(\partial M/\partial T)|_B$. Integration directly provides the uniform magnetisation $M(B,T)$. The necessary integration constant is obtained by a magnetisation measurement at higher temperatures, for example by a vibrating sample magnetometer (VSM). The method was applied to the metal-organic spin ladder material $(C_5H_{12}N)_2CuCl_4$. Magnetisation and MCE data between 0.3 K and 3 K are shown as an example, together with quantitative modeling of these quantities for a perfect spin ladder.

TT 44.60 Thu 10:00 P1

Tensor network states for lattice systems — •Stefan Depenbrock and Ulrich Schollwöck — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, LMU München

Tensor network decompositions offer an efficient description of many-body states on a lattice that can capture the essential physics of these systems. Here, we apply the projected entangled pair state (PEPS) algorithm to finite spin and fermion systems on a square lattice.

TT 44.61 Thu 10:00 P1

Strong correlations in spinful quantum wires with multiple dynamics — •Tobias Meng[1], Mehul Dixit[2], Julia Meyer[3], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [2]Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA — [3]SPSMS, CEA-INAC/UJF-Grenoble 1, 38054 Grenoble, France

We consider a quantum wire of electrons and focus on the quantum phase transition from a strictly one-dimensional to a quasi one-dimensional electron liquid. In the low-density limit, this transition corresponds to the deformation of the 1D Wigner crystal to a zig-zag arrangement of the electrons described by an Ising order parameter. The critical properties are governed by the charge degrees of freedom, of which the spin sector remains essentially decoupled. The interaction between critical fluctuations and the gapless plasmon mode leads to an enhanced SU(2) symmetry and a suppression of the characteristic velocity. At higher densities, the electrons form one-dimensional subbands. At the transition, the second band gets filled as a function of the external gate voltage. Electrons at the bottom of the second band interact strongly due to the diverging density of states and become impenetrable. This stabilizes the electron liquid as it hinders pair-tunneling processes between the bands which generate an attractive interaction. The impenetrable electrons in the second band are further screened by plasmon excitations and the resulting polarons finally undergo a Lifshitz transition. We discuss the resulting phase diagram as a function of transverse confinement and density of the electrons.

TT 44.62 Thu 10:00 P1

Properties of dimerized n-leg spin 1/2 ladders — •Kris Cöster and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The Heisenberg model on quasi one-dimensional ladder structures is expected to be interesting since it interpolates between the purely one-dimensional case having fractional excitations and the two-dimensional system displaying long-range order. In recent years there has been a big process in the theoretical and experimental understanding of the two-leg ladder. But the microscopic determination of the excitation spectrum and the spectral properties of n-leg ladders is very challenging.

Here we approach the general case by studying dimerized n-leg ladders with n=3,4,5,6. To this end we use perturbative continuous unitary transformations (pCUTs) with advanced graph techniques to obtain an effective quasi-particle description. We calculate the one- and two-triplon properties. Special regard is paid to binding effects between two triplons with total spin zero which is of direct relevance for optical spectroscopy on such systems.

TT 44.63 Thu 10:00 P1

Finite-size scaling analysis of the frustrated square-lattice

Heisenberg model — •Burkhard Schmidt, Mohammad Siahatgar, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The two-dimensional frustrated next nearest neighbor Heisenberg model on the square lattice is a prime example for a spin system where quantum fluctuations can either destroy or stabilize magnetic order. The phase boundaries and staggered moment dependence on the frustration ratio J_2/J_1 of the exchange constants are fairly well understood both from approximate analytical and numerical methods. We use exact diagonalization for finite clusters for an extensive investigation of the more general $J_{1a,b}$-J_2 model to clarify the dependence of ground-state energy and ordered moment on exchange frustration and anisotropy. Exact diagonalization is an unbiased approach, however it is restricted to small tiles, and we have to account for finite-size effects. We therefore introduce a systematic way of uniquely generating all possible tilings of the square lattice, define a *compactness* parameter for selecting the tiles to be included into the scaling procedure and, for this low symmetry model, define a controlled procedure for the finite size scaling that is compatible with the possible magnetic phases. We apply the scaling procedure to the ground-state energy, the static structure factor, and the static long-distance correlation function of the $J_{1a,b}$-J_2 model at different characteristic points in the parameter space of the Hamiltonian. The tile size dependence of the ordered moment is derived from the latter two quantities.

TT 44.64 Thu 10:00 P1

Time-dependent exact diagonalization for the simulation of RIXS in 1-D systems — •Stefanos Kourtis, Maria Daghofer, and Jeroen van den Brink — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

We present a method for numerical simulation of resonant inelastic X-ray scattering (RIXS). Using time-dependent exact diagonalization, we take explicitly into account the finite lifetime of the core-hole present in the intermediate state of the process and study its effect on observables. We report preliminary results for the spin and charge excitations of a one-dimensional chain at quarter filling and compare them to various approximations used. In particular, we study to what extent the finite lifetime affects direct RIXS and possibly leads to differences between the expected outcome and the charge response function.

TT 44.65 Thu 10:00 P1

Transport simulations in quasi-one-dimensional correlated quantum systems — •Alex Cojuhovschi[1], Malcolm Einhellinger[1], Eric Jeckelmann[1], Sabine Tornow[2], and Gertrud Zwicknagl[2] — [1]Leibniz Universitaet Hannover — [2]TU Braunschweig

We present a powerful numerical approach for studying spin and charge transport in quasi-one-dimensional correlated quantum many-body systems. The time-evolving block decimation (TEBD) method [1] is used to simulate the quantum dynamics of finite-size systems which are driven out of equilibrium by a sudden change in applied voltage potentials. Thanks to the natural parallelizability of the TEBD algorithm large systems can be simulated efficiently on modern high-performance parallel computers. Using a finite-size analysis based on an analogous classical model, steady-state transport properties are obtained from the quasi-stationary properties calculated with TEBD for finite systems.

To assess the capability and limitation of our approach we investigate the transient and steady-state transport properties of various correlated quantum systems such as Luttinger liquids and dot-lead systems and compare our results with exact results for non-interacting systems as well as field-theoretical predictions and time-dependent numerical renormalization group simulations for interacting systems. \newline
[1] G. Vidal, PRL 91, 147902 (2002); 93, 040502 (2004)

TT 44.66 Thu 10:00 P1

Quantum relaxation in the XY chain with free boundaries — •Benjamin Blass and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

We study the quantum relaxation in the spin-1/2 XY chain with free boundaries in a longitudinal field. The system is described by $\hat{H} = -\frac{J}{2}\sum_{i=1}^{L-1}\left[\frac{1+\gamma}{2}\hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + \frac{1-\gamma}{2}\hat{\sigma}_i^y\hat{\sigma}_{i+1}^y\right] - \frac{h}{2}\sum_{i=1}^{L}\hat{\sigma}_i^z$. By preparing the system in an eigenstate (e.g., the ground state) of the Hamiltonian for given parameters γ_0, J_0 and h_0 and then suddenly changing (i.e., quenching) the parameters to γ, J and h, the system evolves dynamically according to the Schrödinger equation into a stationary (i.e., time translational invariant) state, which is characterized by a length and time scale depending on the quench parameters. Due to the free boundaries, the local order parameter has a time and space dependent profile, which is computed. The issues of thermalization (or the lack thereof) as well as recurrence within a finite system are discussed.

TT 44.67 Thu 10:00 P1

Band renormalization for systems on anisotropic triangular lattices — •Andrea Di Ciolo, Luca F. Tocchio, and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt Am Main, Germany.

We consider electronic systems on anisotropic triangular lattices, i.e. with hopping t on two bonds of the unit cell and t' on the last bond.

We apply the renormalized mean-field theory to the Hubbard model [see F. C. Zhang, et al., Supercond. Sci. Tech. 1, 36 (1988)] and our analytical results are to be compared with Variational Monte Carlo findings.

The renormalization of the band structure and the evolution of the Fermi surface are investigated as due to electronic correlations.

In particular, motivated by former studies for 2D-systems on square lattices [C. Gros et al., Proc. Natl. Acad. Sci. U.S.A. 103, 14928 (2006)] and 1D-systems [L. F. Tocchio et al., Phys. Rev. B 81, 205109 (2010)], we explore the issue of the underlying Fermi surface (Luttinger surface) for insulating states on triangular lattices.

TT 44.68 Thu 10:00 P1

Response of Jahn-Teller inhomogeneities to uniaxial strain. — •Joaquin Miranda Mena — German Research School for Simulation Sciences and RWTH Aachen University, 52425 Jülich

Using Monte Carlo simulations we study the effect of uni-axial strain in a two-dimension electron-phonon Hamiltonian with long-range Coulomb interaction. Lattice effects are introduced in form of Jahn-Teller (JT) polarons. In the absence of strain we observe that charge clustering is accompanied with a strong suppression of single particle density of states (DOS) for high doping and low temperatures. Remarkably, these clusters take stripe forms when the JT attraction and the Coulomb repulsion are similar in magnitude. In this work we report how the map of lattice distortions and DOS are modified in the presence of the uniaxial strain. In the case of ferro-distortive JT attraction we observe orbital ordering and no changes of cluster shapes. The presence of the strain is mainly reflected in DOS of unoccupied states. In the case of antiferro-distortive JT attraction, clusters start to melt with increasing strain.

TT 44.69 Thu 10:00 P1

Functional RG for spin chains — Kimmo Sääskilahti[1], •Stefan Göttel[2], Dirk Schuricht[2], Sabine Andergassen[2], and Carsten Honerkamp[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen, Germany — [2]Institut für Theorie der statistischen Physik, RWTH Aachen, Germany

We apply a recently developed functional RG (fRG) scheme [1] for quantum spin systems to one-dimensional spin chains. Based on an auxiliary fermion representation, the derived flow equations allow for a systematic resummation of perturbation series in the spin-spin interactions. The computed observables include the ground-state energy and the spin-spin correlation function as a function of the spin anisotropy. Comparing to exact results from Bethe Ansatz and DMRG calculations, we assess the accuracy of the obtained results. The importance of the Katanin modification in the truncated fRG scheme is addressed.
[1] J. Reuther und P. Woelfe, Phys. Rev. B 81, 144410 (2010)

TT 44.70 Thu 10:00 P1

Quantum phase transitions in anisotropic Heisenberg antiferromagnetic chains — •David Peters — Institut für Theoretische Physik der Phasenübergänge, RWTH Aachen

Using (infinite) density matrix renormalization group calculations, ground state properties of the spin–1 Heisenberg chain with exchange and quadratic single-ion anisotropies in an external field are studied, for special choices of the two kinds of anisotropies[1]. In particular, the ground state phase diagrams comprise antiferromagnetic, spin-liquid (or spin-flop), half-magnetization-plateau, and supersolid (or biconical) phases. Especially, studying various quantities, including spin-spin correlations, interesting features of the spin-liquid and supersolid phases are identified. Properties of the quantum chains are compared to those of corresponding classical spin chains.
[1] D. Peters, I.P. McCulloch, W. Selke, Phys. Rev. B 79, 132406

(2009); J. Phys.: Conf. Ser. 200, 022046 (2010)

TT 44.71 Thu 10:00 P1

Magnetic susceptibility and spin-wave properties of two-band Hubbard models — •Ernst von Oelsen, Jörg Bünemann, and Götz Seibold — Institut für Physik, BTU Cottbus, Postfach 101334, 03013 Cottbus

We present result on the magnetic susceptibility and the spin-wave properties of two-band Hubbard models in two, three, and infinite dimensions. As a method we use the recently developed generalisation of the time-dependent Gutzwiller theory for multi-band models. Our findings are compared with those of a Hartree-Fock based random phase approximation, which is the standard textbook method for the calculation of two-particle response functions. Like in the corresponding ground-state theories we find significant differences between both methods quantitatively as well as qualitatively.

TT 44.72 Thu 10:00 P1

Investigation of giant spin rings with DMRG — •Jörg Ummethum and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld

Giant antiferromagnetic molecules like Fe_{18} [1], which consists of 18 $s = 5/2$ spins on a ring, are much too large for exact diagonalization so that simplifying models or approximate numerical methods like Quantum Monte Carlo or DMRG have to be used. For one-dimensional systems DMRG is known to yield very accurate results.

We use static and dynamical DMRG methods to investigate the low-lying spectrum of a Heisenberg spin ring consisting of 18 spins (neglecting the small single-ion anisotropy which is present in Fe_{18}) with spin quantum numbers $s = 1/2$ and $s = 5/2$. We calculate the lowest energies in subspaces of total magnetic quantum number, the $T = 0$ magnetization curve, and the spectral function $S^{zz}(q, \omega)$ for different values of q. Since the momentum of the ground state is known, the momenta of low-lying excited states in the $S = 1$ subspace can be calculated by looking for peaks in $S^{zz}(q, \omega)$.

We find that the lowest energies in subspaces of total magnetic quantum number form a rotational band and that transitions from the $S = 0$ ground state to the $S = 1$ ground state within the first rotational band are dominant. This agrees with the results of [2] where much smaller spin rings have been investigated using exact diagonalization.

[1] O. Waldmann, T. C. Stamatatos, G. Christou, H. U. Güdel, I. Sheikin, and H. Mutka, Phys. Rev. Lett. 102, 157202 (2009)
[2] O. Waldmann, Phys. Rev. B 65, 024424 (2001).

TT 44.73 Thu 10:00 P1

Factorization of time-dependent correlation functions for the central spin model — •Fabian Güttge, Jasmin V. Jäger, and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The spin of an electron trapped in a semiconductor quantum dot has been suggested as a possible realisation of a solid-state qubit. The major source of decoherence in such devices is the hyperfine coupling to the nuclear spins. We model this system by a central spin coupled to a finite number of independent nuclear bath spins. The time-dependent two-, three and four-particle correlation functions are calculated using exact diagonalization. We investigate under which conditions the correlation functions can be factorized by neglecting higher order cummulant corrections. This provides information about the applicability of equation of motion decoupling schemes which scale linear with the number of bath spins.

TT 44.74 Thu 10:00 P1

Thermal relaxation and heat transport in spin ice $Dy_2Ti_2O_7$ — •Bastian Klemke[1,2], M. Meissner[1,2], P. Strehlow[2,3], K. Kiefer[1], S. A. Grigera[4,5], and D. A. Tennant[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Technische Universität Berlin — [3]Physikalisch Technische Bundesanstalt, Institut Berlin — [4]School of Physics and Astronomy, St. Andrews, UK — [5]Instituto de Física de Líquidos y Sistemas Biológicos, CONICET, UNLP, La Plata, Argentina

The thermal properties of single crystalline $Dy_2Ti_2O_7$ have been studied at temperature below 30 K and magnetic fields applied along [110] direction up to 1.5 T. Based on a thermodynamic field theory (TFT) various heat relaxation and thermal transport measurements were analysed. So we were able to present not only the heat capacity of $Dy_2Ti_2O_7$, but also for the first time the different contributions of the magnetic excitations and their corresponding relaxation times in the spin ice phase. In addition, the thermal conductivity and the shortest relaxation time were determined by thermodynamic analysis of steady state heat transport measurements. Finally, we were able to reproduce the temperature profiles recorded in heat pulse experiments on the basis of TFT using the previously determined heat capacity and thermal conductivity data without additional parameters. Thus, TFT has been proved to be thermodynamically consistent in describing three thermal transport experiments on different time scales. The observed temperature and field dependencies of heat capacity contributions and relaxation times indicate the magnetic excitations in the spin ice $Dy_2Ti_2O_7$ as thermally activated monopole-antimonopole defects.

TT 44.75 Thu 10:00 P1

Collective orbital excitations in $GdVO_3$ — •Michael Voigt[1], Luis Mäder[1], Konstantin Shportko[1], Graeme R. Blake[2], Nandang Mufti[2], Agustinus A. Nugroho[2,3], Thomas T. M. Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]University of Groningen — [3]Institut Teknologi Bandung

In the vanadates (RVO_3) orbital interactions are expected to be especially strong. In the compounds YVO_3 and $HoVO_3$ these interactions lead to two different phases of orbital ordering (OO), one in an intermediate temperature range with G-type OO and one low-temperature phase with C-type OO. [1] In these orbitally ordered states, one expects novel collective excitations, so called orbitons, which are analogous to spin waves in a magnetically ordered state.

Previous optical measurements of YVO_3 and $HoVO_3$ have shown a striking feature at 0.4 eV with polarization $E \parallel c$ in the intermediate phase which is interpreted as bi-orbiton excitation. [2] Furthermore a second interesting feature at 0.55 eV with polarization $E \parallel a$ is observed. The interpretation of this feature is still a puzzle.

We show the optical conductivity $\sigma(\omega)$ of $GdVO_3$ single crystals for the mid-infrared range and temperatures from 10 K to 300 K. In $GdVO_3$, G-type OO (the intermediate phase of YVO_3) extends down to the lowest temperatures, offering additional information on the excitations discussed above.

[1] Blake *et al.*, PRB **79**, 045101 (2009)
[2] Benckiser *et al.*, NJP **10**, 053027 (2008)

TT 44.76 Thu 10:00 P1

Looking for orbiton dispersion features in $GdVO_3$ with the aim of RIXS — •Pasquale Marra[1], Krzysztof Wohlfeld[1], Jeroen van den Brink[1], Luis Maeder[2], Komalavalli Thirunavukkuarasu[2], Marco Moretti Sala[3], Giacomo Ghiringhelli[3], Thorsten Schmitt[4], and Marcus Grueninger[2] — [1]IFW Dresden — [2]Universität zu Köln — [3]Politecnico di Milano — [4]PSI Villigen

We compute the theoretical RIXS spectra for the *dd* excitations at the vanadium L_3 edge in $GdVO_3$, as a function of energy and momentum transfer, by factorizing the RIXS spectral function into two parts: (i) a single-site part with a core hole present and (ii) a lattice part without the core hole. The obtained results are compared with the direct measurements on the compound for four different angles, carried out with SAXES at the ADDRESS beamline (PSI Villigen, Switzerland). The experimental spectra show a shoulder at low energy with a clearly visible shift corresponding to different momentum transfers. We investigate the possible origin of this shift, in order to distinguish between a crystal field effect (weight transfer between two or more different peaks) and an orbiton dispersion feature predicted by the superexchange mechanism for $3d^2$ degenerate electrons in V^{3+} ions.

TT 44.77 Thu 10:00 P1

Spin excitations in the antiferromagnetic and antiferroquadrupolar phase of CeB_6 — •G. Friemel[1], Y. Li[1], A. Invanov[2], V. B. Filipov[3], N. Yu. Shitsevalova[3], N. E. Sluchanko[4], and D. S. Inosov[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Institut Laue-Langevin, 6 rue Jules Horowitz, F-38042 Grenoble Cedex 9, France — [3]I. N. Frantsevich Institute for Problems of Material Science, National Academy of Sciences of Ukraine, ul. Krzhizhanovskogo 3, Kiev, 03680, Ukraine — [4]A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, ul. Vavilova 38, Moscow, 119991 Russia

We present inelastic neutron scattering studies on CeB_6, a rare earth hexaboride. In zero field CeB_6 exhibits a paramagnetic phase at high temperatures and orders antiferromagnetically below $T_N = 2.3$K.

However, below $T_Q = 3.2$K a peculiar "antiferroquadrupolar" (AFQ)-phase of the cerium ions appears, whose nature is so far controversial. Multipolar excitations in zero field have been theoretically predicted and partially studied. The mechanism behind this type of ordering is still in question since spin excitation data is sparsely available. Therefore, we present a first comprehensive temperature and energy dependent mapping of the spin excitations in the AFM and AFQ phases, which are dominated by a pronounced inelastic intensity in the vicinity of the AFQ wavevector (1/2 1/2 1/2) and which quickly disappear in the paramagnetic phase upon warming above T_Q.

TT 44.78 Thu 10:00 P1

Low temperature thermal and electrical transport properties of $ZrZn_2$ in high magnetic field — •Yang Zou[1,3], Mike Sutherland[1], Stephen Hayden[2], Daniel Rothfuss[3], Andreas Fleischmann[3], F. Malte Grosche[1], and Christian Enss[3] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Physics, University of Bristol, United Kingdom — [3]Kirchhoff-Institut, Universität Heidelberg, Germany

Laudau's Fermi-liquid theory has been proven remarkably successful in describing the properties of metals at low temperatures. Unlike most metals, the low temperature band ferromagnet $ZrZn_2$ appears to violate Fermi-liquid behaviour over a wider temperature range at low temperature. In order to investigate the nature of the Fermi-liquid breakdown in this material, the electrical and thermal transport properties of $ZrZn_2$ were investigated over a wide range of magnetic field. An experimental technique to measure the thermal conductivity down to 100 mK has been set up and tested. In zero field our measurements confirm the finding reported in [1] that, to leading order in temperature T, the electrical and effective thermal resistivities at low temperature take a $T^{5/3}$ and T form, respectively. These are the signatures of a marginal Fermi-liquid, predicted to occur close to a ferromagnetic quantum critical point by spin fluctuation theory. In contrast, we find that at finite magnetic field the electrical and effective thermal resistivities assume quadratic temperature dependencies, consistent with a return to conventional Fermi-liquid behaviour.

[1] Smith et al. Nature 455, 7217 (2008)

TT 44.79 Thu 10:00 P1

Low temperature spin excitation spectrum of FeSi by polarized neutron spectroscopy — •Sven Krannich[1], Yvan Sidis[2], Jean-Michel Mignot[2], Daniel Lamago[1,2], Frank Weber[1], Alexander Ivanov[3], and Paul Steffens[3] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, 76021 Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA-Saclay, F-91191 Gif sur Yvette Cedex, France — [3]Institute Laue Langevin, 156X, 38042 Grenoble Cedex 9, France

We investigated the spin excitation spectrum of FeSi using the thermal triple axis neutron spectrometer IN20 at the Institute Laue Langevin, Grenoble, with polarization analysis. FeSi displays a behavior which has, so far, only been observed in f-electron containing Kondo insulators. Therefore, it has often been claimed to be the first 3d system belonging to this class of materials [1]. A temperature dependent energy gap was observed in optical spectroscopy [2], but measurements of inelastic magnetic scattering via neutrons have been restricted to T $\geq$ 150 K so far [3] and did not report gap signatures. We measured magnetic scattering between room temperature and T = 15 K over a large energy range up to energies of 80 meV. Particular attention was devoted to possible spin-exciton formation at energy transfers below the gap value at low temperatures as observed in the Kondo-insulator YbB_{12} [4].

[1] D. Mandrus et al., Phys. Rev. B 51, 4763 (1995)
[2] D. Menzel et al., Phys. Rev. B 79, 165111 (2009)
[3] K. Tajima et al.,Phys. Rev. B 38, 6954 (1988)
[4] K. S. Nemkovski et al., Phys. Rev. Lett. 99, 137204 (2007)

TT 44.80 Thu 10:00 P1

Dynamic triple-helix spin clusters in the paramagnetic phase of MnSi — •A. Hamann[1], D. Lamago[2], Th. Wolf[1], H. v. Löhneysen[1], and D. Reznik[3] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA Saclay, France — [3]Department of Physics, University of Colorado, Boulder, USA

MnSi exhibits helical magnetic order at low temperatures and ambient pressure with underlying Fermi-liquid (FL) properties. At high pressures an exotic magnetic state forms referred to as partial order [1], where the helical propagation vector becomes disordered. Non-FL temperature dependence of the electrical resistivity appears nearby in the phase diagram. Our numerical calculations show that isotropic nearest-neighbor spin interactions in MnSi favor a glassy aggregation of topological magnetic clusters that we call triple-helices. They are similar to double helices well known from blue phases of liquid crystals [2] and have the spectral signature of partial order. Their stability increases as their size decreases. This model may explain most of the puzzling properties of MnSi including the non-FL behavior and the two-component phase transition that was revealed by specific heat [3]. Our detailed neutron scattering measurements in the paramagnetic phase where temperature sets the scale of the size of dynamic spin clusters fully confirm this picture.

[1] C. Pfleiderer, D. Reznik et al., Nature **427**, 227 (2004)
[2] D. C. Wright and N. D. Mermin, Rev. Mod. Phys. **61**, 385 (1989)
[3] D. Lamago et al., Physica B **385-386**, 385 (2006)

TT 44.81 Thu 10:00 P1

Polarized electron currents in the helical magnet MnSi — •Pascal Krautscheid, Karin Everschor, Markus Garst, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The Dzyaloshinskii-Moriya interaction in MnSi results in the formation of helical magnetic phases and even the stabilization of Skyrmion configurations at low temperatures [1]. A polarized electron current couples efficiently to such twisted magnetic structures giving rise to pronounced spin-torques transfer phenomena [2]. We study the interaction of spin currents with the magnetic texture in MnSi in the framework of the Landau-Lifshitz-Gilbert equation. Particular emphasis is put on the influence of spin currents on the pitch of the magnetic helix and its pinning by the underlying crystal structure of MnSi.

[1] S. Mühlbauer et al., Science 323, 915 (2009).
[2] F. Jonietz et al., Science, to be published (2010).

TT 44.82 Thu 10:00 P1

Entanglement spectrum analysis of frustrated Heisenberg antiferromagnets — •Burkhard Scharfenberger[1], Ronny Thomale[2], and Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA

We investigate numerically the entanglement spectra of $S = 1$ chirality - and $S = 1/2$ chiral spin liquids on various lattice geometries ($N = 16, 32$-site square and $N = 18, 36$-site kagome lattices) with cylindrical topology. We compare these spectra to those obtained from groundstates of antiferromagnetic Heisenberg models with either simple nearest neighbour interaction if the lattice geometry already causes frustration (kagome) or next nearest neighbour interaction near the critical coupling strength $J_1 = 2\,J_2$, which introduces frustration via the interaction (square lattice).

On the square lattice we find that both chiral spin liquid and chirality liquid describe the antiferromagnet equally well up to the critical point, despite the fact that the only the chirality liquid has the same symmetries (parity P and time reversal T) as the hamiltonian. In the case of the Kagome lattice, the exponential groundstate degeneracy caused by frustration is mirrored in the exponential freedom we have in writing out our spin liquids for different sublattice configurations. The interesting 'low energy' part of the spectrum proves to be insensitive to this subdivision, which suggests that all these states essentially describe the same phase of the system.

TT 44.83 Thu 10:00 P1

Quantum Phases of the Planar Antiferromagnetic J_1-J_2-J_3 Heisenberg-Model — •Rachid Darradi[1], Johannes Reuther[2], Peter Wölfle[2], Wolfram Brenig[1], Marcelo Arlego[3], and Johannes Richte[4] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Departamento de Física, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina — [4]Institut für Theoretische Physik, Universität Magdeburg, 39016 Magdeburg, Germany

We present results of a complementary analysis of the frustrated planar J_1-J_2-J_3 spin-1/2 quantum-antiferromagnet. Using dynamical functional renormalization group, high-order coupled cluster calculations, and series expansion based on the flow equation method, we have calculated generalized momentum resolved susceptibilities, the ground state energy, the magnetic order parameter, and the elementary exci-

tation gap. From these we determine a quantum phase diagram which shows a large window of a quantum paramagnetic phase situated between the Neel, spiral and collinear states, which are present already in the classical J_1-J_2-J_3 antiferromagnet. Our findings are consistent with substantial plaquette correlations in the quantum paramagnetic phase. The extent of the quantum paramagnetic region is found to be in satisfying agreement between the three different approaches we have employed.

TT 44.84 Thu 10:00 P1

Generalized Magnetic Impurities in Low-Dimensional Quantum Antiferromagnets — •Björn Willenberg[1,3], Wolfram Brenig[1,3], Holger Frahm[2,3], and Eric Jeckelmann[2,3] — [1]Institute for Theoretical Physics, Technische Universität Braunschweig — [2]Institute for Theoretical Physics, Leibniz Universität Hannover — [3]Niedersächsische Technische Hochschule, NTH

We investigate magnetic impurities with extended multiplet structure in contact with spin-1/2 antiferromagnets. First, and using Quantum Monte-Carlo methods based on the stochastic series expansion, we study a spin-1/2 dimer coupled to the two-dimensional (2D) Heisenberg antiferromagnet (HAFM) at finite temperature. Results will be presented for thermodynamic properties as a function of temperature, exchange-coupling constants, and magnetic field. These include the impurity susceptibilities, magnetization, and the static on- and off-dimer correlation functions. Our findings will be contrasted against those for single spin-1/2 impurities in 2D HAFMs. Moreover we will analyze similar properties for S>1/2 edge-spins coupled to 1D HAFMs with open boundary conditions, where a comparison with results from Bethe ansatz and density-matrix renormalization methods is possible in the limit of zero temperature.

Work partially funded by the NTH School for Contacts in Nanosystems.

TT 44.85 Thu 10:00 P1

Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions — Philipp Wissgott[1], Jan Kuneš[2], •Alessandro Toschi[1], Ryotaro Arita[3], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]Department of Applied Physics, University of Tokyo, Japan

We present an interface between the full-potential linearized augmented plane wave package wien2k[1] and the wannier90[2] code for the construction of maximally localized Wannier functions (MLWF). The interface wien2wannier (w2w)[3] computes the necessary input data for the use of wannier90 starting from a wien2k `.vector` file. Scripts and FORTRAN90 programs to simplify the workflow are also provided. The original wannier90 program has been adapted to return the Hamiltonian in the basis of the Wannier orbitals and other useful data. As an application of w2w, we consider[3] two examples: $SrVO_3$ and $FeSb_2$. The latter material has a very complicated bandstructure. Here, the use of a basis set of Wannier functions allows for a deeper understanding and a for the proper input of codes for strongly correlated materials, such as LDA+DMFT.

[1] P. Blaha, *et al.*, Vienna University of Technology, Austria, 2001.
[2]A. A. Mostofi, *et al.* Comput. Phys. Commun. **178**, 685 (2008); www.wannier.org.
[3] Jan Kuneš, *et al.* , Comp. Phys. Comm. **181** 1888 (2010).

TT 44.86 Thu 10:00 P1

Optimized basis in continuous unitary transformations for symmetry-broken groundstates — •Nils A. Drescher and Götz S. Uhrig — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

Continuous unitary transformations (CUT) [1,2] provide a generic, non-perturbative framework to derive effective low-energy models preserving the system's symmetries. We use them to decouple and study low-lying magnetic excitations [3] of low-dimensional, antiferromagnetic spin $\frac{1}{2}$ models. Our special focus is the quantum phase transition between disordered and long-range ordered phases with spontaneous staggered magnetization in two-dimensional dimerized systems. Introducing a variational parameter, the spin symmetry of the original quasiparticle basis can be broken, thus allowing the CUT to deal with a spontaneously symmetry-broken groundstate. Even in the magnetically disordered one-dimensional system, the optimal choice of the variation parameter allows for a gain of accuracy for magnetic properties.

[1] C. Knetter, K.P. Schmidt and G.S. Uhrig, J. Phys. A: Math. Gen. 36, 7889 (2003)
[2] S. Dusuel and G.S. Uhrig, J. Phys. A: Math. Gen. 37, 9275 (2004)
[3] K. P. Schmidt and G.S. Uhrig, Phys. Rev. Lett. 90, 227204 (2003)

TT 44.87 Thu 10:00 P1

Charge self-consistency in an LDA+DMFT framework — •Daniel Grieger, Oleg Peil, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

In recent years, the combination of the local-density approximation (LDA) to density functional theory with the dynamical mean-field theory (DMFT) has proven to be a powerful and reliable tool to describe explicit strong electronic correlations in realistic materials. However in many current implementations thereof, the correlated charge density is not converged within a comprehensive LDA+DMFT interface. Thus the dependence of many observables on self-energy effects connected to the selfconsistent correlated charge density is neglected. We address this problem both within a pseudopotential and a projector-augmented wave (PAW) [1] implementation of the LDA+DMFT framework. This work first illuminates the crucial parts of the theoretical interfacing structure, such as the extraction of a suitable correlated subspace [2] and the representation of the acquired correlated charge density in a way that it can be processed in the conventional LDA portion as well as the DMFT part of the problem (e.g., Ref. [3]). In addition, concrete materials results from investigations using this charge-selfconsistent scheme in the context of strong correlation problems with relevant charge and spin degrees of freedom will be presented.

[1] P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994)
[2] B. Amadon et al., Phys. Rev. B **77**, 205112 (2008).
[3] F. Lechermann et al., Phys. Rev. B **74**, 125120 (2006)

TT 44.88 Thu 10:00 P1

Compression of matrix-product states — •Michael Lee and Michael Potthoff — I. Institut für Theoretische Physik, Jungiusstraße 9, 20355 Hamburg

One-dimensional systems of strongly correlated electrons can efficiently be treated by means of the density-matrix renormalization group (DMRG) [1]. It has been shown [2] that an essentially equivalent formulation of the DMRG is possible using matrix-product states and matrix-product operators.

We propose to employ Krylov-based techniques operating on the space of matrix-product states. This should allow for a calculation of dynamical correlation functions, like the one-particle Green's function, similar to a standard Lanczos calculation without the need for multiple-state targeting. Unlike the correction-vector method this "matrix-product-Lanczos approach" offers the exciting perspective to get the entire frequency dependence of the Green's function from a single calculation.

The iterative algorithm requires a "compression" of matrix-product states of the form $H|\Psi\rangle$ to control the growth of matrix dimensions. Here, we show first results and discuss the accuracy and efficiency of the compression technique.

[1] S. White, Phys. Rev. Lett. 69, 2863 (1992).
[2] S. Östlund and S. Rommer, Phys. Rev. Lett. 75, 3537 (1995).

TT 44.89 Thu 10:00 P1

Dual-Fermion approach to Non-equilibrium strongly correlated problems — •Alexander Lieder, Christoph Jung, Sergej Brener, Alexander Chudnovskiy, and Alexander Lichtenstein — I. Institut für Theoretische Physik Universität Hamburg

We present a generalization of the recently developed Superperturbation solver for the Anderson impurity model for the non-equilibrium case. We show that the general dual perturbation theory can be formulated on the Keldysh contour. Starting from a reference Hamiltonian system, in which the time-dependent solution is found by exact diagonalization, we make a dual perturbation expansion in order to account for the relaxation effects from the fermionic bath. Test cases for closed as well as open quantum systems in a fermionic bath are presented.

TT 45: Focused Session: 100 Years of Superconductivity

Time: Thursday 10:30–12:40 Location: HSZ 03

Invited Talk TT 45.1 Thu 10:30 HSZ 03

Pairing fermions with population imbalance — •Peter Fulde — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

Cooper pairing of fermions starts usually from the premise that the two species forming pairs have equal populations, i.e., that their particle numbers are the same. That need not always be the case, though, and examples to the opposite are known. They concern metals, as well as dense quark matter, nuclear matter or ultracold atoms.

The simplest case is that of a superconductor when a Zeeman term is added to the Hamiltonion. We will show that the Zeeman energy may result in breaking of translational invariance and hence in inhomogeneous superconducting ground states. They are often referred to as FFLO states, since they were first suggested by Fulde and Ferrell and independently by Larkin and Ovchinnikov. Simple arguments will be presented which explain the origin of the symmetry breaking.

The inhomogeneous states are paralleled by the ones caused by a magnetic field acting on the electron orbits, i.e., Abrikosov vortex states. While it took only a few years to verify Abrikosov vortices after they had been predicted, it has taken nearly 40 years to proof the existence of inhomogeneous states caused by population imbalance. In the meantime experiments on $CeCoIn_5$, and the two-dimensional organic superconductors κ-(BEDT-TTF)$_2 \cdot$ Cu(NCS)$_2$, λ-(BETS)$_2$ $FeCl_4$, λ-(BETS)$_2$ $GaCl_4$ and β-(BEDT-TTF)$_2$ $SF_5CH_2CF_2SO_3$ provide very strong evidence in some cases, and still disputed ones in others that a FFLO state is forming in high magnetic fields. However, the most important realization of FFLO-like states is found in pi junctions, which seem to be on the verge of important technical applications. We will briefly describe progress which has been made here, based on ideas of Bulaevskii, Buzdin, Demler and others and realized by Ryazanov, Feofanov, Ustinov and others.

Invited Talk TT 45.2 Thu 11:00 HSZ 03

Unconventional Superconductivity - Aspects of Symmetry and Topology — •Manfred Sigrist — ETH Zürich, Zürich, Switzerland

Unconventional superconductors form coherent states of Cooper pairs whose internal structure gives rise to most intriguing and complex properties. Since the discovery of superfluid He-3 and the early heavy Fermion superconductors this fascinating field has evolved into one of the most active topics of condensed matter physics and has been stimulated by many discoveries of new materials, such as the cuprate and Fe-pnictide high-temperature superconductors, ruthenates and many heavy Fermion compounds. New theoretical insights based on the symmetry and topology of the superconducting order parameters and proposals of novel pairing mechanism enlarge our scope of superconductivity enormously. In this presentation I will give a brief overview on some of the most important concepts and ideas which have emerged during the recent era of research on unconventional superconductivity.

10 min. break

Invited Talk TT 45.3 Thu 11:40 HSZ 03

Large Scale Applications of Superconductors and the Challenges that they have posed — •David Larbalestier — National High Magnetic Field Laboratory, Florida State University

Already in 1913 Onnes envisioned using superconductors to create 100 kGauss fields well beyond any possibility provided by cooling Ag or Cu with liquid helium. Only some "bad places" in his Hg and Pb wires seemed to impede his first attempts at this dream, one that he imagined a short ongoing effort would quickly resolve. In fact, resolution required 50 years, understanding the subtle effects of alloy and compound superconductivity, closure of the theory-experiment gap and inspired experiments with Nb_3Sn. Suddenly in 1961, it all came together and Onnes's dreams of 100 kGauss magnets were soon comfortably surpassed. In the last 45 years virtually all superconducting magnets have been made from just two Nb-base materials, Nb-Ti and Nb_3Sn, operating in liquid He. In 1987 cuprates with $T_c > 100$K suggested that superconducting applications could leave liquid helium behind, and extend well beyond the science to the electrical engineering market. However, making conductors from complex cuprates posed many more challenges than envisaged in 1987 (echoes of Onnes in 1913?). Now that these challenges have largely been met in $REBa_2Cu_3O_7$ coated conductors, it is time to talk too about practical requirements for new superconductors. At 100, one can still be sure that the "right" new superconductor will find broad application and the ubiquity of superconductivity in materials phase space suggests that many new applications lie ahead in the 2nd superconducting century.

Invited Talk TT 45.4 Thu 12:10 HSZ 03

Weak Superconductivity and Superconductor Electronics — •Konstantin Likharev — Stony Brook University, Stony Brook, NY 11794-3800, U.S.A.

I will review the discovery and studies of the Josephson effect and related macroscopic quantum phenomena (including the single-Cooper-pair tunneling), and the development of their electronics applications. The main focus of the talk will be on digital superconductor devices and circuits (such as the latching logic, parametric quantron, and RSFQ technology), but I will also briefly mention the development and current status of superconductor analog devices for dc voltage and current standards, ultrasensitive magnetometry, and electromagnetic wave detection.

TT 46: SC: Tunneling, Josephson Junctions, SQUIDs 1

Time: Thursday 10:30–13:00 Location: HSZ 301

TT 46.1 Thu 10:30 HSZ 301

Quasiparticle tunneling in superconducting qubits — •Juha Leppäkangas, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128, Germany

In this work we consider the effect of quasiparticle tunneling on Josephson qubits in the high E_J/E_C-limit. Such qubits are immune to pure dephasing due to background charge fluctuations or quasiparticle tunneling across the Josephson junctions. However, the induced energy-decay can still be relatively fast in the presence of typical nonequilibrium quasiparticle density. We consider energy-decay rates due to quasiparticle tunneling for both the equilibrium and nonequilibrium quasiparticles in few qubit designs.

TT 46.2 Thu 10:45 HSZ 301

Dependence of the macroscopic quantum tunneling rate on Josephson junction area — •Roland Schäfer[1,2], Christoph Kaiser[3], and Michael Siegel[2,3] — [1]Institut für Festkörperphysik, Karlsruhe Instituteof Technology, 76021 Karlsruhe — [2]Center for Functional Nanostructures, 76128 Karlsruhe — [3]Institut für Mikro- und Nanoelektronische Systeme, Karlsruhe Institute of Technology, 76187 Karlsruhe

We have carried out systematic Macroscopic Quantum Tunneling (MQT) experiments on Nb/Al-AlO_x/Nb Josephson junctions (JJs) of different areas. Employing on-chip lumped element inductors, we have decoupled the JJs from their environmental line impedances at the frequencies relevant for MQT. This allowed us to study the crossover from the thermal to the quantum regime in the low damping limit. A clear reduction of the crossover temperature with increasing JJ size is observed and found to be in accord with theory. Deviations of the observed quantum rate from theoretical predictions are thoroughly analized and discussed in the framework of Kramer's [1] turnover problem. [1] H. A. Kramers, Physica (Utrecht), **7**, 284 (1940).

TT 46.3 Thu 11:00 HSZ 301

Nonreciprocal microwave transmission through a long Josephson junction — •Kirill G. Fedorov, Hannes Rotzinger, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Insti-

tute of Technology, 76131 Karlsruhe, Germany

We are experimentally investigating microwave transmission through a long Josephson junction. In the flux-flow state, the transmission coefficient depends on the direction of fluxon propagation in the junction. This behavior is based on the modulation of the fluxon chain density by the external microwave radiation applied at the junction boundary.

We have measured the transmission characteristics of 10 GHz microwaves through a long Josephson junction embedded into a resonator that facilitates impedance matching. An enhancement of the microwave transmission occurs when the direction of flux flow coincides with the direction of microwave propagation. Reversal of either the in-plane magnetic field or bias current leads to suppression of the transmitted power due to the reversed direction of flux flow. We envision applications of the described effect for designing microwave on-chip isolators, circulators and amplifiers.

TT 46.4 Thu 11:15 HSZ 301

Cooper pair propagation in Josephson junctions chains — Roland Schäfer[1,2], Wanyin Cui[1,3], Birgit Kiessig[1,3], Kai Grube[1], •Jochen Zimmer[2,3], Hannes Rotzinger[2,3], and Alexey V. Ustinov[2,3] — [1]Institut für Festkörperphysik, Karlsruhe Intitute of Technology, 76021 Karlsruhe — [2]DFG-Center for Functional Nanostructures, 76128 Karlsruhe — [3]Physikalisches Institut, Karlsruhe Intitute of Technology, 76128 Karlsruhe

We have studied the transport properties of aluminum SQUID chains comprising 255 loops. The chains form arrays of coupled islands with a charging energy E_c which is of the order of the Josephson coupling E_j at zero magnetic field. E_j can be tuned towards zero by applying a magnetic field amounting to $\Phi_0/2 = h/4e$ per SQUID loop. Our results are in accord with previous observations [1], displaying a pronounced blockade of Cooper-pair transport at low voltages with a hysteretic onset of a resistive branch. Above a destinct threshhold the array is characterized by a field dependent, but in bias constant slope. The branch scales like E_j^2 and gives clear evidence that charge transport is due to the incoherent motion of Cooper pairs.

[1] P. Ågren, K. Andersson, and D. B. Haviland, J. Low Temp. Phys. 124, 291 (2001).

TT 46.5 Thu 11:30 HSZ 301

Observation of phase diffusion in a two-dimensional SQUID potential — •Susanne Butz[1], Alexey K. Feofanov[1], Ralf Dolata[2], Brigitte Mackrodt[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut fürr Technologie, 76131 Karlsruhe, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

We report experiments detecting two different escape mechanisms of a dc-SQUID from the zero voltage to the gap voltage state. The two underdamped Josephson junctions of the SQUID have the same critical current but different shunting capacitors, corresponding to a model of a virtual particle with spatially anisotropic mass moving in a two-dimensional (2D) potential. The measurements show the coexistence of escape either directly from the superconducting to the gap voltage state or from the phase diffusion regime. The latter is dominated by repeated escape and retrapping events and an increased dissipation. This coexistence is explained qualitatively by analyzing the shape of the 2D potential as well as the effect of the anisotropic mass of the phase particle. Using numerical simulations, the motion of the particle in the two different regimes is examined and it is shown that the anisotropy in mass results in anisotropic dissipation.

Measured and simulated switching current histograms and current-voltage characteristics are presented. A qualitative agreement between simulation and measurement is obtained, indicating simultaneously present escape by phase diffusion and the conventional switching from the superconducting state.

15 min. break

TT 46.6 Thu 12:00 HSZ 301

Sensitive dc SQUIDs for detection of small spin systems — •R. Wölbing[1], J. Nagel[1], M. Kemmler[1], K. Konovalenko[1], M. Turad[1], R. Werner[1], R. Kleiner[1], D. Koelle[1], O. Kieler[2], T Weimann[2], J. Kohlmann[2], A. Zorin[2], E. Kleisz[3], S. Menzel[3], B. Büchner[3], and R. Klingeler[3] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, 72076 Tübingen, Germany — [2]Fachbereich 2.4 "Quantenelektronik", Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [3]Leibnitz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany

Investigation on small spin systems, e.g. macromolecules, require ultrasensitive devices for sensing the magnetization reversal of such particles with the ultimate goal of single spin flip detection. For this purpose we examine submicron dimension SQUIDs, which can detect the magnetization reversal of small spin particles directly in strong magnetic fields. We fabricated dc SQUIDs based on Nb/HfTi/Nb Josephson junctions with areas down to 200 nm x 200 nm, as well as on $YBa_2Cu_3O_7$ (YBCO) grain boundary junctions (GBJs) with linewidths down to 80 nm. The critical current densities for both types of junctions are relatively large ($j_c > 10^5 A/cm^2$ at 4.2 K), which provides high critical currents even for submicron sized junctions. The Nb/HfTi/Nb and the YBCO SQUIDs have been characterized by electric transport and noise measurements at low and high fields up to the tesla range, showing low noise performance.

TT 46.7 Thu 12:15 HSZ 301

Thermal and Quantum depinning of a fractional Josephson vortex — •Edward Goldobin[1], Tobias Gaber[1], Kai Buckenmaier[1], Uta Kienzle[1], Hanna Sickinger[1], Dieter Koelle[1], Reinhold Kleiner[1], Max Meckbach[2], Christoph Kaiser[2], Konstantin Il'in[2], and Michael Siegel[2] — [1]Physikalische Institut, University of Tübingen, Auf der Morgenstelle 14, 72076 Tübingen — [2]Institut für Mikro- und Nanoelektronische Systeme, University of Karlsruhe, Hertzstraße 16, 76187, Karlsruhe

We investigate the bias current induced depinning of a fractional Josephson vortex in a 0-κ Josephson junction [1], where the κ-discontinuity of the phase is induced by current injectors. At high temperatures $T \gtrsim 100$ mK the depinning is governed by thermal fluctuations. By measuring a depinning current histogram and extracting the effective barrier height vs. κ, one can see the signatures of fractional vortex escape [2,3]. At low $T \lesssim 100$ mK, the escape is dominated by quantum fluctuations and the histogram width saturates. In spite of large currents involved (bias current ~ 1 mA, injector current ~ 5 mA), advanced experimental techniques such as superconducting bias filters and persistent mode loops for injector currents allow us to argue that the observed histograms correspond to MQT of a fractional vortex. We also discuss the particular histogram shape in this quantum regime.

[1] E. Goldobin et al., Phys. Rev. B **70**, 174519 (2004).
[2] U. Kinzle et al., Phys. Rev. B **80**, 014504 (2009).
[3] K. Vogel et al., Phys. Rev. B **80**, 134515 (2009).

TT 46.8 Thu 12:30 HSZ 301

Spin Currents in TFT-Josephson Junction — •Dirk Manske[1] and Philip Brydon[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]TU Dresden, Germany

The spin of the Cooper pair in a triplet superconductor provides a new degree of freedom in Josephson junction physics. This can be accessed by using a magnetically-active tunneling barrier, leading to a rich variety of unconventional Josephson effects. Because of the triplet state of the pairing wavefunction, triplet superconductor junctions in general also display a Josephson spin current, which can flow even when the equilibrium charge current is vanishing. Using the quasiclassical Green's function theory, we have examined the more general situation of a magnetically-active barrier which does not conserve the spin of a tunneling Cooper-pair [1]. We demonstrate that the Josephson spin currents on either side of the barrier need not be identical, with the magnitude, sign and orientation all allowed to differ. Not only do our calculations enhance the physical understanding of transport through triplet superconductor junctions, but they also open the possibility of novel spintronic Josephson devices [2,3].

[1] P.M.R. Brydon, C. Iniotakis, D. Manske, and M. Sigrist, Phys. Rev. Lett. 104, 197001 (2010).
[2] P.M.R. Brydon and D. Manske, Phys. Rev. Lett. 103, 147001 (2009).
[3] P.M.R. Brydon, C. Iniotakis, and D. Manske, New J. Phys. 11, 055055 (2009).

TT 46.9 Thu 12:45 HSZ 301

Long-range spin-triplet proximity effect in Josephson junctions with multilayered ferromagnets — •Luka Trifunovic[1,2] and Zoran Radovic[1] — [1]Department of Physics, University of Belgrade, Serbia — [2]Department of Physics, University of Basel, Switzerland

We study theoretically the Josephson effect and pairing correlations

in planar SF_1F_2S junctions that consist of conventional superconductors (S) connected through two metallic monodomain ferromagnets (F_1 and F_2) with transparent interfaces. We solve self-consistently the Eilenberger equations for arbitrary orientation of in-plane magnetizations in the clean limit and for moderate disorder in ferromagnets. Both singlet and triplet pair amplitudes and the Josephson current-phase relations are calculated numerically. It is shown that for equally thick ferromagnetic layers (symmetric junctions) the long-range spin-triplet correlations are not dominant: For thin ferromagnetic layers all amplitudes are equally large, while for thick layers the long range triplet amplitude is very small. It is shown that for noncollinear magnetizations the long-range proximity effect can be dominant in highly non-symmetric SF_1F_2S junctions with particularly thin F_1 and thick F_2 ferromagnetic layers. We find that dominant triplet correlations in Josephson junctions with ferromagnetic bilayer always give dominant second harmonics in current-phase relations at low temperatures.

TT 47: TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1

Time: Thursday 10:30–13:00 Location: HSZ 304

TT 47.1 Thu 10:30 HSZ 304

Universal relaxation resistance in the interacting resonant level model — •Oleksiy Kashuba, Herbert Schoeller, and Janine Splettstoesser — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

We calculated relaxation resistance, capacitance and relaxation time for the quantum dot interacting with a single-channel spin-polarised contact using the interacting resonant level model[1]. Extending the real-time renormalisation group method[2] for the case of adiabatic time depending parameters we confirmed the prediction of the universal relaxation resistance which was made for the non-interacting system[3]. We also expanded our model allowing adiabatic time dependence in interaction strength as well as in the escape rate and the level position. We found the corrections to the transport coefficients and showed that the relaxation time is less sensitive to the adiabatic time dependence then the resistance and capacitance, and the calculation of the correction to the relaxation time cannot be made in the frame of perturbation expansion with renormalised parameters requiring renorm-group approach.

[1] S.Andergassen, M.Pletyukhov, D.Schuricht, H.Schoeller, and L.Borda, arXiv:1010.5666 (2010).
[2] H.Schoeller, Eur. Phys. J. Special Topics 168, 179 (2009).
[3] M.Buttiker, H.Thomas, and A.Pretre, Mesoscopic capacitors, Phys. Lett. A 180, 364 (1993).

TT 47.2 Thu 10:45 HSZ 304

Obtaining the Full Counting Statistics from Time Dependent Simulations for Strongly Correlated Systems — Dmitry Bagrets[1], Sam Carr[2], and •Peter Schmitteckert[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology

Recent advances in the simulation of time evolution of correlated electron systems led to progress in understanding transport properties of nano scale systems attached to leads. Time dependent simulations enable the extraction of the IV characteristic [1,2] and noise correlations [3] from the transient evolution of a charge imbalanced quench. In this work we extend the idea of obtaining the Full Counting Statistics (FCS) from time dependent simulations [4] of the cumulant generating function and apply it to model systems such as the interacting resonant level model. The simulations are performed within the framework of the density matrix renormalization group approach.

[1] E. Boulat, H. Saleur, and P. Schmitteckert, Phys. Rev. Lett. 101, 140601 (2008).
[2] A. Branschädel, G. Schneider, and P. Schmitteckert; Ann. Phys. 522, 657 (2010).
[3] A. Branschädel, E. Boulat, H. Saleur, and P. Schmitteckert; Phys. Rev. B 82, 205414 (2010); Phys. Rev. Lett. 105, 146805 (2010).
[4] K. Schönhammer; Phys. Rev. B 75, 205329 (2007).

TT 47.3 Thu 11:00 HSZ 304

Full counting statistics of a molecular quantum dot with strong electron-phonon interaction — •Stefan Maier and Andreas Komnik — Institut für Theoretische Physik, Heidelberg, Germany

We investigate the non-equilibrium charge transfer properties of a single level quantum dot with a local bosonic degree of freedom (aka Holstein phonon) coupled to metallic reservoirs. Using the Lang-Firsov transformation we have derived a diagrammatic scheme for the calculation of the full counting statistics. Our approach is exact in the electron-phonon interaction and resums a certain diagram subset with respect to the tunneling amplitude. A comparison with Monte-Carlo simulation data shows that the formalism captures basic properties of the strong electron-phonon coupling regime. In addition to the nonlinear current-voltage relation we analyze noise properties and higher order cumulants of the system.

TT 47.4 Thu 11:15 HSZ 304

Full counting statistics for the Kondo dot coupled to normal as well as ferromagnetic electrodes — •Henning Soller and Andreas Komnik — Ruprecht-Karls-Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

We investigate the interplay of the Kondo effect, superconductivity and ferromagnetic correlations in a quantum dot coupled to metallic electrodes. We concentrate on the non-equilibrium transport properties and calculate the full counting statistics of the structure in the different parameter regimes. We take into account the full energy dependence of the superconductor DOS and use an effective model for the quantum dot in the Kondo regime. We achieve good agreement with the experimental data for the non-linear current-voltage relations in the case of a normal as well as a ferromagnetic electrode coupled to the Kondo dot. This allows us to make reliable predictions for the noise and higher order cumulants. All analyzed structures represent basic building blocks of devices for generation and detection of entanglement via crossed Andreev reflection.

TT 47.5 Thu 11:30 HSZ 304

Real time Effective-action approach to the Anderson quantum dot — •Denes Sexty, Thomas Gasenzer, and Jan Pawlowski — ITP Uni Heidelberg, Deutschland

The non-equilibrium time evolution of an Anderson quantum dot coupled between two leads forming a chemical-potential gradient for fermions is investigated. We use Kadanoff-Beym dynamic equations derived from the two-particle irreducible effective action with a non-perturbative resummation of the s-channel bubble chains. The effect of the resummation is shown to be equivalent to the introduction of a frequency dependent 4-point vertex. The tunneling to the leads is taken into account exactly, without further approximations. The method allows the determination of the transient as well as stationary transport through the quantum dot, and results are compared to different schemes (fRG, ISPI, tDMRG and QMC) for different values of the interactions between the fermions.

15 min. break

TT 47.6 Thu 12:00 HSZ 304

Anderson impurity model in nonequilibrium: analytical results versus quantum Monte Carlo data — Lothar Mühlbacher[1], •Daniel F. Urban[1], and Andreas Komnik[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany — [2]Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, D-69120 Heidelberg, Germany

We analyze the spectral function of the single-impurity two-terminal Anderson model at finite voltage using the recently developed diagrammatic quantum Monte Carlo technique as well as perturbation theory. In the (particle-hole-)symmetric case we find an excellent agreement of the numerical data with the perturbative results of second order up to interaction strengths $U/\Gamma \approx 2$, where Γ is the transparency of the impurity-electrode interface. The analytical results are obtained in form of the nonequilibrium self-energy for which we present explicit formulas in the closed form at arbitrary bias voltage. We observe an increase of the spectral density around zero energy brought about by the Kondo effect. Our analysis suggests that a finite applied voltage

V acts as an effective temperature of the system. We conclude that at voltages significantly larger than the equilibrium Kondo temperature there is a complete suppression of the Kondo effect and no resonance splitting can be observed. We confirm this scenario by comparison of the numerical data with the perturbative results.
[1] L. Mühlbacher, D. F. Urban, and A. Komnik, arXiv:1007.1793.

TT 47.7 Thu 12:15 HSZ 304

Correlated current- and spin dynamics in a quantum dot with magnetic impurity — •Daniel Becker, Stephan Weiss, Michael Thorwart, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg

Based on the numerically exact, non-perturbative scheme of iterative summation of path integrals (ISPI)[1,2], the fully correlated dynamics of a single-level quantum dot is studied, which contains a quantum spin-1/2 magnetic impurity, interacting with the dot-electron spins, and is in contact with unpolarized, metallic leads. The main focus lies on the charge current and electron-induced dynamics of the impurity spin. Their dependence on crucial model parameters, such as the on-dot interaction strengths (Coulomb, electron-impurity), the bias voltage, and the temperature is systematically investigated in the non-perturbative regime, where all appearing energy scales are of the same order of magnitude. Due to flip-flop processes between electron- and impurity spins and stochastic tunneling of electrons onto and off the dot, a polarization of the impurity spin decays exponentially, even for vanishing charge current. The current, in turn, is solely affected by the longitudinal part of the electron-impurity interaction, which acts as an effective magnetic field. From the dependence of the impurity relaxation time on the bias voltage, conclusions about the nontrivial energy level structure can be drawn, while the charge current shows a monotonic dependence on the bias voltage.
[1] S. Weiss et al., Phys. Rev. B 77, 195316 (2008)
[2] D. Becker et al., J. Phys.: Conf. Ser. 245 012021 (2010)

TT 47.8 Thu 12:30 HSZ 304

Transport through quantum-dot spin valves with a magnetic impurity — •Björn Sothmann and Jürgen König — Theoretische Physik, Universität Duisburg-Essen

Quantum-dot spin valves, i.e., quantum dots coupled to ferromagnetic electrodes with noncollinear magnetizations exhibit a number of interesting effects. On the one hand, spin accumulates on the dot and blocks further transport. On the other hand, an effective exchange field gives rise to a precession of the accumulated spin thereby lifting the spin blockade [1].

Here, we investigate transport through a quantum-dot spin valve with a side-coupled spin on the dot using a real-time diagrammatic approach. We find that for a large external magnetic field, the current is insensitive to the coherent dynamcis of the two spins on the dot. In contrast, the finite-frequency noise acquires a peak at the precession frequency of the spins. For a small magnetic field, the system exhibits a nontrivial spin dynamics due to the interplay between exchange coupling, external magnetic field and exchange field. We show how this spin dynamics can be studied in the finite-frequency noise.
[1] M. Braun, J. König, J. Martinek, Phys. Rev. B **70**, 195345 (2004).
[2] B. Sothmann, J. König, arXiv:1009.5901, Phys. Rev. B in press.

TT 47.9 Thu 12:45 HSZ 304

Nonequilibrium Zeeman-splitting in quantum transport through nanoscale junctions — •Sebastian Schmitt and Frithjof B. Anders — Theoretische Physik II, Technische Universität Dortmund

We study an interacting quantum dot –modeled by a single impurity Anderson model– coupled to two different leads where a finite bias voltage is applied. The quantum transport through such a device is governed by the charging energy U of the dot. We employ the scattering-states numerical renormalization-group approach to open quantum systems to study nonequilibrium Green functions and current-voltage characteristics of such a junction. At intermediate to large values of U considerable voltage-dependent redistribution of spectral weight occurs. In a finite magnetic field the Zeeman-split Kondo resonance is rapidly destroyed upon increasing the bias voltage. The nonlinear differential conductance of a particle-hole symmetric as well as particle-hole asymmetric quantum dot is studied for various coupling asymmetries. In contrast to maxima derived from charge-excitations of the quantum dot, the position of the Zeeman-split zero-bias anomaly is independent of these asymmetries. Additionally, at large magnetic fields its position can even exceed the value given by the Zeeman-energy. The results are discussed in connection with recent experiments where similar behavior was encountered.

TT 48: CE: Metal-Insulator Transition 2

Time: Thursday 10:30–13:00 Location: HSZ 105

TT 48.1 Thu 10:30 HSZ 105

The x-ray induced Mott-Anderson scenario in organic charge-transfer salts studied by noise spectroscopy — •Robert Rommel[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Goethe-Universität Frankfurt, SFB/TR49, Frankfurt am Main — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic molecular conductors (BEDT-TTF)$_2$X are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. With respect to the amount of disorder, different types of metal-to-insulator transitions (MIT) can occur. We will focus on the bandwidth-controlled Mott transition due to external pressure or chemical substitution and disorder-induced carrier localization caused by x-ray irradiation. We will discuss comparative studies of the clean correlation-driven Mott MIT and the Anderson scenario originating from the randomness in the lattice potential. To extract information about the influence of disorder on the electron dynamics we employ noise/fluctuation spectroscopy. The technique was systematically applied after subsequent doses of x-ray irradation of the pristine superconductor κ-(ET)$_2$-Cu[N(CN)$_2$]Br. We find that the increase of insulating behavior in the resistance is accompanied by the emergence of new energy scales pointing to distinct changes in the dynamic properties of the correlated charge carriers.

TT 48.2 Thu 10:45 HSZ 105

Localization-delocalization transition in the κ-(ET)$_2$X salts: Evidence from fluctuation spectroscopy — •Jens Brandenburg[1], Jens Müller[1], and John A. Schlueter[2] — [1]Johann Wolfgang Goethe-Universität, Frankfurt am Main — [2]Argonne National Laboratory, Argonne, IL, USA

Quasi-2D organic conductors κ-(ET)$_2$X with X = Cu[N(CN)$_2$]Cl, Cu[N(CN)$_2$]Br and Cu(NCS)$_2$ are model systems for low-dimensional metals exhibiting both strong electron-electron and electron-phonon interactions. The interplay of charge, spin, and lattice degrees of freedom lead to a variety of different magnetic-insulating, metallic, and superconducting ground states. The normal-conducting state shows anomalous behavior at a temperature scale $T^* \sim 35 - 50\,\mathrm{K}$ interpreted, e.g., as a crossover from coherent to incoherent transport.
Fluctuation spectroscopy is a new powerful tool to study the intrinsic charge-carrier dynamics in these materials [1,2]. Systematic investigations of four compounds, situated at different positions in the generalized phase diagram, show clear signatures in the temperature dependence of the relative noise amplitude $a_R = S_R \cdot f/R^2$ at T^* depending on the correlation strength characterized by the ratio of bandwidth to on-site Coulomb interaction W/U_{eff}. This indicates a localization-delocalization transition in the interlayer transport on the metallic side of the phase diagram as a function of temperature or electronic correlation strength. Funded by SFB/TR 49
[1] PRB 79 (2009), 214521
[2] PRL 102 (2009), 047004

TT 48.3 Thu 11:00 HSZ 105

Scaling Theory of the Mott Transition and Breakdown of the Grüneisen Scaling Near a Finite-Temperature Critical End Point — •Lorenz Bartosch[1], Mariano de Souza[2], and Michael Lang[2] — [1]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Physikalisches Institut, Goethe-Universitat, 60438 Frankfurt am Main, Germany

We discuss a scaling theory of the lattice response in the vicinity of a finite-temperature critical end point. The thermal expansivity is shown

to be more singular than the specific heat such that the Grüneisen ratio diverges as the critical point is approached, except for its immediate vicinity. More generally, we express the thermal expansivity in terms of a scaling function which we explicitly evaluate for the two-dimensional Ising universality class. Recent thermal expansivity measurements on the layered organic conductor κ-(BEDT-TTF)$_2X$ close to the Mott transition are well described by our theory.

TT 48.4 Thu 11:15 HSZ 105

Interacting electrons in a random potential: Absence of thermodynamic signatures of a metal-insulator transition in two dimensions — •Prabuddha Chakraborty[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135, Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, 00-681, Warszawa, Poland

The properties of a quantum phase transition where a two-dimensional metallic phase arises out of an Anderson insulator as a consequence of short-range electronic interactions are investigated using quantum Monte Carlo simulations. We present results for the compressibility and the antiferromagnetic and uniform susceptibilities. We demonstrate that, in contrast to predictions made using perturbative Renormalization Group calculations, the susceptibilities show no signature of the metal-insulator transition. To explore the nature of the metallic state itself the behaviour of thermodynamic quantities deep in the metallic phase is also explored.

TT 48.5 Thu 11:30 HSZ 105

Metal-insulator transition in 2D disordered bipartite systems — •Elio König[1], Pavel Ostrovsky[2], Ivan Protopopov[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 predict the novel type of metal-insulator transition in 2D disordered systems with a bipartite structure. This in particular applies to graphene with vacancies and/or ripples and to topological insulators of unconventional symmetry. We use the σ-model description of these disordered systems and identify specific vortex-like excitations giving rise to the Berezinsky-Kosterlitz-Thouless-type transition. This results in appearence of the minimal metallic conductivity and insulating phase at sufficiently strong disorder. Our results are in agreement with available numerical simulations and motivate further theoretical and experimental studies of exotic disordered systems.

15 min. break

TT 48.6 Thu 12:00 HSZ 105

Effective spin Hamiltonian for the spin liquid of the Hubbard model on the honeycomb lattice — •Hong-Yu Yang[1], Andreas Läuchli[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany — [2]MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany

Motivated by the spin liquid phase unveiled by quantum Monte Carlo simulations of the Hubbard model on the honeycomb lattice at intermediate values of U, we derive the effective spin-only model from the strong-coupling limit using continuous unitary transformations (CUTs). It turns out that the spin liquid phase is located in the non-perturbative regime. We therefore apply a recently developped non-perturbative extension of CUTs named graph-based CUT (gCUTs) in order to obtain a pure spin model as effective Hamiltonian for the intermediate U regime. We use exact diagonalizations to check the validity of the effective spin model by comparing its low-energy properties to the one of the Hubbard model on small clusters. Surprisingly, we find that besides a frustrating next-nearest neighbor two-spin exchange a family of six-spin interactions are the dominant corrections to the nearest-neighbor Heisenberg model.

TT 48.7 Thu 12:15 HSZ 105

Orbital selective phase transitions observed in dynamical cluster approximation calculations — Hunpyo Lee[1], Yu-Zhong Zhang[2], •Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Department of Physics, Tongji University, Shanghai 200092, PR China

We study a two-orbital Hubbard model with unequal bandwidths on the square lattice using the dynamical cluster approximation (DCA) based on the hybridization expansion continuous-time quantum Monte Carlo method. In the case of four site clusters, the competition between Slater and Mott physics leads to orbital selective phases for intermediate values of the interaction strength. We also investigate a two-orbital Hubbard model with equal bandwidths where we allow one orbital to have an antiferromagnetic solution (AF orbital) while we constrain the other orbital to be paramagnetic (PM orbital). We find an interesting phase diagram with orbital selective phases that are caused by the different magnetic states in the two orbitals: As function of the interaction strength, the PM orbital undergoes a transition from a Fermi liquid to a Mott insulator through an intermediate non-Fermi liquid phase while the AF orbital shows a transition from a Fermi liquid to an antiferromagnetic insulator through an intermediate antiferromagnetic metallic phase.

TT 48.8 Thu 12:30 HSZ 105

Giant Chemical Shifts of the Sulphur 2*s*-Line Close to the Glass-Like Transition of CT Salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br- a Hard X-ray Photoemission Study — •G. Schönhense[1], M. de Souza[2], K. Medjanik[1], A. Gloskovskii[3], H.J. Elmers[1], J. Müller[2], and M. Lang[2] — [1]Institut für Physik, J. Gutenberg Univ. Mainz — [2]Institut für Physik, J. Wolfgang von Goethe Universität Frankfurt — [3]Institut für Anorganische und Analytische Chemie, J. Gutenberg Univ. Mainz

The organic (super-)conductors of the κ-(ET)$_2$-X family are characterized by a strongly-correlated π - electron system with close proximity of superconductivity and antiferromagnetic insulating states and a half-filled quasi-2D metallic conduction band. HAXPES was performed at beamline P09 of PETRA III [1]. In the regions of $T^* \sim 45$ K (anomalous metallic state) and $T_g \sim$77K (thermal glass-like transition), the S 2s core level spectrum changes dramatically in warming-up series: around T^*, the main-line intensity drops to 80 % of its initial value and a high-binding-energy shoulder arises. When approaching T_g, it further drops to 40 % and several new peaks appear, being strongly shifted by up to more than 10eV. Above the glass-transition, all satellites disappear instantaneously and the main line intensity jumps back to its initial value. This gives further evidence for changes in the electronic degrees of freedom at the T^* transition and indicates that the latter may be involved in the glass-like transition, as was already speculated in literature.
Funded by DFG/TR49, Graduate School of Excellence MAINZ, and COMATT.
[1] A.Gloskovskii et al., this conference;

TT 48.9 Thu 12:45 HSZ 105

Long range order effects in the Mott-Hubbard transition and the variational lattice approach — •Aljoscha Wilhelm[1], Christoph Jung[1], Hartmut Hafermann[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9 — [2]Centre de Physique Théorique (CPHT), École Polytechnique, 91128 Palaiseau Cedex, France

We introduce an efficient strategy to treat long ranged correlations in fermionic lattices, the so called variational lattice approach (VLA). The VLA combines the recently developed dual fermion approach for k-dependent problems and the exact diagonalization technique. We present first benchmark results. The phase diagram of the half-filled paramagnetic Mott-Hubbard transition is discussed and compared results to CDMFT and DCA calculations.

TT 49: CE: Spin Systems and Itinerant Magnets 2

Time: Thursday 14:00–18:45 Location: HSZ 03

TT 49.1 Thu 14:00 HSZ 03

Theory of disordered stripes in hole-doped $La_{2-x}Sr_xCoO_4$ — •Matthias Vojta — Technische Universität Dresden, Germany

The compounds $La_{2-x}Sr_xCoO_4$ are isostructural to the 214 family of cuprate superconductors, but remain insulating over a wide doping range. Recently, the x=1/3 compound was found to display a peculiar type of magnetism, with short-ranged static antiferromagnetic order and an hour-glass-like excitation spectrum, not unlike some cuprates. We argue that a scenario of disordered charge stripes, formed by Co^{2+} and Co^{3+} ions, is consistent with the experimental data. In particular, we calculate the magnetic excitation spectrum in the disordered charge background and discuss possible origins of the stripe disorder.

TT 49.2 Thu 14:15 HSZ 03

Vacancies in non-collinear antiferromagnets — •Alexander Wollny[1], Lars Fritz[1], and Matthias Vojta[2] — [1]Institut für theoretische Physik, Universität zu Köln, 50937 Köln — [2]Institut für theoretische Physik, Technische Universität Dresden, 01062 Dresden

We study a single vacancy in the 2D quantum Heisenberg antiferromagnet on the triangular lattice.

We observe that the classical 120 degree ordered state is distorted in the vicinity of the vacancy. We determine that the deviation from the bulk ordered state decays as $1/r^3$ also upon inclusion of quantum corrections controlled in 1/S. The distortion and the $1/r^3$-decay can be understood as the response to a local transversal field generated by the vacancy.

We use both spin wave and Monte Carlo methods to determine the impurity contribution to the uniform susceptibility at zero and finite temperatures respectively.

TT 49.3 Thu 14:30 HSZ 03

Spin dephasing through a nuclear spin bath — •Jasmin V. Jäger, Fabian Güttge, and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

In semiconducting quantum dots the electron spin coherence time is limited due to interactions of the confined electron with its environment. The most relevant decoherence mechanism in such devices is the interaction between the nuclear spins and the central electronic spin. We focus on the time-evolution of a single electron spin interacting with a bath of nuclear spins via the hyperfine interaction. Initially, the nuclear spins are unpolarized and couple to the central spin with a random distribution of hyperfine coupling constants. This central spin model has been solved exactly for a few bath spins by using the exact diagonalization method. By solving equations of motion numerically, we compute the time evolution of the electron spin interacting with a bath of nuclear spins. Because of many-particle correlations the exact equations have to be replaced by approximated equations using a cluster expansion method. In this work, we investigate the quality of the approximation by comparing the results of both methods.

TT 49.4 Thu 14:45 HSZ 03

Valence Bond Crystal on the Hyperkagome Antiferromagnet — •Emil Bergholtz, Andreas Läuchli, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

We describe our recent work that indicates that the ground state of the antiferromagnetic spin-1/2 Heisenberg model on the highly frustrated, three-dimensional, hyperkagome lattice is a valence bond crystal (VBC) [1]. Performing a series expansion around an arbitrary dimer covering on the hyperkagome we find that a ground state with a huge (72 site) unit cell is selected by the quantum fluctuations. The regularity and favorable energetics of our series expansion establishes the VBC as a serious contender to the earlier spin liquid proposals. We find that the ground state supports many, very low lying, excitations in the singlet sector and that the low energy spinful excitations (spinons and triplons) are effectively confined to various emergent lower-dimensional structures. If applicable to the recently studied sodium iridate compound, $Na_4Ir_3O_8$, this scenario has interesting observable implications, such as spatially anisotropic neutron scattering spectra and possibly multiple finite temperature signatures in the magnetic specific heat due to a multi-step breaking of discrete symmetries. Most saliently, here—as for several proposed states for analogous kagome and pyrochlore magnets—one might expect a clearly resolved Ising transition at relatively high temperature.

[1] E.J. Bergholtz, A.M. Läuchli and R. Moessner, Phys. Rev. Lett., in press (2010) [arXiv:1010.1345]

TT 49.5 Thu 15:00 HSZ 03

Numerical studies of the metallic and insulating phases of a spinless fermion model on a kagome lattice — Aroon O'Brien[1], Frank Pollmann[1], •Satoshi Nishimoto[2], Masaaki Nakamura[3], and Peter Fulde[1,4] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, 01187 Dresden, Germany — [2]IFW Dresden, Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [3]Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan — [4]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Geometrically frustrated models exhibit many fascinating physical properties such as highly degenerate ground states and even the possible existence of fractionally charged excitations. Both phenomena are consequences of the frustrated electronic interactions.

We present a model of spinless fermions on the 2D kagome lattice. In this model a metal-insulator transition occurs as nearest-neighbour interactions are tuned into the strongly correlated regime. We consider the nature of the transition for positive and negative hopping matrix elements; differences between the two cases are attributable to the form of the band structure.

In the insulating phase fractionally charged excitations occur at certain filling factors. An investigation of the dynamical properties of the fractional charges is discussed. Particular focus is given to signatures of the confined collective excitations as observed in numerically calculated spectral densities.

TT 49.6 Thu 15:15 HSZ 03

Thermodynamics of quantum magnets at large S — •Andreas Honecker[1], Mike Zhitomirsky[2], Johannes Richter[3], and Moritz Härtel[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Commissariat à l'Energie Atomique, DSM/INAC/SPSMS, Grenoble, France — [3]Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany

Experiments demand efficient methods to compute thermodynamic properties of quantum magnets in arbitrary dimensions and with arbitrary interaction geometries as well as spin quantum numbers S at moderate to high temperatures. Using the example of the square lattice, we start by generating reference data for $S \leq 5/2$ by Quantum Monte Carlo simulations and for $S = \infty$ by classical Monte Carlo simulations. Next, we perform a phenomenological scaling analysis with spin quantum number S. We then explore other, mainly semiclassical methods, which avoid expensive numerical simulations. The methods investigated include linearized spin-wave theory, equations of motion for the Green functions, and a Monte-Carlo evaluation of a cumulant expansion in a spin-coherent-states representation. We compare advantages and shortcomings of the different methods.

15 min. break

TT 49.7 Thu 15:45 HSZ 03

Series Expansion Analysis of a Four-Spin Tube — Marcelo Arlego[1] and •Wolfram Brenig[2] — [1]Departamento de Física, Universidad Nacional de La Plata, 1900 La Plata, Argentina — [2]Institute for Theoretical Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany

We analyze a four-legged anisotropic triangular spin ladder with transverse periodic boundary conditions leading to a frustrated four-spin tube. In the limit of strong rung coupling, and starting from decoupled four-spin plaquettes, we study the zero temperature properties of this quantum spin model, using a series expansion based on the flow equation method. Results will be reported for the ground state energy, as well as for the dispersion of the one- and the two-particle excitations. The effective two-particle interactions will be analyzed and are shown to induce several types of (anti)bound states. In sharp contrast to conventional spin ladders, the renormalized plaquette regime of the four-spin tube is unstable to quantum-phase transitions at finite

leg couplings. These are reported to be of first order and their critical lines will be determined using the density-matrix renormalization group.

TT 49.8 Thu 16:00 HSZ 03

Coherent spin-current oscillations in transverse magnetic fields — •Robin Steinigeweg[1], Stephan Langer[2], Fabian Heidrich-Meisner[2], Ian P. McCulloch[3], and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Department of Physics, Ludwig-Maximilians-Universitaet Muenchen, D-80333 Muenchen, Germany — [3]School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072, Australia

This work addresses coherence properties in the dynamics of spin-currents with components transverse to an externally applied magnetic field for the spin-1/2 Heisenberg chain. We study two cases, first, the linear-response regime at finite temperatures, and second, the real-time dynamics of spin currents during the evolution from initial states with an inhomogeneous transverse magnetization. Apart from a coherent oscillation at the Larmor frequency linked to the integrability of the model we find a second nontrivial collective oscillation at higher frequencies, emerging at low temperatures. We clarify that this oscillation is a many-magnon effect and also becomes coherent at lower temperatures. The collective oscillation frequency and life-time is investigated as a function of temperature and magnetic field, with a satisfying agreement between the two approaches employed.

TT 49.9 Thu 16:15 HSZ 03

Entanglement Spectra and Entanglement Hamiltonians for quantum spin chains — •Ronny Thomale[1], Stephan Rachel[2], Daniel P. Arovas[3], and B. Andrei Bernevig[1] — [1]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [3]Department of Physics, University of California at San Diego, La Jolla, California 92093, USA

We give a complete definition of the entanglement gap separating low-energy, CFT levels, from high-energy, generic ones, in the "entanglement spectrum" in the momentum cut of gapless quantum spin chains. The approach allows to study the dimerization transition, bulk excitation state counting, and the manifestation of logarithmic CFT corrections purely from the ground state wave function. It provides a new formulation of non-local order in quantum spin chains.

From a different angle, we address the question of how to define Hermitian operators which would serve as entanglement Hamiltonians for spin chains and discuss correspondences and differences between energy and entanglement spectra.

TT 49.10 Thu 16:30 HSZ 03

Derivation of effective microscopic models for the frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 from first principles — •Kateryna Foyevtsova, Ingo Opahle, Yu-Zhong Zhang, Harald O. Jeschke, and Roser Valentì — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

We report on the density functional theory (DFT) investigations of the frustrated triangular-lattice antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4, which in particular focus on derivation of effective models for the two compounds. The drastic disagreement between the Heisenberg model that we derived for Cs_2CuCl_4 using its X-ray structural data and the experimentally established model motivated us to perform a detailed study of the crystal structure optimization effects on the exchange couplings with a number of exchange-correlation functionals for Cs_2CuCl_4 as well as for Cs_2CuBr_4. We find that, in order to obtain results that are consistent with experiment, one has to consider during the optimization an insulating state, appearing only with a spin-polarized exchange-correlation functional, and electronic correlations (within the LDA+U approach). We will in addition discuss the effect of interlayer couplings as well as longer-ranged couplings in both systems.

As the mixed $Cs_2CuCl_{4-x}Br_x$ ($0 < x < 4$) systems have been gaining a lot of attention recently, we also present some DFT insights on the distribution of either of the halide atoms at various mixing factors.

TT 49.11 Thu 16:45 HSZ 03

Magnetic and structural properties of AFe_4X_2 (A = Y, Sc, Lu, and Zr; X = Ge and Si) — •Nandang Mufti[1], Til Dellmann[2], Philipp Materne[2], Hans H. Klauss[2], Graeme Blake[3], Thomas T. M. Palstra[3], and Christoph Geibel[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

The compound RFe_4Ge_2 (R = Dy, Ho, Er, Y) have been reported to crystallize with the tetragonal $ZrFe_4Si_2$ structure type and to show interesting magnetic properties. In YFe_4Ge_2, antiferromagnetic ordering with small ordered moment $\sim 0.63\ \mu_B$ occurs simultaneously with a large (2.5 %) first order structural distortion from tetragonal to orthorhombic at 43.5 K. The presence of a large structural distortion despite a weak antiferromagnetic ordering with low T_N and small moments is reminiscent of observations in Fe-arsenides. Here, we will present magnetic and structural properties of AFe_4X_2 (A = Y, Sc, Lu and Zr; X = Ge and Si) based on magnetic susceptibility, specific heat, resistivity and low temperature X-ray diffractometer measurements. Our results indicate the occurrence of a transition in all compounds at critical temperatures between 30 K and 75 K depending on the compounds. There is no systematic relationship between T_N and and the lattice parameters of AFe_4X_2. However, magnetic order and structural distortion seems generally to be connected. The relation between structural, electronic, and magnetic properties will be discussed.

TT 49.12 Thu 17:00 HSZ 03

Mössbauer Spectroscopic Study of Spin and Orbital Order in $FeCr_2S_4$ — •Josefin Engelke[1], Jochen Litterst[1], Alexander Krimmel[2], Alois Loidl[2], Friedrich Wagner[3], Michael Kalvius[3], and Vladimir Tsurkan[2,4] — [1]IPKM TU Braunschweig, Germany, e-mail: j.engelke@tu-bs.de — [2]Experimentalphysik V, Universität Augsburg, Germany, e-mail: alois.loidl@physik.uni-augsburg.de — [3]Physics-Department TU München, Germany, e-mail:kalvius@ph.tum.de — [4]Inst. Applied Physics, Acad. Sciences Moldava, Republic of Moldava

The spinel $FeCr_2S_4$ has been studied intensely in the past for its peculiar magnetic and local structural changes, which are sensitively influenced by the Jahn- Teller properties of Fe^{2+} in tetrahedral sulphur coordination. Recent muon spin rotation data [1] give strong evidence that the collinear ferrimagnetism found below $T_C = 165\ K$ changes to an incommensurate structure below 50 K. Recent high resolution X-ray studies reveal a broadening of Bragg peaks below 50 K and a maximum of mean square displacement around 15 K [2]. Below 10 K orbital order is concluded from specific heat data [2].

We present Mössbauer spectroscopic data taken on the same samples as used in [1, 2]. The influence on spectral shape by changing Jahn-Teller dynamics will be discussed. Special emphasis is placed on the interpretation of the spectra close to the magnetic and orbital transitions.

[1] G. M. Kalvius et al., J. Phys.: Condens. Matter 22, 052205 (2010)
[2] V. Tsurkan et al., Phys. Rev. B81, 184486 (2010)

15 min. break

TT 49.13 Thu 17:30 HSZ 03

Exchange driven phonon splitting in transition-metal monoxides — •Christian Kant[1], Franz Mayr[2], Joachim Deisenhofer[2], and Alois Loidl[2] — [1]TU Wien, Wien, Österreich — [2]Center for Electronic Correlations, Universität Augsburg, Augsburg, Deutschland

The interplay of magnetism and the underlying crystal lattice is a topical issue of condensed-matter physics. It can relieve frustration in the magnetic sector via a spin-driven Jahn-Teller effect in frustrated lattices, leads to novel excitations such as electromagnons in multiferroics, and bears the potential for future applications via magnetodielectric effects. A conceptual understanding of the coupling of spins and phonons is, however, often hampered by the complexity of the interactions. For transition-metal monoxides, which are model systems to study the effects of electronic correlations, a magnetism-induced anisotropy in the lattice response was predicted theoretically. We report optical evidence for a linear dependence of the phonon splitting on the nearest-neighbour exchange coupling in the monoxides MnO, $Fe_{0.92}O$, CoO and NiO. Our results directly confirm the seminal theoretical prediction of a purely exchange induced splitting of the zone-centre optical phonon and pave a new path for the understanding of spin-phonon coupling effects.

TT 49.14 Thu 17:45 HSZ 03

Bose-Einstein Condensation in the Han purple compound:

a high field NMR study — •Steffen Krämer[1], Mladen Horvatic[1], Claude Berthier[1], Raivo Stern[2], and Tsuyoshi Kimura[3] — [1]Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble, France. — [2]NICPB, Tallinn, Estonia. — [3]Osaka University, Osaka, Japan.

The quasi-2D, antiferromagnetic exchange coupled spin-1/2 dimer compound $BaCuSi_2O_6$ (Han purple) is considered as a prototype of the magnetic field induced Bose-Einstein Condensation (BEC) of triplet excitations on a lattice. Recently, $BaCuSi_2O_6$ has been claimed to exhibit an unusual reduction of dimensionality of the BEC from 3D to 2D when lowering the temperature, induced by frustration between adjacent planes. However, due to a structural transformation at 90 K, different intradimer exchange couplings and different gaps ($\Delta_B/\Delta_A = 1.16$) exist in every second plane along the c axis. First Nuclear Magnetic Resonance (NMR) experiments have shown that this leads to a population of bosons in the B planes, n_B, much smaller than in A planes in the field range $\Delta_A/g\mu_B < H < \Delta_B/g\mu_B$ where $n_B = 0$ is expected in a model of uncoupled planes. More recently, a better model has been presented, which takes into account both frustration and quantum fluctuations. This leads to a non-zero population n_B of uncondensed bosons in the B plane, increasing quadratically with $(H - H_{c1})$, as compared to the linear dependence of n_A. In our contribution we compare our new NMR results, obtained at high magnetic fields (23-27 T) and low temperatures (50 mK), to these models.

TT 49.15 Thu 18:00 HSZ 03

Vibrating coil magnetometry of the spin ice state in $Ho_2Ti_2O_7$ — •C. Krey[1], S. Legl[1], S. R. Dunsiger[1], C. Pfleiderer[1], J. S. Gardner[2], and J. Roper[3] — [1]Physik Department E21, Technische Universität München, Germany — [2]NIST, Center for Neutron Research, Gaithersburg, Maryland, USA — [3]Los Alamos National Laboratory, Los Alamos, USA

The 'spin ice' model highlights the strong analogy between spin ordering in Ising magnets and proton ordering in ice. Recently, it has been proposed that the excitations may be described in terms of magnetic point defects or emergent magnetic monopoles [1]. The cubic pyrochlore systems $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ are excellent experimental realizations of spin ice, where the local $\langle 111 \rangle$ Ising anisotropy of the rare earth sites in combination with net ferromagnetic interactions give rise to a highly degenerate ground state. The similarities with water ice are the observation of a first order transition terminating in a critical point in the magnetization of $Dy_2Ti_2O_7$ for applied magnetic fields along the global $\langle 111 \rangle$ direction. We report a comprehensive study of the magnetization at mK temperatures of $Ho_2Ti_2O_7$ by means of a vibrating coil magnetometer [2]. We observe considerable qualitative similarities with $Dy_2Ti_2O_7$ but also distinct differences. We consider the role of strong hyperfine interactions associated with Ho compounds.

[1] Ryzhkin, J Exp and Theor Physics 101, 481 (2005), Castelnovo et al., Nature 451, 42 (2008)
[2] Legl et al., Rev. Sci. Instrum. 81, 043911 (2010)

TT 49.16 Thu 18:15 HSZ 03

Probing the local magnetic structure of a quasi-1D cuprate with Resonant Inelastic X-Ray Scattering — Claude Monney[1], Valentina Bisogni[2], Kejin Zhou[1], Roberto Kraus[2], Vladimir Strocov[1], Jochen Geck[2], and •Thorsten Schmitt[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]IFW, Dresden, Germany

The quasi-one-dimensional cuprate Li_2CuO_2 is a prototype edge-sharing chain compound. The Cu^{2+} ions in this strongly correlated material give rise to one spin 1/2 per CuO_4 plaquette with a nearest neighbor Cu-O-Cu bond angle close to 90° implying weak superexchange between Cu spins. As a result, spins order antiferromagnetically between the chains below $T_N \sim 9$K, but ferromagnetically in the chains. We have performed Resonant Inelastic X-ray Scattering (RIXS) at Cu L_3 and O K-resonances at the ADRESS beamline of the Swiss Light Source on this compound. Our momentum resolved RIXS measurements at the Cu L_3-edge allow analyzing orbital excitations with high sensitivity. At the O K-edge, the RIXS spectra display a complicated interplay of low-energy excitations from charge, orbital and lattice degrees of freedom. In particular, we discuss charge transfer related spectral components in the scenario of exotic Zhang-Rice (ZR) singlet and triplet excitations which can be reached in the final state with O K-edge RIXS. The intensity of the ZR features can be related to the thermodynamics of domain walls in one dimension. This establishes RIXS as an excellent probe for investigating local magnetic order.

TT 49.17 Thu 18:30 HSZ 03

The effect of interchain coupling on multipolar phases in quasi-1d quantum helimagnets — •S. Nishimoto[1], S.-L Drechsler[1], R.O. Kuzian[1], J. Richter[2], and J. van den Brink[1] — [1]IFW Dresden, Germany — [2]Universität Magdeburg, Germany

Coupled frustrated spin-1/2 chains in high magnetic fields described within the ferro- antiferromagnetic J_1-J_2 Heisenberg model are studied by DMRG, hard core boson, and spin wave theory approaches. Multipolar phases related to magnon bound states are destroyed (supported) by weak antiferromagnetic (ferromagnetic) interchain couplings J_{ic}. We show that quantum spin nematics might be found for $LiVCuO_4$ whereas for $Li(Na)Cu_2O_2$ it is prevented by a sizeable antiferromagnetic J_{ic}. Also for Li_2ZrCuO_4 with a small antiferromagnetic J_{ic} expected triatic or quartic phases are unlikely, too. The saturation field is found to be strongly affected even by a relatively small J_{ic}.

[1] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. Richter, and J. van den Brink, arXiv:1005.5500v2.
[2] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. van den Brink, J. Richter, W.E.A. Lorenz, Y. Skourski, R. Klingeler, B. Büchner, arXiv:1004.3300v2.
[3] S.-L. Drechsler, S. Nishimoto, R.O. Kuzian, J. Malek, W.E.A. Lorenz, J. Richter, J. van den Brink, M. Schmitt, H. Rosner, arXiv:1006.5070v2.

TT 50: SC: Tunneling, Josephson Junctions, SQUIDs 2

Time: Thursday 14:00–15:15 Location: HSZ 301

TT 50.1 Thu 14:00 HSZ 301

Probing the superconducting state of $CeCoIn_5$ by quantum interferometry — •Oleksandr Foyevtsov, Fabrizio Porrati, and Michael Huth — Johann Wolfgang Goethe University, Frankfurt am Main, Germany

Josephson junction based structures provide a pathway to investigation of the superconducting state of unconventional superconductors. A superconducting quantum interference device (SQUID) structure was fabricated on micro-crystals of the heavy-fermion superconductor $CeCoIn_5$. Photo-lithography and ion beam milling/induced deposition were used to prepare the structure on a thin film of $CeCoIn_5$ grown via molecular beam epitaxy. The interferometer was characterized with regard to the SQUID properties. The unconventional nature of superconducting state in $CeCoIn_5$, the implications of the normal-state electronic properties, as well as the weak-link characteristics of the SQUID structure itself lead to a wealth of different features in the I(V) and dI/dV(V) characteristics.

TT 50.2 Thu 14:15 HSZ 301

Magnetic field sensors based on growth modified bi-crystal grain boundaries — •Peter Michalowski, Christian Katzer, Daniel Kuhwald, Matthias Schmidt, Veit Grosse, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

During the pulsed laser deposition of $YBa_2Cu_3O_{7-\delta}$ (YBCO) gold nano clusters forming from an intermediate gold layer can modify the growth and crystalline structure of the YBCO film [1]. In a similar way also the properties of grain boundaries of films grown on bi-crystal substrates can be modified by gold nano clusters. As a result Josephson junctions fabricated from these films typically show changes in their superconducting properties, especially in the critical current I_C, normal state resistance R_N and the $I_C R_N$ product.

Based on the experimental results of simple dc-Superconducting QUantum Interference Device (SQUID) structures with and without crystalline gold clusters we produced and analysed dc-SQUID gradiometers.

We present results of the temperature dependence of the critical current, the SQUID modulation (transfer function) depending on bias current and temperature as well as the London penetration depth as a function of temperature.
[1] Grosse, V. et al. (2010), Formation of gold nano-particles during pulsed laser deposition of $YBa_2Cu_3O_{7-\delta}$ thin films. Phys. Status solidi (RRL) - Rapid Research Letters, 4: 97-99.

TT 50.3 Thu 14:30 HSZ 301

Systematic investigation of the current injection effect in $Bi_2Sr_2CaCu_2O_{8+\delta}$ — •S. Probst, X. Y. Jin, Y. Simsek, C. Steiner, and P. Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

By current injection we can change the properties of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals electronically in a wide range [1]. In order to investigate the doping process in greater detail, we have performed automated current injection experiments in very small bias current/voltage steps. By measuring the IV characteristics as well as doping current and doping voltage simultaneously, the change of superconducting properties is monitored. We were able to determine precisely the threshold-bias region where doping starts. We will discuss the observed phenomena and give an estimate for the depth of trap levels, which is crucial to understand the doping process.
[1] Y. Koval, X. Y. Jin, C. Bergmann, Y. Simsek, L. Ozyuzer, P. Müller, H. B. Wang, G. Behr, B. Büchner, Appl. Phys. Lett. **96**, 082507 (2010).

TT 50.4 Thu 14:45 HSZ 301

Superconductivity induced by current injection into non-superconducting $Bi_2Sr_2CaCu_2O_8$ — •Y. Simsek, Y. Koval, X. Y. Jin, S. Probst, and P. Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

We already have shown that we can change the carrier concentration of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals by current injection along the c-axis [1]. In this work, we focus on the interesting question: Can we induce superconductivity in non-superconducting $Bi_2Sr_2CaCu_2O_8$ merely by current injection? We report on current-injection experiments of fully oxygen depleted $Bi_2Sr_2CaCu_2O_8$ in which superconductivity was not observed down to 4.2 K. In order to eliminate the contact resistance of the highly resistive depleted material, we have fabricated double cross-bar crystal stacks. We have increased the c-axis conductivity by carrier injection until superconductivity above 4.2 K was observed. Doping the sample further by current injection, optimum-doped and even overdoped states were obtained. The current injection effect was persistent up to annealing temperatures of approximately 270 K.
[1] Y. Koval, X.Y. Jin, C. Bergmann, Y. Simsek, L. Ozyuzer, P. Müller, H. B. Wang, G. Behr, B. Büchner, Appl. Phys. Lett. **96**, 082507, 2010.

TT 50.5 Thu 15:00 HSZ 301

The tunnel barrier of intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_{8+\delta}$ after doping by current injection — •X. Y. Jin, S. Probst, Y. Simsek, C. Steiner, Y. Koval, and P. Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

Superconductivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals can be tuned electronically in a wide range by current injection along the c-axis [1]. We investigate the change of superconducting properties after current injection by performing macroscopic quantum tunneling experiments of intrinsic Josephson junctions. An exponential increase of critical current density j_c with increase of hole concentration was observed. At the same time, microwave spectroscopy has shown that the junction capacitance per unit area increased by a factor of 5. Both experiments indicate that the tunnel barrier of intrinsic Josephson junction was significantly modified by the increase of the doping level.
[1] Y. Koval, X. Y. Jin, C. Bergmann, Y. Simsek, L. Ozyuzer, P. Müller, H. B. Wang, G. Behr, B. Büchner, Appl. Phys. Lett. **96**, 082507 (2010).

TT 51: TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2

Time: Thursday 14:00–15:30 Location: HSZ 304

TT 51.1 Thu 14:00 HSZ 304

Correlation of quantum transport and tip-enhanced Raman spectroscopy on carbon nanotubes — •Karin Goss[1], Niculina Peica[2], Sebastian Smerat[3], Martin Leijnse[4], Maarten R. Wegewijs[1,5], Christian Thomsen[2], Janina Maultzsch[2], Claus M. Schneider[1], and Carola Meyer[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich & JARA Jülich Aachen Research Alliance, Jülich, Germany — [2]Institut für Festkörperphysik, TU Berlin, Germany — [3]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, LMU München, Germany — [4]Niels Bohr Institute & Nano-Science Center, University of Copenhagen, Denmark — [5]Institut für Theoretische Physik A, RWTH Aachen, Germany

Carbon nanotube (CNT) ropes offer a generic system to study the interactions of molecules with their environment. We show quantum transport spectra of a contacted rope, which consists of several CNT strands forming parallel quantum dots at low temperature. From their distinct interaction properties, we count at least five parallel dots. In order to attribute these to the different strands within the rope, it is characterized using tip-enhanced Raman spectroscopy. This method offers both an increased spatial resolution and a high signal enhancement. From the diameter dependent Raman modes in combination with a tentative chiral assignment, we identify several CNTs with different diameters and electronic properties. This correlation of transport with Raman spectroscopy illustrates a useful principle for molecular electronics, where an understanding of strong perturbations by environmental effects is required for the interpretation of transport data.

TT 51.2 Thu 14:15 HSZ 304

Spin current polarization due to spin orbit interaction in carbon nanotubes — •Miriam del Valle, Magdalena Margańska, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, Germany

Finite carbon nanotubes placed in a magnetic field parallel to their axes develop localized states and an associated suppression of current. The current is completely blocked for magnetic fields beyond a certain value which depends on the length and chirality of the tube. We will focus on the interplay of this blocking mechanism with the spin orbit interaction and the Zeeman effect. We observe in particular reversible spin polarization of the current, controlled by the bias applied to the tube. The analytical results are supported by numerical simulations for different lengths and chiralities.

TT 51.3 Thu 14:30 HSZ 304

Magnetic field-induced localization in carbon nanotubes — •Magdalena Marganska, Miriam del Valle, Sung Ho Jhang, Christoph Strunk, and Milena Grifoni — University of Regensburg, Regensburg, Germany

The electronic spectra of long carbon nanotubes (CNTs) can, to a very good approximation, be obtained using the dispersion relation of graphene with both angular and axial periodic boundary conditions. In short CNTs one must account for the presence of open ends, which in some CNTs may give rise to states localized at the edges. We show that when a magnetic field is applied parallel to the tube axis, it modifies both momentum quantization conditions, causing hitherto extended states to localize near the ends. The localization is gradual and at low magnetic fields the involved states are still extended. This effect occurs in nanotubes of any size and chirality except armchair. We derive our results using the tight-binding model including the nanotube curvature.

TT 51.4 Thu 14:45 HSZ 304

Pseudo-spin-dependent scattering in carbon nanotubes — •Leonhard Mayrhofer[1] and Dario Bercioux[2,3] — [1]Fraunhofer IWM, Wöhlerstrasse 11, D-79108 Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [3]Physikalisches Institut, Albert-Ludwigs- Universität, D-79104 Freiburg, Germany

We investigate the electronic scattering properties of defected armchair single-walled carbon nanotubes with analytical and numerical methods [1]. By analyzing the local density of states and its Fourier transform we show that electron scattering at defects in carbon nanotubes is strongly affected by the pseudo-spin of the electrons. Depending on the defect symmetry pseudo-spin is conserved or not. In addition, the investigation reveals that the lattice reconstruction of the energetically favored 5-8-5 di-vacancy defects, breaking particle-hole symmetry, is responsible for the pseudo-spin selection rules observed in the experiments by Ouyang *et al.* [2]. Comparison with other experiments is also reported [3,4].

[1] L. Mayrhofer and D. Bercioux, arXiv:1009.4839.
[2] M. Ouyang *et al.*, Phys. Rev. Lett. **88**, 066804 (2002).
[3] J. Lee *et al.*, Phys Rev Lett. **93**, 166403 (2004).
[4] G. Buchs *et al.*, Phys. Rev. Lett. **102**, 245505 (2009).

TT 51.5 Thu 15:00 HSZ 304

Defect-Induced Electron Scattering in Single-Walled Carbon Nanotubes — •Dario Bercioux[1,2], Gilles Buchs[3], Hermann Grabert[1,2], and Oliver Groening[4] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universitat, D-79104 Freiburg, Germany — [3]Kavli Institute of Nanoscience, TU-Delft, P.O. Box 5046, 2600 GA Delft, The Netherlands — [4]EMPA Swiss Federal Laboratories for Materials Testing and Research, nanotech@surfaces, Feuerwerkerstr. 39, CH-3602 Thun, Switzerland

We present a detailed comparison between theoretical predictions on electron scattering processes in metallic single-walled carbon nanotubes with defects and experimental data obtained by scanning tunneling spectroscopy of Ar^+ irradiated nanotubes [1,2]. To this purpose we first develop a formalism for studying quantum transport properties of defected nanotubes in presence of source and drain contacts and an STM tip. The formalism is based on a field theoretical approach describing low-energy electrons. We account for the lack of translational invariance induced by defects within the so called extended $\mathbf{k}\cdot\mathbf{p}$ approximation. The theoretical model reproduces the features of the particle-in-a-box-like states observed experimentally. Further, the comparison between theoretical and experimental Fourier-transformed local density of state maps yields clear signatures for inter- and intra-valley electron scattering processes depending on the tube chirality.

[1] D. Bercioux *et al.*, arXiv:1011.1423.
[2] G. Buchs *et al.*, Phys. Rev. Lett. **102**, 245505 (2009).

TT 51.6 Thu 15:15 HSZ 304

Multi-level carbon nanotube quantum dots: reservoir-coupling induced renormalization effects — •Stephan Grap[1], Sabine Andergassen[1], Volker Meden[1], Kasper Grove-Rasmussen[2], Jens Paaske[2], Karsten Flensberg[2], Henrik Jørgensen[2], Poul Lindelof[2], Koji Muraki[3], and Toshimasa Fujisawa[4] — [1]RWTH Aachen and JARA-Fundamentals of Future Information Technology, Germany — [2]Niels Bohr Institute, Copenhagen, Denmark — [3]NTT Basic Research Laboratories, Japan — [4]Tokyo Insitute of Technology, Japan

In carbon nanotube dots the fourfold level degeneracy with respect to the spin and valley index K, K' is lifted by intervalley coupling, resulting from disorder, the confining potential, spin-orbit interactions due to the tube curvature, or a magnetic field. In the basis of single-particle eigenstates of the isolated dot the inner four levels lead to pairs of strongly and weakly coupled levels in absence of magnetic field. In addition to the Kondo ridges at zero field, the crossings of levels originating from different shells give rise to Kondo ridges at finite magnetic field. The observed bending with respect to the Kondo ridges at zero field turns out be a consequence of the magnetic-field dependence of the level-reservoir coupling strengths. Theoretical understanding is provided by using the functional renormalization-group approach, which reproduces the features of the linear conductance measurements as a function of the applied gate voltage and magnetic field. In particular the bending of the Kondo ridges at finite magnetic field is traced back to the renormalization of the couplings.

TT 52: CE: Low-dimensional Systems - Models 1

Time: Thursday 14:00–16:15 Location: HSZ 105

TT 52.1 Thu 14:00 HSZ 105

Spectral functions with the DMRG in frequency space — •Piet Dargel and Thomas Pruschke — Institut für theoretische Physik, Universität Göttingen, Deutschland

Standard methods for calculating spectral functions with the DMRG in frequency space have to include an artificial broadening (Correction vector) or will have bad resolution for low energies (Fourier transform of TDMRG data). We use an adaptive Lanczos method to calculate iteratively the coefficients of the continued fraction expansion of the spectral function. We show that the spectral weights and poles for the discrete system can be extracted by this method and compare this method to other DMRG methods for calculating spectral functions in frequency space.

TT 52.2 Thu 14:15 HSZ 105

Disordered groundstate phase for 2D-lattice models of hard-core bosons — •Ansgar Kalz, Andreas Honecker, Sebastian Fuchs, and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen

We present Quantum Monte-Carlo data for frustrated models on 2D-lattices. The spin-1/2-Heisenberg model with antiferromagnetic S^z-interaction and ferromagnetic interactions in the x-y–plane can be rewritten as model of hard-core bosons with repulsive density-interactions. Longer-range interactions, i.e., next-nearest neighbor interactions introduce frustration for the square lattice as well as for the hexagonal lattice. Depending on the strength of the frustration we find different classical groundstates which are seperated by a critical point. The frustration yields a large degeneracy that hinders the classical ordering process in the vicinity of the critical point.

For the square lattice with nearest neighbor and competing next-nearest neighbor interactions we calculated magnetic observables and higher-order correlation functions. We show finite temperature phase diagrams and the groundstate phase diagram where we identified a finite region without any order.

On the honeycomb lattice we included interactions up to third nearest neighbors and find a similar scenario as for the frustrated square lattice. In the vicinity of the ciritical point of the model we find a region without classical order and present measurements of higher-order correlation functions.

TT 52.3 Thu 14:30 HSZ 105

Ground states with spontaneous breaking of translational symmetry in orthogonal-dimer chain with Ising and Heisenberg bonds — •Vadim Ohanyan[1] and Andreas Honecker[2] — [1]Department of Theoretical Physics, Yerevan State University, Alex Manoogian 1, 0025, Yerevan, Armenia — [2]Institut für Theoretische Physik Universität Göttingen, Friedrich-Hund-Platz 1 37077 Göttingen, Germany

Considering the exactly solvable model of orthogonal-dimer chain with Ising and Heisenberg bond we investigate the issue of vast variety of its ground states, especially ones with spontaneous breaking of translational symmetry. Analyzing ground states properties we obtain several $T = 0$ ground states phase diagrams corresponds to different sets of parameters. We demonstrate the appearance of magnetization plateaus at $M/M_{sat} = 0, 1/4$ which are connected with the breaking of translational symmetry of the lattice, more precisely, with the doubling of unit cell. The general mechanism of unit cell doubling in the lattice models with block structure and left-right asymmetry is discussed. Calculation the partition function exactly we also obtain analytic expressions for free energy and all thermodynamic function, presenting the plots of magnetization processes for finite temperature displaying magnetization plateaus at $M/M_{sat} = 0, 1/4, 1/2$.

TT 52.4 Thu 14:45 HSZ 105

Low-energy spectral weights of the 1D Hubbard chain — •Stefan Söffing[1,3], Imke Schneider[2], Alexander Struck[1], and Sebastian Eggert[1] — [1]Fachbereich Physik und Forschungszentrum Optimas, Technische Universität Kaiserslautern, Deutschland — [2]Universität Dresden, Deutschland — [3]Graduiertenschule MAT-

COR/MAINZ

We investigate the low-energy spectral weights of the 1D Hubbard chain by means of Density Matrix Renormalization Group (DMRG) calculations in comparison with Bosonization results. We identify the bosonic excitations of the underlying Luttinger liquid and analyze their evolution upon increasing the interaction strength in terms of their density of states (DOS). Comparing analytical and numerical results we point out the competition of spin/charge degrees of freedom vs. non-interacting spin up and down particles, which here become important due to the lattice nature of the model and higher order operators. Furthermore, we discuss the spatially resolved (local) DOS that can be calculated analytically by a recursive formula vs. numerically using DMRG.

15 min. break

TT 52.5 Thu 15:15 HSZ 105

A study of coupled spin-orbital physics in a one-dimensional model — •Alexander Herzog[1,2], Andrzej Michal Oles[1,3], Peter Horsch[1], and Jesko Sirker[2] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Physics and Research Center Optimas, University of Kaiserslautern, Kaiserslautern, Germany — [3]Marian Smoluchowski Institute of Physics, Krakow, Poland

We study the dynamics and thermodynamics of a one-dimensional spin-orbital model relevant for transition metal oxides. For antiferromagnetic superexchange we investigate how spin-wave excitations are affected by coupled spin-orbital excitations using a boson-fermion representation. We contrast a mean-field decoupling approach with results obtained by treating the spin-orbital coupling perturbatively. Within the latter approach we find a significant broadening and additional structures in the dynamical spin structure factor caused by the coupling of spin excitations to orbital fluctuations leading to a Kohn anomaly in the spin-wave dispersion. Moreover the spin-orbital coupling induces a redistribution of entropy from low to intermediate temperatures as is confirmed by comparing our perturbative results for the specific heat with a numerical solution of the model obtained by the density-matrix renormalization group.

TT 52.6 Thu 15:30 HSZ 105

Finite-size scaling analysis of the spatially anisotropic frustrated $S = 1/2$ Heisenberg model — •Mohammad Siahatgar, Burkhard Schmidt, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We investigate the ground-state properties of the $S = 1/2$ frustrated Heisenberg model on a 2D lattice with orthorhombic symmetry. This model, known as the $J_{1a,b} - J_2$ model, is studied using exact diagonalization technique on finite clusters, as well as introducing a systematic way to construct finite clusters to tile the square lattice. For this low symmetry model, a controlled procedure for the finite-size scaling analysis is defined for the tiles which are compatible with corresponding magnetic phase. We calculate the ground-state energy, structure factors and ordered moment, and compare these numerical results with spin-wave calculations as well. In particular, the finite-size behavior of the system in the disordered regions between ordered ferromagnetic and Néel and columnar antiferromagnetic phases is discussed more carefully. We conclude that the effect of spatial anisotropy $J_{1a,b}$ is stabilizing the columnar antiferromagnetic order for all frustration parameters, notably in the spin-nematic phase of the isotropic model.

TT 52.7 Thu 15:45 HSZ 105

Non-equilibrium effects of open boundary in spin chains — suppression of magnon propagation. — •Masud Haque — Max Planck Institut - Physics of Complex Systems Dresden

In the open XXZ spin chain, I will present boundary-induced structures in the energy spectrum. A dramatic series of dynamics-suppression effects arise due to these spectral structures.

TT 52.8 Thu 16:00 HSZ 105

Energy dynamics out of equilibrium in low dimensional quantum magnets — •Stephan Langer[1], Markus Heyl[1], Ian McCulloch[2], and Fabian Heidrich-Meisner[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, LMU München, Germany — [2]School of physical Sciences, The University of Queensland, Brisbane, Australia

We investigate the real-time dynamics of the energy density in spin-1/2 chains and ladders, starting from initial states with an inhomogeneous profile of bond energies, extending our previous work on the dynamics of spin-density wave packets [1]. These simulations are carried out using the adaptive time-dependent density matrix renormalization group algorithm. We analyze the time-dependence of the spatial variance of the bond energies which yields necessary criteria for ballistic or diffusive energy dynamics. In the case of the XXZ chain, our results are consistent with ballistic behavior, both in the massless and the massive phase. For the massless regime, we compare our numerical results to predictions from bosonization for, e.g., the velocity that the initial perturbation spreads with. In the case of ladders, we find an involved dynamics whose qualitative interpretation is still under scrutiny.

[1] Langer et al. Phys. Rev. B 79, 214409 (2009)

TT 53: Graphene (jointly with DY, DS, HL, MA, O)

Time: Thursday 15:15–17:00 Location: HSZ 401

TT 53.1 Thu 15:15 HSZ 401

Tunable edge magnetism in graphene — •Manuel J. Schmidt[1], Daniel Loss[1], David J. Luitz[2], and Fakher F. Assaad[2] — [1]Universität Basel, Switzerland — [2]Universität Würzburg, Germany

Edge states with nearly zero energy that are exponentially localized at zigzag edges of graphene ribbons, in combination with electron-electron interactions give rise to edge magnetism. We show how the characteristic momentum-dependence of the transverse wave function of the edge states may be exploited in order to manipulate the edge state bandwidth [1]. This allows to tune graphene edges from the usual edge magnetism regime, over a regime of itinerant one-dimensional ferromagnetism, down to the non-magnetic Luttinger liquid regime. As an example we discuss graphene/graphane interfaces for which we propose an experimental setting in which the bandwidth may be tuned in situ by means of electrostatic gates [2]. We introduce an effective one-dimensional model for the edge states, on the basis of which we investigate the tunability of edge magnetism. Our analysis uses essentially three techniques: by a mean-field treatment of the effective interaction, the phase diagram is established. Quantum fluctuations, which may not be neglected in one dimension, are taken into account on the basis of a bosonization technique. Finally, these analytical calculations are complemented by an exact diagonalization analysis of the effective edge state model.

[1] M.J. Schmidt and D. Loss, Phys. Rev. B 81, 165439 (2010).

[2] M.J. Schmidt and D. Loss, Phys. Rev. B 82, 085422 (2010).

TT 53.2 Thu 15:30 HSZ 401

Ballistic transport at room temperature in micrometer size multigraphene — •Srujana Dusari[1], José Luis Barzola Quiquia[1], Pablo Esquinazi[1], and Nicolas Garcia[2] — [1]Division of Superconductivity and Magnetism, Universität Leipzig, Faculty of Physics and Earth Sciences, Institute for Experimental Physics II, Linnéstr. 5, 04103 Leipzig, Germany — [2]Laboratorio de Física de Sistemas Pequeños y Nanotecnología, Consejo Superior de Investigaciones Científicas, Serrano 144, E-28006 Madrid, Spain

As an emergent material for electronic applications, graphite and graphene and their electrical transport properties have become a subject of intense focus. By performing transport measurements through micro and submicro constrictions in ~10 nm thick graphite samples, we observe drastic increase in the resistance decreasing the constriction width. Our experimental observations indicate that electrons behave ballistically even at room temperature and with mean free path of the order of microns. The values obtained for the mobility (~10^7 cm^2 v^-1 s^-1) and density of the electrons (~10^8 cm^-2) indicates that the graphene layers inside graphite are of higher quality than single ones. The decrease of magneto resistance with decreasing constriction width also indicates that the carrier mean free path is larger than few microns at room temperature.

TT 53.3 Thu 15:45 HSZ 401

Long spin relaxation times in bilayer graphene — •Frank Volmer[1,2], Tsung-Yeh Yang[1,2], Jayakumar Balakrishnan[3], Ahmet Avsar[3], Manu Jaiswal[3], Julia Samm[1,2], Syed Rizwan Ali[1,2], Alexandre Felix Pachoud[3,4], Ming-Gang Zeng[3,5], Mihaita Popinciuc[1,2], Barbaros Özyilmaz[3,4,5], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany — [3]Department of Physics, National University of Singapore, 117542 Singapore — [4]NUS Graduate School for Integrative Sciences and Engineering (NGS), Centre for Life Sciences (CeLS), 117456 Singapore — [5]Nanocore, National University of Singapore, 117576 Singapore

The demonstration of micrometer long spin relaxation lengths in graphene at room temperature has made this material a promising candidate for spintronic applications. We investigated the spin transport in the non-local spin valve geometry in bilayer graphene using MgO barriers for spin injection. We demonstrate that the dominant spin relaxation mechanism in bilayer graphene is of the D'yakonov-Perel' type. In this case the spin dephasing time scales inversely with the charge carrier mobility. At room temperature spin dephasing times of up to 2 ns are measured in samples with the lowest mobility.

This work has been supported by DFG through FOR 912.

TT 53.4 Thu 16:00 HSZ 401

The graphene Landau quartet unveiled — •Sander Otte[1,2,3], Young Jae Song[2,3], and Joseph Stroscio[2] — [1]Delft University of Technology, The Netherlands — [2]National Institute of Standards and Technology (NIST), USA — [3]Maryland NanoCenter, University of Maryland, USA

Some of the unique properties of graphene come to expression when its electrons are locked into Landau levels in an external magnetic field. Due to spin-degeneracy in combination with the two-atom unit cell of the hexagonal lattice (valley degeneracy), each Landau level is expected to host four electrons. We use a newly completed dilution refrigerator cooled STM system to study epitaxial graphene at 10 mK in magnetic fields up to 15 T. The unparalleled energy resolution of this instrument enables us to break the predicted fourfold Landau level degeneracy and to measure the sublevel splittings as a function of the magnetic field. Surprisingly large splittings are found for the valley states, which are not magnetic by nature. In addition, intriguing partial filling of the sublevels is observed, yielding access to promising electron correlation effects.

TT 53.5 Thu 16:15 HSZ 401

Emergent magnetism of *5d* transition-metal adatoms on Graphene — •Hongbin Zhang[1], Cesar Lazo[2], Stefan Blügel[1], Stefan Heinze[2], and Yuriy Mokrousov[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098 Kiel, Germany

Owing to its peculiar electronic structure, graphene serves as a playground for many interesting physical properties and has drawn a lot of attention recently [1]. In this work, using the first principles FLAPW methods, we investigate the magnetism of 5*d* transition metal (TM) atoms from Hf to Pt deposited on graphene in different supercell geometries. By taking into account the effect of atomic relaxations, we find that most of the 5*d* TMs exhibit strong local magnetism when deposited on graphene. A combination of large spin moments with strong spin-orbit coupling in considered adatoms leads to gigantic values of the magnetic anisotropy energies, reaching values as large as 30 meV/atom. We also investigate the influence of external electric fields on the magnetic properties of 5*d* TM adatoms and discuss possible transport applications. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] A. H. C. Neto, *et al.*, Rev. Mod. Phys. **81**, 109 (2009).

TT 53.6 Thu 16:30 HSZ 401

Anisotropic magnetoresistance observed in graphite flakes — •Jose Barzola-Quiquia, Andreas Schadewitz, Winfried Böhlmann, and Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany

The possibility to have magnetic order at room temperature in a system without 3d metallic magnetic elements attracts the interest of the solid state physics community. Experimental evidence for the existence of ferromagnetism in virgin and proton-irradiated graphite samples was published based on SQUID [1] and XMCD [2] measurements. An alternative method to detect magnetic order is to measure the magnetoresistance (MR). The MR develops a characteristic butterfly loop when measured vs. magnetic field. In this work we have studied the magnetotransport properties of micrometer-size and ˜10 nm thick graphite flakes as a function of temperature, magnetic field applied in- and out-plane configurations. We investigated especially the MR as a function of the angle between current and applied field in order to study the anisotropic magnetoresistance (AMR). Virgin graphite flakes show a small AMR and flakes treated with H_2SO_4 show an increase in the AMR signal. The observed behavior provides evidence for intrinsic and induced ferromagnetism at the surface of graphite samples. This investigation also was complemented using SQUID magnetometry on graphite powder in virgin state and after treatment with H_2SO_4 resulting in a clear ferromagnetic signal. [1] P. Esquinazi et al., Phys. Rev. B 66, 024429 (2002), Phys. Rev Lett. 91, 227201 (2003). [2] H. Ohldag et al., Phys. Rev. Lett. 98, 187204 (2007).

TT 53.7 Thu 16:45 HSZ 401

Magnetic clusters on graphene flakes — •Wolfgang Landgraf, Sam Shallcross, and Oleg Pankratov — Lehrstuhl fur Theoretische Festkorperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany.

We present an investigation of the properties of magnetic ad-atoms and clusters on graphene flakes. We consider clusters of 1-7 atoms of metals from the 3d series assembled on graphene flakes composed of the order of 100 carbon atoms. All calculations are performed within the spin density functional theory formalism in the local density approximation. We elucidate the range of the magnetic interaction for pairs of magnetic ad-atoms on graphene flakes, as well as the equilibrium magnetic structure for various cluster types. By a comparison of such clusters on flakes with their counterparts on extended sheets, we are able to elucidate the role of the flake shape upon the magnetic interaction. In this way we determine the role of confinement on the magnetic interaction, and comment on the possibility of using flake shape as a design parameter of magnetic nanostructures on graphene flakes.

TT 54: SC: Heterostructures, Andreev Scattering, Proximity Effect

Time: Thursday 15:30–17:15 Location: HSZ 301

TT 54.1 Thu 15:30 HSZ 301

Observation of Andreev bound states at spin-active interfaces — •Florian Hübler[1,2], Michael J. Wolf[1], Detlef Beckmann[1], and Hilbert von Löhneysen[2,3] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie — [2]KIT, Institut für Festkörperphysik — [3]KIT, Physikalisches Institut

Spin-active interfaces, for instance between superconductors and ferromagnets are characterized by spin-dependent transmission amplitudes as well as phase shifts[1]. The relative phase shift between spin-up and -down, the so-called spin-mixing angle θ_s, is an important parameter for the triplet proximity effect. So far, little quantitative information is available about θ_s. Recent theoretical models indicate that θ_s may actually be quite large in structures with ultra-thin tunnel barriers[2]. One of the consequences of finite θ_s in S/F hybrids is the presence of bound states at the interface[3], at energies which have a particularly simple relation to θ_s, $\epsilon = \pm\Delta cos(\theta_s/2)$. We report here the experimental observation of Andreev bound states induced by spin-mixing in Al/Al2O3/Fe structures. From the energy of the bound states, we can determine θ_s with great accuracy. As predicted theoretically, we find examples of $\theta_s \approx \Pi$, but also a significant spread from contact to contact, even within the same fabrication batch. The large spread indicates that spin mixing in real structures depends in a subtle way on details of the interface, and is possibly controlled by defects.

[1] Millis et al., Phys. Rev. B 38, 4504 (1988)
[2] Grein et al., Phys. Rev. B 81, 094508 (2010)
[3] Zhao et al., Phys. Rev. B 70, 134510 (2004)

TT 54.2 Thu 15:45 HSZ 301

Nonlocal conductance via overlapping Andreev bound states in ferromagnet-superconductor heterostructures — •Georgo Metalidis[1], Matthias Eschrig[1,2], Roland Grein[1], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

In a setup where two ferromagnetic electrodes are attached to a superconductor, Andreev bound states are induced at both ferromagnet/superconductor interfaces. We study how these states propagate through the superconductor and interact with each other. We find that the energetic positions of the Andreev states are not anymore determined solely by the magnetic properties of a single interface, but depend on the interface distance and the relative magnetization orientation of the ferromagnetic contacts as well. These bound states show up as distinct peaks in the nonlocal conductance signal and lead to marked asymmetries with respect to the applied voltage. Our results are related to nonlocal crossed Andreev and elastic co-tunneling processes.

TT 54.3 Thu 16:00 HSZ 301

Experimental Observation of the Spin Screening Effect in Superconductor/Ferromagnet Thin Film Heterostructures — •Ruslan Salikhov[1,2], Ilgiz Garifullin[2], Nadir Garifyanov[2], Lenar Tagirov[3], Kurt Westerholt[1], and Hartmut Zabel[1] — [1]Experimental Physics, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Zavoisky Physical-Technical Institute, Russian Academy of Science, 420049 Kazan, Russia — [3]Kazan State University, 420008 Kazan, Russia

We have studied the nuclear magnetic resonance (NMR) of 51V nuclei in the superconductor/ferromagnet thin film heterostructures $Pd_{1-x}Fe_x$/V/$Pd_{1-x}Fe_x$ and Ni/V/Ni in the normal and superconducting state. Whereas the position and shape of the NMR line in the normal state for the trilayers is identical to that observed in a single V layer, in the superconducting state the line shape definitely changes, developing a systematic distortion of the high-field wing of the resonance line. By varying the thickness of the superconducting V layer for Ni/V/Ni trilayer samples we observed that the distortion of the high-field wing of the resonance line has an obvious trend to disappear with increasing V layer thickness. We consider this as the first experimental evidence for the penetration of ferromagnetism into the superconducting layer, a phenomenon which has been theoretically predicted recently and dubbed the spin screening effect.

TT 54.4 Thu 16:15 HSZ 301

Andreev reflection with semiconductor-valence-band carriers — •David Futterer[1], Michele Governale[2], Ulrich Zülicke[3], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg Essen and CeNIDE, 47048 Duisburg, Germany — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington, New Zealand — [3]Institute of Fundamental Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Massey University

We investigate Andreev reflections through a hybrid semiconductor/superconductor interface within the Bogoliubov-de Gennes formalism. In particular we focus on valence-band carriers of p-doped semiconductors with large spin-orbit coupling, approaching the junction under an arbitrary angle.

The spin-orbit coupling leads to a mixing between the energy bands. This allows four possibilities of reflection for an injected light-hole (heavy-hole) carrier. It can be normal reflected into the light-hole (heavy-hole) band or the heavy-hole (light-hole) band as well as Andreev reflected into each of the two bands. The reflection depends strongly on the angle of injection. Though Andreev reflection of heavy-hole carriers is in general possible, these carriers can only be normal reflected into the heavy-hole band in the case of perpendicular injection.

TT 54.5 Thu 16:30 HSZ 301

Adiabatic Cooper pair pumping through quantum dots — •Bastian Hiltscher[1], Michele Governale[2], Janine Splettstoesser[3], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CeNIDE — [2]School of Chemical and Physical Sciences, Victoria University of Wellington — [3]Institut für Theoretische Physik A, RWTH Aachen University

Motivated by recent experimental work [1] we investigate splitting of Cooper pairs in adiabatic pumping. We consider (i) a quantum dot with Zeeman split levels tunnel coupled to a normal and a superconductor and (ii) two quantum dots tunnel coupled to the same superconductor and each dot coupled to a normal conductor.

We combine the means of two different theories. On the one hand a systematic perturbation expansion in tunnel-coupling strength between quantum dots and superconductors [2] and on the other hand an adiabatic expansion using that the pumping period is small compared to the lifetime of a certain state [3].

We find that the pumped charge and the linear conductance show the same dependence on the average dot level position. The underlying tunneling processes are discussed. In order to figure out processes where a Cooper pair is split we compare the properties of Cooper pair pumping with single-electron pumping. The dependence on the average dot-level position turns out to be the main distinguishing feature.

[1] Hofstetter *et al.*, Nature **461**, 960 (2009); Herrmann *et al.*, PRL **104**, 026801 (2010).
[2] Governale *et al.*, PRB **77**, 134513 (2008).
[3] Splettstoesser *et al.*, PRB **74**, 085305 (2006).

TT 54.6 Thu 16:45 HSZ 301

Controlling the Conductance and Thermopower of Chaotic Quantum Dots — •Thomas Engl, Jack Kuipers, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Transport through quantum cavities, like quantum dots, has raised much interest in physics in recent decades. When attaching superconductors to the cavity, these transport properties are substantially changed, known to be caused by Andreev reflection on the interface between the normal region and the superconductor.

Using a semiclassical framework for ballistic systems, so called Andreev billiards with chaotic dynamics, we show how Andreev reflection along with the interference due to subtle correlations between the classical paths of electrons and holes inside the system affects the conductance of the system and see how these combined cause large quantum corrections to the conductance like its reduction by a phase difference between the superconductors. Furthermore we show that the thermopower requires an asymmetry with respect to an exchange of the superconducting leads in order to be nonzero. Moreover, we are able to see what happens if the temperature is increased or a magnetic field is applied.

TT 54.7 Thu 17:00 HSZ 301

Chain of Majorana States from Superconducting Dirac Fermions at a Magnetic Domain Wall — •Titus Neupert[1], Shigeki Onoda[2], and Akira Furusaki[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [2]Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan

We study theoretically a strongly type-II s-wave superconducting state of two-dimensional Dirac fermions in proximity to a ferromagnet having in-plane magnetization. It is shown that a magnetic domain wall can host a chain of equally spaced vortices in the superconducting order parameter, each of which binds a Majorana-fermion state. The overlap integral of neighboring Majorana states is sensitive to the position of the chemical potential of the Dirac fermions. Thermal transport and scanning tunneling microscopy experiments to probe the Majorana fermions are discussed.

TT 55: TR: Topological Insulators 1 (jointly with HL and MA)

Time: Thursday 16:00–17:00 Location: HSZ 304

TT 55.1 Thu 16:00 HSZ 304

Topological phases in three-dimensional superconductors — •Andreas Schnyder — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We examine different topological phases in three-dimensional noncentrosymmetric superconductors with time-reversal symmetry by using three different types of topological invariants. Due to the bulk boundary correspondence, a non-zero value of any of these topological numbers indicates the appearance of zero-energy Andreev surface states. In fully gapped phases the presence of these surface states is independent of the surface orientation, whereas in nodal superconducting phases the Andreev states appear only for certain orientations of the surface. We find that some of these boundary modes in nodal superconducting phases are dispersionless, i.e., they form a flat surface band. These dispersionless Andreev surface bound states have many observable consequences. In particular, they lead to a zero-bias conductance peak in the scanning tunneling spectra. Furthermore, we discuss the appearance of surface Majorana modes in gapless superconducting phases.

TT 55.2 Thu 16:15 HSZ 304

Symmetry protected topological phases: An entanglement point of view — •Frank Pollmann[1], Ari Turner[2], Erez Berg[3], and Masaki Oshikawa[4] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley CA 94720, USA — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [4]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581 Japan

We propose a scheme to characterize topological phases in one dimensional systems in terms of properties of the entanglement spectrum. We discuss the application of this scheme in two specific examples. The first example is the Haldane phase for a S=1 chain. We show that the Haldane phase is protected by certain symmetries and characterized by a double degeneracy of the entanglement spectrum. The degeneracy cannot be lifted unless either a phase boundary to another, "topologically trivial", phase is crossed or the symmetry is broken. In the second example we apply these concepts to classify systems of interacting fermions in one dimension in the presence of time reversal and parity symmetry.

TT 55.3 Thu 16:30 HSZ 304

Electronic scattering and phonons in the 3D topological insulators Bi_2Se_3 and $Cu_{0.07}Bi_2Se_3$ — •Peter Lemmens[1,2], Vladimir Gnezdilov[1,3], Dirk Wulferding[1,2], and Helmuth Berger[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]NTH, Germany — [3]ILTPE NAS, Ukraine — [4]EPFL, Lausanne, Switzerland

The Raman-active lattice vibrations of three dimensional topological insulators Bi_2Se_3 and $Cu_{0.07}Bi_2Se_3$ (R-3m) are investigated by Raman spectroscopy. All four expected Raman modes, $2A_{1g}$ and $2E_g$, were determined for the first time and compared with the theoretical predictions. Electronic scattering is observed as a quasielastic response in the doped material at higher temperatures.

Work supported by DFG and NTH.

TT 55.4 Thu 16:45 HSZ 304

Multidimensional Angle-Resolved Photoemission Spectroscopy: Application to Topological Insulators — •Ovsyannikov R.[1], Lupulescu C.[1,2], Rienks E.D.L.[1], Fink J.[1], King P.D.C.[3], Baumberger F.[3], Hatch R.C.[4], Hofmann P.[4], Mi J.[4], Iversen B.B.[4], Lindblad A.[5], Svensson S.[5,6], and Eberhardt W.[1,2] — [1]Helmholtz Zentrum Berlin, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany — [3]University of St Andrews, St Andrews, UK — [4]Aarhus University, Aarhus, Denmark — [5]MAX-lab, Lund, Sweden — [6]Uppsala University, Uppsala, Sweden

We will present a novel approach of performing photoelectron spectroscopy experiments and demonstrate its potential on the prototype topological insulator Bi_2Se_3. We use VG Scienta's ARTOF 10k, a time-of-flight electron spectrometer which combines position-sensitive detection with an advanced focusing electron lens system. The instrument allows the simultaneous recording of kinetic energy and the angular pattern of photoelectrons in a cone of up to 30° opening angle with very high resolution. Additionally, the temporal evolution of the sample electronic structure can be easily extracted from the corresponding data set. The experiments were carried out at the 10m NIM beamline at the BESSY II synchrotron facility, when operating in single bunch mode. We will show the temporal evolution of the topological state and the subsequent formation of a two-dimensional electron gas at the (0001) surface of the topological insulator Bi_2Se_3. We will also discuss the overall time resolution of the experimental setup.

TT 56: CE: Heavy Fermions

Time: Thursday 16:30–19:00 Location: HSZ 105

TT 56.1 Thu 16:30 HSZ 105

Symmetry enhancement at Kondo destroyed quantum critical points — •S. Kirchner[1,2], J.H. Pixeley[3], and Q. Si[3] — [1]Max-Planck-Institut PKS, Dresden, Germany — [2]Max-Planck-Institut CPfS, Dresden, Germany — [3]Physics & Astronomy, Rice University, Houston, USA

Recent studies in quantum critical heavy fermion metals have pointed towards a global phase diagram [1]. There is growing experimental evidence, that rare earth intermetallic systems in the vicinity of a quantum critical point show a linear in temperature magnetic and single-particle relaxation rate[2]. Among the proposed mechanisms is the critical destruction of the Kondo effect. We address this issue in several quantum impurity systems by a combination of techniques and determine the full scaling functions. In each case, the quantum relaxational regime is characterized by linear-in-temperature relaxation rates. This is naturally explained in terms of an emerging conformal symmetry at the quantum critical point that is absent in the bare models[3,4,5].

[1] Q. Si & F. Steglich, Science **329**, 1161 (2010).
[2] A. Schröder et al., Nature (London) **407**, 351 (2000); S. Friedemann et al. Proc. Natl. Acad. Sci. USA **107**, 14547 (2010).
[3] S. Kirchner & Q. Si, Phys. Rev. Lett. **100**, 026403 (2008).
[4] M. T. Glossop, S. Kirchner, J. H. Pixley and Q.Si, arXiv:0912.4521, to be published (2010).
[5] J. H. Pixley, S. Kirchner and Q.Si, arXiv:1010.3024, to be published (2010).

TT 56.2 Thu 16:45 HSZ 105

Hot lines on quantum critical Fermi surfaces from magneto oscillation measurements — •Lars Fritz and Achim Rosch — Universität zu Köln, Institut für theoretische Physik

Quantum criticality in electronic systems figures prominently in so-called heavy fermion systems. Many of these systems can be driven by either pressure, magnetic field, or chemical doping towards a point, where the anitferromagnetic Néel temperature is suppressed to zero resulting in a quantum critical point. One of the major questions which occur in the context of this quantum critical point is by which mechanism the antiferromagnetic state is converted into the heavy Fermi liquid. There exist two extreme cases: one in which the heavy Fermi liquid state is obtained in the framework of a spin density wave (SDW) scenario in the spirit of the Hertz-Millis-Moriya theory as opposed to a scenario of breakdown of the Kondo effect. On an elementary level, the scenarios also differ in the way the Fermi surface becomes critical. Whereas in a SDW scenario hot lines due to overdamping by spin density wave at certain points of the Fermi surface have to be expected, in more exotic scenarios the whole Fermi surface becomes critical ("hot"). It is thus desirable to have a probe which is sensitive to the existence or nonexistence of hot lines on the Fermi surface. We discuss the possibility to locate hot regions and extract the ordering wave vector in strongly correlated fermionic systems close to a collective instability

by means of angle dependent magneto-oscillations measurements of the de-Haas-van-Alphen or Shubnikov-de-Haas type.

TT 56.3 Thu 17:00 HSZ 105

Interplay between Kondo effects in a Kondo lattice with two in-equivalent local moments — •Adel Benlagra[1], Lars Fritz[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, TU Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany

Usual theoretical studies of Kondo systems often assume the presence of a single spin$-1/2$ local moment per unit cell and little is known about the behavior of a Kondo lattice with multiple distinct local moments. Motivated by the recently studied family of ternary compounds $(RE)_3Pd_{20}X_6$ (Re=rare-earth, X=Ge, Si), which have two inequivalent Kondo sites per unit cell, we study a Kondo lattice Hamiltonian with two local moments coupled to the sea of conduction electrons with different Kondo couplings ($J_2 < J_1$). In particular, we investigate the interplay between the resulting Kondo screenings and explore the thermodynamic properties of the heavy Fermi liquid regime using slave bosons in the mean-field approximation. It is found that the two effects compete or cooperate depending on the electronic filling number. The coherence scale governing the low temperature behavior of the heavy Fermi liquid is affected and, in particular, its ratio to the Kondo scales is not generically independent of the Kondo couplings as is the case for the standard Kondo lattice problem.

TT 56.4 Thu 17:15 HSZ 105

Tracing the Kondo Lattice in $YbRh_2Si_2$ — •Stefan Ernst[1], Stefan Kirchner[2,1], Steffen Wirth[1], Cornelius Krellner[1], Christoph Geibel[1], Frank Steglich[1], and Gertrud Zwicknagl[3] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]Max-Planck-institut für Physik Komplexer Systeme, Dresden — [3]Institut für Mathematische Physik, TU Braunschweig

Heavy fermion (HF) metals are often characterized by a variety of relevant energy scales and competing interactions which may result in the emergence of novel states of condensed matter. Therefore, these materials have advanced to suitable model systems by means of which electronic correlations can be studied in detail. For a further in-depth understanding of the underlying physics, the application of local electronic probes is of major importance.

We present recent results of Scanning Tunneling Microscopy and Spectroscopy (STM/S) at low temperature conducted on the prototypical HF compound $YbRh_2Si_2$. The topography confirms an excellent low temperature *in situ* cleave of the single crystals. The hybridization of conduction and $4f$ electrons results in a gap-like feature in the tunneling conductance. In addition, the crystal field excitations are unambiguously reflected in our STS data and hence, bulk properties are predominatly probed. A strongly temperature-dependent peak in the tunneling conductance is attributed to a Kondo–lattice resonance.

TT 56.5 Thu 17:30 HSZ 105

Magnetic ac susceptibility of $YbRh_2Si_2$ at ultra-low temperatures — •Lucia Steinke[1,2], Erwin Schuberth[2], Stefan Lausberg[1], Christoph Klingner[1], Cornelius Krellner[1], Manuel Brando[1], Christoph Geibel[1], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Walther Meissner Institut, 85748 Garching, Germany

Recent magnetization measurements on the heavy fermion compound $YbRh_2Si_2$ at ultra-low temperatures (ULT) below 1 mK show that the weak antiferromagnetic phase, which forms at $B = 0$ below $T_N = 70$ mK, is not the $T = 0$ ground state of the system. Instead, two additional ULT regimes were discovered [1]: a new phase below $T_A = 2.2$ mK, where the phase transition is observed as a pronounced magnetization peak, and a second regime below $T_B = 15$ mK, where zero-field-cooled / field-cooled measurements begin to show a hysteresis. To clarify the origin of these two new ULT regimes, particularly to seek evidence for possible superconducting states in $YbRh_2Si_2$, we measured the magnetic ac susceptibility at $B = 0$. Initial results indicate a decrease in the real part χ' of the ac susceptibility as the sample temperature is lowered beyond $T_B = 15$ mK and a pronounced drop in χ' as T drops below the transition temperature $T_A = 2.2$ mK. Whether the response is indeed diamagnetic depends on the yet unknown background signal.

[1] E. Schuberth *et al.*, J. Phys. C **150**, 042178 (2009)

15 min. break

TT 56.6 Thu 18:00 HSZ 105

Magnetic field dependence of the antiferromagnetic order in $YbCo_2Si_2$ — •A. Haase[1], O. Stockert[1], N. Mufti[1], C. Krellner[1], J.-U. Hoffmann[2], A. Hoser[2], S. Capelli[3], and C. Geibel[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Helmholtzzentrum Berlin, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France

One of the model compounds to study quantum critical behaviour is $YbRh_2Si_2$, which orders antiferromagnetically at a very low $T_N \approx 0.07$ K. Due to the small ordered moment and the high neutron absorption of Rh the magnetic structure of $YbRh_2Si_2$ is still unknown. $YbCo_2Si_2$ with its body-centered tetragonal crystal structure is isoelectronic to $YbRh_2Si_2$ and serves as a reference system. $YbCo_2Si_2$ orders antiferromagnetically below $T_N = 1.7$ K with an additional first order transition at $T_L = 0.9$ K. This compound exhibits a complex magnetic (B, T) phase diagram for applied magnetic field and shows a pronounced basal plane anisotropy observed in magnetisation and magnetoresistance measurements. While at lowest temperature the magnetic order is commensurate with $\tau_1 = (0.25\ 0.25\ 1)$, the magnetic structure becomes incommensurate above T_L with $\tau_2 = (0.08\ 0.25\ 1)$. Using neutron diffraction we studied the magnetic structure in magnetic fields applied along [100], [110] and [001]. While in the commensurate phase no hysteresis was observed for all three directions of applied magnetic fields, a pronounced hysteresis of the intensity was detected in the incommensurate phase for fields along [100], which most likely can be attributed to different domain population.

TT 56.7 Thu 18:15 HSZ 105

Magnetically driven superconductivity in $CeCu_2Si_2$ — •S. Kirchner[1,2], O. Stockert[2], J. Arndt[2], E. Faulhaber[3,4], C. Geibel[2], H.S. Jeevan[2], M. Loewenhaupt[4], K. Schmalzl[5], W. Schmidt[5], Q. Si[6], and F. Steglich[2] — [1]Max-Planck-Institut PKS, Dresden, Germany — [2]Max-Planck-Institut CPfS, Dresden, Germany — [3]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [4]Gemeinsame Forschergruppe Helmholtz-Zentrum Berlin – TU Dresden, Garching, Germany — [5]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France — [6]Dept. of Physics and Astronomy, Rice Univ., Houston, USA

The origin of unconventional superconductivity, including high-temperature and heavy-fermion superconductivity, is still a matter of controversy. Spin excitations instead of phonons are thought to be responsible for the formation of Cooper pairs. Based on inelastic neutron scattering data, we present the first in-depth study of the magnetic excitation spectrum in momentum and energy space in the superconducting and the normal state of $CeCu_2Si_2$ [1]. A clear spin excitation gap is observed in the superconducting state. Our findings identify the antiferromagnetic excitations as the major driving force for superconducting pairing in this prototypical heavy-fermion compound located near an antiferromagnetic quantum critical point. This study represents the first thorough comparison of the competing energetics for a superconductor near an antiferromagnetic quantum critical point, as well as for any unconventional low-temperature superconductor. [1] accepted for publication in Nature Physics.

TT 56.8 Thu 18:30 HSZ 105

Magnetic Phase Diagram of $CeAu_2Ge_2$ — •Veronika Fritsch, Bernd Pilawa, Peter Schweiss, Peter Pfundstein, and Hilbert v. Löhneysen — Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany

$CeAu_2Ge_2$ single crystals (tetragonal $ThCr_2Si_2$ structure) have been grown in Au-Ge flux (AGF) as well as in Sn flux (SF). X-ray powder diffraction measurements and EDX measurements indicate that in the latter case Sn atoms from the flux are incorporated in the samples, leading to a decrease of the lattice constants by $\approx 0.3\%$ compared to AGF samples. The magnetization M demonstrates a strong dependence of the magnetic properties on the flux employed. While the SF samples adopt simple antiferromagnetic order below 9 K, a sequence of metamagnetic transitions with increasing magnetic field in the AGF samples points towards a more complex magnetic structure for $\mathbf{B}\|\mathbf{c}$. One the basis of the neutron scattering data of Loidl et al. (PRB **46**, 9341, 1992) we calculated the field-dependence of the magnetization at $T = 20$ K in the paramagnetic regime, as well as the temperature dependence, and found good agreement with our measured data for $\mathbf{B}\|\mathbf{c}$ and $\mathbf{B} \perp \mathbf{c}$. The complex phase diagram of the AGF samples in comparison to the simpler one of the SF samples is discussed within

the framework of the ANNNI model, making $CeAu_2Ge_2$ a possible candidate for a Devil's Staircase.

TT 56.9 Thu 18:45 HSZ 105

Spin dynamics in $EuCu_2Si_{2-x}Ge_x$: from mixed valence to magnetic instability — •Kirill Nemkovski[1], Pavel Alekseev[2], Jean-Michel Mignot[3], Ross Stewart[4], Robert Bewley[4], and Alexandr Gribanov[5] — [1]Jülich Centre for Neutron Science, Forschungszentrum Jülich, Germany — [2]RRC "Kurchatov Institute", Moscow, Russia — [3]Laboratoire Léon Brillouin, CEA/Saclay, France — [4]ISIS, Rutherford Appleton Laboratory, Didcot, UK — [5]Department of Chemistry, Moscow State University, Russia

$EuCu_2Si_{2-x}Ge_x$ series represents the only known case among Eu- and Sm-based systems, where the state in the phase diagram is tuned from the valence-fluctuating one to heavy-fermion, and then to magnetic-ordered state, with quantum critical point near x=0.7. Here we present the inelastic neutron scattering study of spin dynamics in $EuCu_2Si_{2-x}Ge_x$ (x=0, 0.2, 0.5, 0.8), performed in a wide temperature range (5-200K). At x=0 the magnetic excitation spectrum was found to be represented by the double-peak structure just below the energy range of the Eu^{3+} spin-orbit (SO) excitation $^7F_0 \rightarrow ^7F_1$, so that at least the high-energy spectral component can be assigned to the renormalized SO transition. Change of the Eu valence towards 2+ with increase of the temperature and/or Ge concentration results in further renormalization (lowering the energy) and gradual suppression of both inelastic peaks in the spectrum, along with developing sizeable quasielastic signal. The origin of the spectral structure and its evolution is discussed in terms of excitonic model for the mixed-valence state. This work was supported by RFBR grant No. 11-02-00121.

TT 57: SC: Fe-based Superconductors - 122 - Thin Films

Time: Thursday 17:15–18:45 Location: HSZ 304

TT 57.1 Thu 17:15 HSZ 304

New routes for epitaxial thin films of Fe-based superconductors — Thomas Thersleff, •Silvia Haindl, Kazumasa Iida, Fritz Kurth, Jan Engelmann, Martin Kidszun, Sascha Trommler, Jens Hänisch, Alexander Kauffmann, Elke Reich, Ruben Hühne, Darius Pohl, Andreas Hartmann, Bernd Rellinghaus, Ludwig Schultz, and Bernhard Holzapfel — Institute for Metallic Materials, IFW Dresden

With the recent discovery of the Fe-based superconductors, a major question raised is their suitability for applications. Many of the most interesting devices require the controlled production of thin films with clean interfaces. During the laboratory production of Fe-based superconductor thin films, a detailed analysis by TEM of the substrate/film interface revealed evidence for secondary phase formation. On the basis of the observation of the formation of an Fe layer at the substrate/film interface for Co-doped $BaFe_2As_2$, we designed a bonding scheme between Fe and the iron pnictide phase, resulting in a new thin film architecture we have termed the 'Fe/Ba-122' bilayer system. The first results from this system reveal greatly enhanced growth properties and critical current densities with regard to deposition on pure oxide substrates and may provide a key to understanding a more general growth mechanism in this system.

TT 57.2 Thu 17:30 HSZ 304

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

The interplay between structural parameters and superconducting properties attracts high interest in particular regarding the iron based superconductors. In contrast to the cuprate family, superconductivity of the latter can be induced using either pressure or chemical substitution. Nevertheless little is known about this relationship when biaxial strain is applied. The generation of biaxial strain by the preparation of thin films on substrates with different lattice mismatch is well established for cuprates. However, high quality films are necessary to correlate structural changes with electronic properties. In this work an alternative approach is used. Single crystalline piezoelectric substrates offer the unique opportunity to tune the lattice parameters continuously using the inverse piezoelectric effect. We prepared thin epitaxial $La_{1-x}Sr_xCuO_4$ and $BaFe_{2-x}Co_xAs_2$ films on piezoelectric (001) $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (PMN-PT) substrates. A reversible shift of the superconducting transition has been achieved with a value of 0.44 K for $La_{1.85}Sr_{0.15}CuO_4$ and 0.2 K for $BaFe_{1.8}Co_{0.2}As_2$ for a biaxial strain of 0.022% and 0.017%, respectively.

TT 57.3 Thu 17:45 HSZ 304

Epitaxial growth of superconducting $Ba(Fe_{1-x}Co_x)_2As_2$ thin films on IBAD-MgO buffered metallic substrates — •Jens Hänisch[1], Kazumasa Iida[1], Sascha Trommler[1], Vladimir Matias[2], Tom Thersleff[1], Fritz Kurth[1], Irene Lucas del Pozo[1], Jan Engelmann[1], Silvia Haindl[1], Ruben Hühne[1], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]IFW Dresden, P. O. Box 270116, 01171 Dresden, Germany — [2]MPA-STC, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Recently we have shown that thin Fe buffer layers are beneficial for the growth of high-quality $Ba(Fe_{1-x}Co_x)_2As_2$ (Ba-122) thin films.[1] Even on MgO with large lattice mismatch, epitaxial growth can be achieved with Fe buffer. Here, we report on the biaxially textured growth of superconducting Ba-122 thin films on metallic technical tapes with an ion beam assisted deposition MgO (IBAD-MgO) and Fe buffer architecture. The epitaxial relation was confirmed to (001)[100]Ba-122‖(001)[110]Fe‖(001)[100]MgO by XRD θ-2θ scans and pole figure measurements. The iron pnictide layer showed a T_c of 21.5 K, which is only slightly lower than on single-crystal MgO substrates. The angular-dependent critical current density, $J_c(\theta)$, showed a broad maximum at $\theta = 90°$ and a lower J_c anisotropy than films on single-crystalline substrates. A self-field J_c of $8{\times}10^5$ A/cm^2 has been achieved at 4 K.

[1] T. Thersleff et al., APL 97, 022506 (2010);
K. Iida et al., APL 97, 172507 (2010)

TT 57.4 Thu 18:00 HSZ 304

Transport properties of thin $Ba(Fe,Co)_2As_2$ film microbridges — •Dagmar Rall[1,2], Konstantin Il'in[1], Kazumasa Iida[3], Silvia Haindl[3], Fritz Kurth[3], Thomas Thersleff[3], Ludwig Schultz[3], Bernhard Holzapfel[3], Uli Lemmer[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Hertzstrasse 16, 76187 Karlsruhe — [2]Lichttechnisches Institut (LTI), Karlsruher Institut für Technologie, Engesserstrasse 13, 76131 Karlsruhe — [3]Institute for Metallic Materials (IMW), IFW Dresden, p. o. box 270116, 01171 Dresden

The critical current density of $Ba(Fe,Co)_2As_2$ thin film microbridges was evaluated from current-voltage characteristics measured using the standard four-probe technique. The $Ba(Fe,Co)_2As_2$ films were deposited by pulsed-laser deposition on heated $(La,Sr)(Al,Ta)O_3$ substrates and patterned by means of photolithography and ion milling. The critical current density at T = 4.2 K reaches about 3 MA/cm^2. The experimentally obtained temperature dependence of the critical current density is described by $(1-T/T_c)^{1.5}$ in the unexpectedly wide temperature range $0.4 < T/T_c < 1$. The results can be explained in the frame of Ginzburg-Landau theory for the de-pairing critical current. The expulsion of magnetic vortices is considered as a mechanism which is responsible for overcoming Likharev's limit for observation of the de-pairing critical current.

TT 57.5 Thu 18:15 HSZ 304

Thin film hybrid Josephson junctions with Co doped Ba-122. — •Stefan Schmidt[1], Sebastian Döring[1], Frank Schmidl[1], Volker Tympel[1], Veit Grosse[1], Silvia Haindl[2], Kazumasa Iida[2], Fritz Kurth[2], Ingolf Mönch[3], Bernhard Holzapfel[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institut für metallische Werkstoffe, Helmholtzstrasse 20, 01069 Dresden, Germany — [3]IFW Dresden, Institut für Integrative Nanowissenschaften, Helmholtzstrasse 20, 01069 Dresden, Germany

Josephson junctions are a strong tool to investigate fundamental su-

perconducting properties, such as gap behaviour, dependencies from external fields and the order parameter symmetry. Finding secure values enables the possibility of theoretical descriptions to understand the physical processes within the new iron-based superconductors. Based on Co-doped $BaFe_2As_2$ (Ba-122) layers produced via pulsed laser deposition (PLD) on (La,Sr)(Al,Ta)O_3 substrates, we manufactured superconductor-normal conductor-superconductor (S-N-S) junctions structures by using photolithography, ion beam etching as well as insulating SiO_2 layers. We present working Ba-122 / Au / PbIn thin film Josephson junctions with different contact areas and barrier thicknesses, their temperature dependence and response to microwave irradiation. The calculated I_cR_N product is in the range of a couple of microvolts.

TT 57.6 Thu 18:30 HSZ 304

Tunnelling spectroscopy of $BaFe_2As_2$ / Au / PbIn thin film junctions — •Sebastian Döring[1], Stefan Schmidt[1], Frank Schmidl[1], Volker Tympel[1], Veit Grosse[1], Silvia Haindl[2], Kazumasa Iida[2], Fritz Kurth[2], Bernhard Holzapfel[2], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena — [2]IFW Dresden, Institut für metallische Werkstoffe, Helmholtzstrasse 20, 01069 Dresden

Tunnelling spectroscopy is an important tool to investigate the properties of iron-based superconductors. In contrast to commonly used point contact Andreev reflection (PCAR) technique, we fabricated hybrid superconductor / normal metal / superconductor (SNS) thin film structures, with tunable barrier thickness and area.

For the base electrode we use $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin films, produced via pulsed laser deposition (PLD). A gold layer was sputtered to form the barrier, while the counter electrode material is the conventional superconductor PbIn with a T_c of 7.2 K.

For temperatures below 7.2 K the spectrum shows a subharmonic gap structure (SGS), described by an extended model of Octavio, Tinkham, Blonder and Klapwijk (OTBK), while at higher temperatures the SGS vanishes and an SN-like behaviour can be observed.

TT 58: SC: Vortex Dynamics, Vortex Phases, Pinning

Time: Thursday 17:30–19:00 Location: HSZ 301

TT 58.1 Thu 17:30 HSZ 301

Study of the imperfect Meissner effect in niobium — •Sarah Aull, Oliver Kugeler, and Jens Knobloch — Helmholtz-Zentrum Berlin

When cooling niobium below the critical temperature T_c in the presence of a magnetic below H_{c1}, the magnetic field is expected to be expelled from the sample via the Meissner effect.

However, even below H_{c1} one observes flux trapping - presumably at pinning centers such as impurities and lattice defects - leading to an incomplete Meissner effect or even suppression of the Meissner effect entirely.

We measured the level of flux trapping in niobium samples that have undergone several different treatments commonly employed for the production of superconducting RF cavities, such as chemical and heat treatment. The dependance on the material crystallinity and the influence of spatial and temperoral temperature gradients during cooldown were investigated as well.

TT 58.2 Thu 17:45 HSZ 301

The $I_c(H)$-$T_c(H)$ phase boundary of superconducting Nb thin films with periodic and quasiperiodic antidot arrays — •D. Bothner[1], M. Kemmler[1], R. Cozma[1], V. Misko[2], F. Peeters[2], F. Nori[3], R. Kleiner[1], and D. Koelle[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]Departement Fysica, Universiteit Antwerpen, Belgium — [3]Advanced Science Institute, RIKEN, Japan

The magnetic field dependent critical current $I_c(H)$ of superconducting thin films with artificial defects strongly depends on the symmetry of the defect arrangement. Likewise the critical temperature $T_c(H)$ of superconducting wire networks is heavily influenced by the symmetry of the system. Here we present experimental data on the $I_c(H)$-$T_c(H)$ phase boundary of Nb thin films with artificial defect lattices of different symmetries. For this purpose we fabricated 60 nm thick Nb films with antidots in periodic (triangular) and five different quasiperiodic arrangements. The parameters of the antidot arrays were varied to investigate the influence of antidot diameter and array density. Experiments were performed with high temperature stability ($\Delta T < 1\,\mathrm{mK}$) at $0.5 \leq T/T_c \leq 1$. From the I-V-characteristics at variable H and T we extract $I_c(H)$ and $T_c(H)$ for different voltage and resistance criteria. The experimental data for the critical current density are compared with results from numerical molecular dynamics simulations. We focus on novel quasicrystalline ordering phenomena and the efficient suppression of vortex mobility as reported in V. Misko *et al.*, Phys. Rev. B **82**, 184512 (2010).

TT 58.3 Thu 18:00 HSZ 301

Vortex attraction and vortex clusters — •Ernst Helmut Brandt — Max-Planck-Institut für Metallforschung, Stuttgart

While the Abrikosov vortices in superconductors usually repel each other, there are cases when the vortex interaction has an attractive tail and thus a minimum. This may lead to vortex clusters and chains. Decoration pictures then may look like in the intermediate state of type-I superconductors, showing lamellae or islands of Meissner state or surrounded by Meissner state, but now the normal regions are filled with Abrikosov vortices that are typical for type-II superconductors in the mixed state. Such intermediate-mixed state was observed and investigated in detail in pure Nb, TaN and other materials 40 years ago [1-3]. Recently it was possibly also observed in MgB_2 [4] where it was simply ascribed to the existence of two superconducting electron bands, one of type-I and one of type-II. We expect [5] that the complicated two-band electronic structure of MgB_2 possessing a single transition temperature may indeed lead to vortex interaction with an attractive tail if evaluated numerically.

[1] U. Essmann and H. Träuble, Sci. Am. **224**, 75 (1971).
[2] J. Auer and H. Ullmaier, Phys. Rev. B **7**, 136 (1973).
[3] E. H. Brandt and U. Essmann, phys. stat. sol.(b) **144**, 13-38 (1987).
[4] V. Moshchalkov et al., Phys. Rev. Lett. **102**, 117001 (2009).
[5] E. H. Brandt and M. P. Das, Journal of Superconductivity and Novel Magnetism, in print.

TT 58.4 Thu 18:15 HSZ 301

Quantitative interpretation of the flux lines arrangement and their physical properties in superconducting materials. — •Henry Stopfel[1], Tetyana Shapoval[1], Dmytro S. Inosov[2], Volker Neu[1], Ulrike Wolff[1], Silvia Haindl[1], Jan Engelmann[1], Bernhard Holzapfel[1], Ji Tae Park[2], Dunlu L. Sun[2], Chengtian T. Lin[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

In superconducting thin films as well as in non-ideal single crystals the distribution of magnetic flux quanta is affected by existing defects. This interplay between repulsive vortex-vortex interaction and attractive pinning ends up in a strongly disordered vortex arrangement. Visualization of flux lines with magnetic force microscopy (MFM) followed by the quantitative analysis of data offers direct insight into pinning mechanism on a local scale. We have performed quantitative analysis of MFM images of two superconductors: single crystalline $BaFe_{2-x}Co_xAs_2$ and NbN thin films. Statistical evaluation of the images allows us to conclude about the existence of a short range hexagonal order in the FeAs crystal with strong pinning sites[1]. Evaluation of the measured signal in NbN thin films gives us an information about the local pinning force as well as the magnetic penetration depth.

[1] Inosov et al. PRB 81 014513 (2010)

TT 58.5 Thu 18:30 HSZ 301

Formation and propagation of flux avalanches in MgB_2 films — •Sebastian Treiber[1], Claudia Stahl[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Hochschule Aalen, Beethovenstrasse 1, 73430 Aalen, Germany

Devices made of MgB_2 are substantially limited by the presence of magnetic flux avalanches at temperatures below 10 K. In this case,

quickly moving magnetic vortices create large amounts of heat and magnetic noise.

We found out, that it is necessary to distinguish between mechanisms which are responsible for the formation and the propagation of these avalanches [1]. In addition to the existing knowledge, described in Ref. [2], avalanches form preferably in granular areas with lower current density. This makes a nonlocal description for avalanche-formation necessary. Mechanisms for avalanche-propagation are still under discussion. Since propagation depends on many factors, one has to consider thermal, electrical and superconducting properties as well as the microstructure of the sample. The diverse consequences on formation and propagation explains the preference of avalanches for inhomogeneous superconductors.

[1] S. Treiber and J. Albrecht, New J. Phys. **12**, 093043 (2010)
[2] J. Albrecht *et al.*, Phys. Rev. Lett. **98**, 117001 (2007)

TT 58.6 Thu 18:45 HSZ 301

Influence of dissipation on flux patterns in type-II superconductors — •Constantin Tomaras and Stefan Kehrein — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, D- 80333 München, Germany

Topological quantum field theories constitute the present frontier of theoretical physics [1]. Quite the *oldest* example is the theory of superconductivity, where the appropriate topological charge is just the number of condensed gauge bosons. We formulate a non-equilibrium BCS theory ($d \geq 2$) in presence of a continuous measurement of the local order parameter $\Delta_{BCS} = \langle \Psi_\downarrow^\dagger \Psi_\uparrow^\dagger \rangle$. This allows for local annihilation of pairs of vortices with opposing winding number, while the global phase (∼number of particles-number of holes) is conserved. Depending on the initial flux pattern, the constraint yields to domain wall formation and eventually a percolation transition. Our theory is in agreement with the seminal paper of Toussiant and Wilczek [2], and relevant for recent Hall probe microscopy experiments [3].

[1] E. Witten, Comm. Math. Phys. 121, 3, 351-399 (1989).
[2] D. Toussaint, F. Wilczek, J. Chem. Phys. 78, 2642 (1983).
[3] A. Silhanek et al., Phys. Rev. Lett. 104, 017001 (2010).

TT 59: TR: Topological Insulators 2 (jointly with HL and MA)

Time: Friday 10:30–13:00 Location: HSZ 03

TT 59.1 Fri 10:30 HSZ 03

New Family of Materials for Three-Dimensional Topological Insulators in the Antiperovskite Structure — •Yan Sun[1], Xing-Qiu Chen[1], Dianzhong Li[1], Yiyi Li[1], and Seiji Yunoki[2] — [1]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China — [2]Computational Condensed Matter Physics Laboratory, RIKEN ASI, Saitama 351-0198, Japan

Up to now, all known topological insulators found experimentally and theoretically are related to two families with distinct crystal structures, i.e., one being a cubic non-centrosymmetric zinc-blende HgTe type and the other being a hexagonal centrosymmetric Bi_2Se_3 type. Here, we propose a new family of materials for topological insulators in the antiperovskite structure. Through first-principles calculations, we show evidences that under a proper uniaxial strain, cubic ternary centrosymmetric antiperovskite compounds (M_3N)Bi (M = Ca, Sr, and Ba) are three-dimensional (3D) topological insulators. We also discuss other related materials of the same antiperovskite structure which are good candidates for 3D topological insulators. This proposed family of materials is chemically inert and the lattice structure is well matched to important semiconductors, which provides a rich platform to easily integrate with electronic devices. This work was supported by the "Hundred Talents Project" of Chinese Academy of Sciences and by startup funding of the Institute of Metal Research, CAS in China.

TT 59.2 Fri 10:45 HSZ 03

Transport signatures of Majorana bound states in disordered superconducting nanowires — •Jan Dahlhaus, Michael Wimmer, Fabian Hassler, Anton Akhmerov, and Carlo Beenakker — Instituut-Lorentz, Universiteit Leiden, The Netherlands

Superconducting wires without time-reversal and spin-rotation symmetries can be driven into a topological phase that supports Majorana bound states. We show that the phase transition is signaled by a quantized thermal conductance and electrical shot noise power, irrespective of disorder. In a ring geometry, it is signaled by a period doubling of the magnetoconductance oscillations. Furthermore the influence on the Andreev reflection process at the Fermi level is addressed.

TT 59.3 Fri 11:00 HSZ 03

Majorana bound states without vortices in topological superconductors with electrostatic defects — •Michael Wimmer[1], Anton Akhmerov[1], Maryia Medvedyeva[1], Jakub Tworzydlo[2], and Carlo Beenakker[1] — [1]Universiteit Leiden, The Netherlands — [2]University of Warsaw, Poland

Vortices in two-dimensional superconductors with broken time-reversal and spin-rotation symmetry can bind states at zero excitation energy. These socalled Majorana bound states transform a thermal insulator into a thermal metal and may be used to encode topologically protected qubits. We identify an alternative mechanism for the formation of Majorana bound states, akin to the way in which Shockley states are formed on metal surfaces: An atomic-scale electrostatic line defect can have a pair of Majorana bound states at the end points. The Shockley mechanism explains the appearance of a thermal metal in vortex-free lattice models of chiral p-wave superconductors and (unlike the vortex mechanism) is also operative in the topologically trivial phase.

TT 59.4 Fri 11:15 HSZ 03

Zoology of topological phases and Chern number transfer in an exactly solvable spin model — Graham Kells[1,2], •Janik Kailasvuori[3], Joost Slingerland[1,4], and Jiri Vala[1,4] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Department of Mathematical Physics, National University of Ireland, Maynooth, Ireland — [3]Max-Planck-Institut für Physik komplexer Systeme, Germany — [4]Dublin Institute for Advanced Studies, School of Theoretical Physics, Dublin, Ireland

Exactly solvable models in spin lattices are an important playground for the study of topological phases. A primary tool for identifying these phases is the Chern invariant. For spin lattice models mapping to spinless p-wave fermions as well as for related models of topological insulators the Chern numbers for the ground states have mainly been restricted to $\nu = 0, \pm 1$, although general symmetry arguments would allow for more. With the rich phase zoology of spin-triplet p-wave fermions in mind we look at the square-octagon (4-8) variant of Kitaev's honeycomb lattice model. It allows for a mapping to spinful paired fermions and indeed, the phase diagram of the model turns out to be of unprecedented richness, possessing distinct Abelian and non-Abelian phases with total Chern number $\nu = 0, \pm 1, \pm 2, \pm 3$ and ± 4. Furthermore, we provide details on how the higher Chern numbers are reached by stepwise transfer of Chern numbers between the individual bands.

TT 59.5 Fri 11:30 HSZ 03

Topological phase transitions in quantum spin Hall lattices — •Dario Bercioux[1,2], Nathan Goldman[3], and Daniel F. Urban[2] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universitat, D-79104 Freiburg, Germany — [3]Center for Nonlinear Phenomena and Complex Systems - Universit*é* Libre de Bruxelles (U.L.B.), Code Postal 231, Campus Plaine, B-1050 Brussels, Belgium

Physical phenomena driven by topological properties, such as the quantum Hall effect, have the appealing feature to be robust with respect to external perturbations. Lately, a new class of materials has emerged manifesting their topological properties at room temperature and without the need of external magnetic fields. These topological insulators are band insulators with large spin-orbit interactions and exhibit the quantum spin-Hall (QSH) effect. Here we investigate the transition between QSH and normal insulating phases under topological deformations of a two-dimensional lattice. We demonstrate that the QSH phase present in the honeycomb lattice looses its robustness as the occupancy of extra lattice sites is allowed [1]. Furthermore, we propose a method for verifying our predictions with fermionic cold atoms in op-

tical lattices. In this context, the spin-orbit interaction is engineered via an appropriate synthetic gauge field [2].
[1] D. Bercioux, N. Goldman, and D.F. Urban, arXiv:1007.2056.
[2] N. Goldman *et al.*, arXiv:1011.3909 Phys. Rev. Lett. (2010) *in press.*

15 min. break

TT 59.6 Fri 12:00 HSZ 03

Bound states and persistent currents in topological insulator rings — •Patrik Recher and Paolo Michetti — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

We analyze theoretically the bound state spectrum of an Aharonov Bohm (AB) ring in a two-dimensional topological insulator using the four-band model of HgTe-quantum wells as a concrete example. We calculate analytically the circular helical edge states and their spectrum as well as the bound states evolving out of the bulk spectrum as a function of the applied magnetic flux and dimension of the ring. We also analyze the spin-dependent persistent currents, which can be used to measure the spin of single electrons. We further take into account the Rashba spin-orbit interaction which mixes the spin states and derive its effect on the ring spectrum. The flux tunability of the ring states allows for coherent mixing of the edge- and the spin degrees of freedom of bound electrons which could be exploited for quantum information processing in topological insulator rings.

TT 59.7 Fri 12:15 HSZ 03

Dephasing of spin and charge interference in helical Luttinger liquids — •Pauli Virtanen and Patrik Recher — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We consider a four-terminal Aharonov-Bohm interference setup formed out of two edges of a quantum spin Hall insulator, supporting helical Luttinger liquids (HLLs). We show that the temperature and bias dependence of the interference oscillations are linked to the amount of spin flips in tunneling between two HLLs which is a unique signature of a HLL. We predict that spin dephasing depends on the electron-electron (e-e) interaction but differently from the charge dephasing due to distinct dominant tunneling excitations. In contrast, in a spinful Luttinger liquid with SU(2) invariance, uncharged spin excitations can carry spin current without dephasing in spite of the presence of e-e interactions.

TT 59.8 Fri 12:30 HSZ 03

Helical modes in carbon nanotubes generated by strong electric fields — •Jelena Klinovaja, Manuel J. Schmidt, Bernd Braunecker, and Daniel Loss — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Helical modes, conduction channels transporting opposite spins in opposite directions, naturally lead to spin filtering, but they have also potential application as Cooper pair splitters and, if in proximity with a superconductor, lead to Majorana bound states at the edges of the conductor. Helical modes have also attracted much attention recently in the context of topological insulators. Such physics may be achieved in CNTs [1]. This is a consequence of the interplay between spin-orbit interaction and strong electric fields. Starting from a tight-binding model we derive the effective low-energy Hamiltonian and the resulting spectrum. Helical modes are shown to exist in metallic armchair nanotubes in an all-electric setup. The helical regime can also be obtained in chiral metallic nanotubes by applying an additional magnetic field. In particular, it is possible to obtain helical modes at one of the two Dirac points only, while the other one remains gapped.
[1] Jelena Klinovaja, Manuel J. Schmidt, Bernd Braunecker, and Daniel Loss, arXiv:1011.3630

TT 59.9 Fri 12:45 HSZ 03

Chirality Induced Tilted-Hill Giant Nernst Signal — •Panagiotis Kotetes[1], Gerd Schön[1,3], Alexander Shnirman[2,3], and Georgios Varelogiannis[4] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [3]DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany — [4]Department of Physics, National Technical University of Athens, GR-15780 Athens, Greece

We reveal a novel source of giant Nernst response exhibiting strong non-linear temperature and magnetic field dependence including the mysterious tilted-hill temperature profile observed in a pleiad of materials [1]. The phenomenon can originate either from a topological insulator or from the formation of a chiral order parameter. Particular examples are the Quantum Anomalous Hall state and the chiral d-density wave, respectively. The occurence of this giant thermoelectric response is distinctly different from the usual quasiparticle and vortex Nernst mechanisms. Our picture provides a unified understanding of the anomalous thermoelectricity observed in materials as diverse as hole doped cuprates [1] and heavy-fermion compounds like URu2Si2 [2]. Moreover, fingerprints of this phenomenon could be observed on the surface of several 3D topological insulators.
[1] P. Kotetes and G. Varelogiannis, Phys. Rev. Lett. 104, 106404 (2010).
[2] P. Kotetes, A. Aperis, and G.Varelogiannis, arXiv:1002.2719.

TT 60: SC & MLT: Cryodetectors

Time: Friday 10:30–13:15 Location: HSZ 301

TT 60.1 Fri 10:30 HSZ 301

Ultra-thin TaN films for infrared Superconducting Nanowire Single-Photon Detectors — •Konstantin Ilin[1], Dagmar Rall[1,4], Matthias Hofherr[1], Michael Siegel[1,5], Alexei Semenov[2], Heinz-Wilhelm Hübers[2], Andreas Engel[3], Kevin Inderbitzin[3], Adrian Aeschbacher[3], and Andreas Schilling[3] — [1]IMS, Karlsuher Institut für Technologie, Karlsruhe, Deutschland — [2]DLR Institut für Planetenforschung, Berlin, Deutschland — [3]Physik-Institut der Universität Zürich, Zürich, Schweiz — [4]LTI, KIT, Karlsruhe, Deutschland — [5]DFG CFN, Karlsruhe, Deutschland

The quest for the development of superconducting nanowire single-photon detectors (SNSPD) with higher intrinsic detection efficiency in a wider spectral range stimulates the study of ultra-thin films of different superconducting materials. Tantalum nitride (TaN) is considered as a promising candidate for the development of SNSPDs for infra-red radiation. Thin superconducting TaN films were deposited by reactive magnetron sputtering from a pure Ta target in a gas mixture of Ar and N_2. The films were deposited on sapphire substrates heated to about 550 C. The transition temperature T_c of the thickest films (15 nm) was about 9.6 K. It decreased with the thickness remaining larger than 7 K for films with a thickness of 4 nm. SNSPDs made from TaN films have a critical current density of a few MA/cm^2 at 4.2K and T_c only slightly less than T_c of non-patterned films. Superconducting and normal state properties of micrometer and sub-micrometer sized TaN structures will be discussed in details. The single-photon response of TaN SNSPDs will be presented for the first time.

TT 60.2 Fri 10:45 HSZ 301

Microwave Kinetic Inductance Detectors for astronomy and particle detection — •Christian Hoffmann[1], Alessandro Monfardini[1], Markus Roesch[2], and Karl Schuster[2] — [1]Institut Néel, CNRS & Université J. Fourier, BP 166, 38042 Grenoble, France — [2]IRAM, 300 rue de la piscine, 38406 St. Martin d'Hères, France

A new type of superconducting detector, the Microwave Kinetic Inductance Detector, has recently drawn the attention of the low-temperature detector community. Easy fabrication, high sensitivity, low time constants and most notably the intrinsic capability to frequency multiplexing open new possibilities to applications that need very large array sizes and/or high speed read-out. We develop detector arrays for applications in the domain of astronomy, particle detection, phonon imaging and Helium-physics based on Lumped Element KIDs (LEKIDs). In a LEKID a resonant circuit composed of a discrete inductance and capacitance is coupled to a transmission line. The constant current density in the inductive part makes it a very efficient detector for em-radiation and particles. In this contribution we discuss detector principle, design and measured characteristics. Then we

focus on the application for a millimeter wavelength camera, successfully tested at the IRAM 30-meter telescope at Pico Veleta, Spain in October 2010. The current instrument contains two arrays at 100 mK with more than 100 pixels on one read-out-line each for observations at 1.3 and 2 mm. The performances are the best achieved as of today for groundbased KIDs with sensitivities already comparable with existing (horns-coupled bolometers) instruments.

Invited Talk TT 60.3 Fri 11:00 HSZ 301

Engineering Atomic-Scale Spin Systems — •Sebastian Loth — IBM Research - Almaden, San Jose, CA

When magnetic structures shrink to a point where they consist of only a few atoms, their continuously variable magnetization transforms into a spin with quantized states. Their dynamical behavior is determined by the energetic distribution of these states. We demonstrate that low temperature scanning tunneling microscopy can access both the energetic and dynamical properties of electron spins in transition metal atoms that were placed on a Cu_2N overlayer on Cu(100).

Inelastic electron tunneling spectroscopy measures the transition energies of the atomic spins. Fe atoms experience large easy-axis anisotropy leading to a potentially bistable configuration, whereas Mn atoms in high magnetic field form a uniform ladder of spin states that is inherently unstable. The STM gains access to the corresponding dynamical evolution by all-electronic pump-probe spectroscopy. We measure the spin relaxation time of individual atoms or nanostructures with nanosecond precision and find that placing Cu atoms in decreasing distances to Fe atoms successively boosts the Fe atom's magnetic anisotropy energy and increases the spin relaxation time beyond 200 ns.

For potential spintronics applications, these experiments demonstrate the ability to manipulate the energetic structure of individual atomic spins and to directly monitor the resulting effect on the spin dynamics.

TT 60.4 Fri 11:30 HSZ 301

Cryogenic single-photon detector on the base of a S-I-N-I-S type single-electron trap — •Sergey V. Lotkhov[1], Antti Kemppinen[2], Olli-Pentti Siara[3], Jukka P. Pekola[3], and Alexander B. Zorin[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Brausnchweig — [2]Centre for Metrology and Accreditation (MIKES), P.O. Box 9, 02151 Espoo, Finland — [3]Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 AALTO, Finland

For a long time, extremely high sensitivity of the single-electron circuits in respect to their electromagnetic environment was considered as a bottle neck for realization of a quantum current standard. For example, our recent experiments with the so-called hybrid superconductor-normal metal electron turnstiles on the base of Al and AuPd revealed an inherent relation of the pumping accuracy to the quality of noise filtering for such a device. In the current work, we generalize the task and regard our single-electron trapping circuit as a detector of single noise quanta, reaching the sample even in a well-filtered cryogenic setup at T $\sim$ 100 mK. Owing to simplicity of the hybrid approach: our trap is built on a basic two-junction hybrid device controlled by a single gate, we can characterize not only the average noise level, but to conclude on the noise spectrum of the particular setup as well, on the frequency scale around $f \sim (E_c + \Delta)/h \sim$100-200 GHz, where E_c is the charging energy barrier in the trap, and Δ is a superconducting energy gap of Al.

15 min. break

TT 60.5 Fri 12:00 HSZ 301

Physics and Applications of Metallic Magnetic Calorimeters — •C. Pies, S. Heuser, A. Kampkötter, S. Kempf, J.-P. Porst, P. Ranitzsch, S. Schäfer, S. Vick, T. Wolf, L. Gastaldo, A. Fleischmann, and C. Enss — Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

Metallic Magnetic Calorimeters (MMCs) are calorimetric particle detectors which are typically operated at temperatures below 100 mK. A paramagnetic sensor material is used to convert the temperature rise due to the absorbtion of a massive particle or photon to a change of magnetic flux which is detected by a SQUID magnetometer.

Since the thermodynamic properties of the detectors can be predicted with confidence, MMCs can be designed for specific applications with optimized performance concerning detection efficiency and energy resolution. Currently, an energy resolution of 2.7 eV (FWHM) for x-ray photons with energies of 6 keV has been achieved with fully micro-fabricated detectors and resolutions below 1 eV are expected for the next generation of devices. MMCs are being developed for a wide range of applications including x-ray spectroscopy of highly charged ions, direct neutrino mass measurements by beta spectroscopy, x-ray cameras for astronomy, calibration of radiation standards in metrology and spatially resolved detection of molecular fragments.

We present an introduction to the physics of MMCs and detector geometries for a variety of applications and discuss design considerations and micro-fabrication processes of current devices and their experimental performance.

TT 60.6 Fri 12:15 HSZ 301

Development of non-hysteretic unshunted rf-SQUIDs for multiplexed MMC readout — •S. Kempf, A. Fleischmann, L. Gastaldo, S. Heuser, A. Kampkötter, C. Pies, J.-P. Porst, P. Ranitzsch, S. Schäfer, S. Vick, T. Wolf, and C. Enss — Kirchhoff Institute for Physics, Heidelberg University.

Metallic magnetic calorimeters (MMCs) are energy dispersive particle detectors with a high resolving power that are operated at temperatures below 100 mK. Presently single channel MMCs are proving to be promising detectors in areas diverse as atomic and nuclear physics or x-ray astronomy, while many of those experiments would greatly benefit from large detector arrays. However, array readout poses a significant challenge since a multiplexing scheme is required. A promising approach employs a microwave SQUID multiplexer consisting of non-hysteretic unshunted rf-SQUIDs that are coupled to high Q tank circuits with unique resonance frequencies. By coupling all tank circuits to a common transmission line and injecting a microwave frequency comb it is possible to monitor all detectors simultaneously.

We discuss design, fabrication and operation of a microwave SQUID multiplexer for the readout of MMC detector arrays. For our present devices we used SNEAP to produce micron-size Nb/Al-AlO_x/Nb Josephson junctions with low critical current densities. The quality of the fabricated Josephson junctions is discussed. Finally we outline the expected performance of a detector array that is read out with the designed SQUID multiplexer as derived from numerical optimization calculations.

TT 60.7 Fri 12:30 HSZ 301

3D power distribution scan of Gaussian beams and THz-antennas — •Christian Brendel, Alexander Guillaume, 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 power distribution of far infrared Gaussian beams in the free space. Close to the beam waist we irradiated different THz antennas from below and scanned the radiation pattern in the 3D half space above the antennas. As scanning sensor we employ a Josephson-junction from the high-temperature superconductor $YBa_2Cu_3O_7$ on cantilever prepared from a $LaAlO_3$-bicrystal. The antenna on the Josephson-junction has to be smaller than the wavelength to achieve high spatial resolution but large enough to be able to detect sufficient power. Also the characteristic frequency, antenna impedance, bandwidth up to 1 THz and connection filters have to be optimized for a $LaAlO_3$-bicrystal substrate. The setup is mounted inside a vacuum chamber on x-, y- and z-tables with 15 mm scan length and is cooled down to a temperature of 38 K by a cryocooler. 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. We realized a quasi-optic THz-lens system to transfer the far infrared beam into the vacuum chamber.

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

TT 60.8 Fri 12:45 HSZ 301

Coherent broadband THz spectrometer using photomixers in combination with magneto-cryostats: A compact solution for spectroscopy at low temperature and high magnetic field — •Komalavalli Thirunavukkuarasu[1], Andreas Janssen[1], Malte Langenbach[1], Holger Schmitz[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Axel Roggenbuck[3], Anselm Deninger[3], Markus Grüninger[1], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln, Germany — [2]Max-Planck Institute for Radio Astronomy, Auf dem Hügel

69, D-53121 Bonn, Germany — [3]TOPTICA Photonics AG, Lochhamer Schlag 19, D-82166 Gräfelfing, Germany

We present the first results of the integration of a cw THz spectrometer together with magneto-cryostats for use at low temperatures and high magnetic fields. The high-resolution spectrometer employs photomixing of two NIR-DFB lasers for generation and phase sensitive detection of THz radiation in the frequency range from 60 GHz to 1.5 THz. A fiber-based phase modulation technique is used to accurately determine the amplitude and the phase at a given frequency. The complex optical functions can be evaluated from the full phase information of the THz beam. Recently, this compact spectrometer was successfully integrated within a magneto-cryostat. This system is one of the very few experimental realizations that allow for investigations at magnetic fields up to 16 T and temperatures down to 3 K with excellent reliability. The response of photomixers and the general operation of the spectrometer in these experimental conditions will be outlined.

TT 60.9 Fri 13:00 HSZ 301

Micro-Hall Magnetometer for Molecular Nanomagnets — •Alexander Sundt and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany

In recent years the molecular nanomagnets (MNMs), e.g., the single-molecule magnets, have been the subject of many studies, as they exhibit phenomena such as magnetic hysteresis and quantum tunneling of the magnetization, which make them candidates for single molecule data storage devices and bits for quantum computing. To investigate this class of materials it is of apparent importance to measure their magnetization. The micro-Hall probes have been proven to be a highly sensitive and robust method in this direction. In this talk we will present the latest improvements of our in-house built magnetometer. The setup provides now an extended temperature range from 1.4 to 300 K and higher magnetic fields up to 7 T. However, the main improvements were to use: 1) novel micro-Hall sensors providing an increased sensitivity of up to 10^{-9} emu, 2) a double micro-Hall sensor configuration as well as a mimic, which allows for an in-situ adjustment of the orientation of the micro-Hall sensors to compensate for the main magnetic field, and 3) an improved scheme to measure light-induced magnetism in molecular clusters. The data recorded on several MNMs will be shown and discussed.

TT 61: TR: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3

Time: Friday 10:30–12:45 Location: HSZ 304

TT 61.1 Fri 10:30 HSZ 304

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, 93040 Regensburg, Germany — [2]Physics Department, University of Arizona, AZ 85716, USA

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 [1] 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 systems using analytical models and numerical methods. This work is supported by the DFG under grant SPP 1285.

[1] D. Loss, and D. P. DiVincenzo, Quantum computation with quantum dots, Phys. Rev. A 57, 120 (1998)

TT 61.2 Fri 10:45 HSZ 304

Negative differential conductance with symmetric set-up ? — •Andrea Donarini, Abdullah Yar, and Milena Grifoni — Universität Regensburg, Germany

We consider a minimal model of transport through a nano-junction in the single electron tunneling regime. We prove that the source-drain asymmetric is not a necessary condition for the appearance of negative differential conductance (NDC). The latter is obtained even for a completely symmetric set up under specific conditions over the "geometrical component" of the tunneling rates. We apply the theory to study the transport characteristics of suspended carbon nanotube quantum dots. The electron-phonon coupling tunes in this case the "geometrical component" of the rates and determines the presence of NDC. Moreover, the interplay of Franck-Condon factors and spin/pseudo-spin degeneracies generates gate asymmetries in the stability diagram.

TT 61.3 Fri 11:00 HSZ 304

Decoherence in a Double-Dot Aharonov-Bohm Interferometer — •Björn Kubala[1], David Roosen[2], Michael Sindel[3], Walter Hofstetter[2], and Florian Marquardt[1] — [1]Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Goethe Universität, 60438 Frankfurt/Main, Germany — [3]Physics Department, ASC and CeNs, Ludwig-Maximilians-Universität, 80333 Munich, Germany

Coherence in electronic interferometers is typically believed to be restored fully in the limit of small voltages, frequencies and temperatures. However, it is crucial to check this essentially perturbative argument by nonperturbative methods. Here, we use the numerical renormalization group to study ac transport and decoherence in an experimentally realizable model interferometer, a parallel double quantum dot coupled to a phonon mode. The model allows to clearly distinguish renormalization effects from decoherence. We discuss finite frequency transport and confirm the restoration of coherence in the dc limit.

TT 61.4 Fri 11:15 HSZ 304

Adiabatic State Evolution: a new route to nonequilibrium physics — •Marion Moliner and Peter Schmitteckert — Karslruhe Institute of Technology

In recent years, the development of time dependent simulations of quantum systems have led to major steps in understanding non-equilibrium quantum systems. In these simulations, one typically studies the evolution of a system after a quench. In contrast, analytical approaches like Keldysh techniques can be traced back to the Lippmann-Schwinger equation, which itself is based on the concept of switching on perturbations adiabatically. In this work we present an approach which combines concepts of both techniques. By tracking the response of a system to an external perturbation adiabatically, we are able to access the non-equilibrium regime of a quantum system. We apply this method to interacting fermions in one dimension within the framework of the Density Matrix Renormalization Group technique.

TT 61.5 Fri 11:30 HSZ 304

Time-convolutionless master equation for quantum dots to all orders in the tunneling — •Carsten Timm — Technische Universität Dresden, Germany

Master equations describing the non-equilibrium dynamics of a quantum dot coupled to metallic leads are considered. I derive an exact time-convolutionless master equation for the probabilities of dot states, i.e., a *Pauli* master equation. The derivation naturally leads to an expansion in the tunneling amplitudes between dot and leads, which is obtained to arbitrary order. Relations to the time-nonlocal Nakajima-Zwanzig master equation and to the T-matrix approach are exhibited. The absence of divergences in the time-convolutionless and Nakajima-Zwanzig formalisms is demonstrated for all orders.

15 min. break

TT 61.6 Fri 12:00 HSZ 304

Modeling a scanning tunneling microscope: a nano-DΓA study — •Viktoria Motsch, Angelo Valli, Giorgio Sangiovanni, Alessandro Toschi, and Karsten Held — Institut für Festkörperphysik, TU Wien, Österreich

We apply nano-DΓA [1], a new approach to nanoscopic systems based on Dynamical Vertex Approximation (DΓA)[2], to study the tip of a

scanning tunneling microscope (STM). Due to the geometrical confinement, we expect electronic correlations to play a more pronounced role in such a system. Decreasing the hybridization strength between the tip and the surface, the atom forming the contact undergoes a local Mott-Hubbard crossover (i.e. we observe a suppression of the spectral weight at the Fermi level). We study this phenomena and compute the conductance through the tip for different lattice structures and set of parameters.Our finding has important implications for interpreting STM images: The presumed proportionality of the conductance to the local density of states of the material scanned does not necessarily hold for STM tips made out of transition metals.

[1] A. Valli, *et al.*, Phys. Rev. Lett. **104**, 246402 (2010)
[2] A. Toschi, *et al.*, Phys. Rev. B **75**, 045118 (2007)

TT 61.7 Fri 12:15 HSZ 304

Transport measurements on single Bi nanowires at temperatures below 1 K — •C. Reiche[1], T. Peichl[1,2], S. Mueller[3], M.E. Toimil-Molares[3], R. Neumann[3], and G. Weiss[1,2] — [1]Physikalisches Institut, KIT Karlsruhe — [2]Centrum für funktionelle Nanostrukturen, KIT Karlsruhe — [3]GSI Darmstadt

With its large Fermi wavelength and long mean free paths, Bi is a fascinating metal for studies of transport phenomena in samples of reduced dimensions. Previous transport measurements on bundles of crystalline Bi wires with diameters around 100 nm found a remarkable decrease of sample resistance below 300 mK. Localization effects were ruled out as a cause of this decrease, so one might speculate that surface states are able to change the electronic structure of Bi in a way that it may exhibit superconductive properties. Very recently other groups have conducted measurements on single Bi nanowires and found that their data also fit superconductivity, probably induced by a surface layer of Bi oxide or other contaminants on the surface of the wires. Our samples are produced by a template method, using an ion track etched polycarbonate membrane. It has been shown that using these membranes it is possible to extract single wires without oxidation of the surface. From these samples we are preparing single Bi wires and contact them in 2- or 4-point contact geometry. We are conducting transport measurements to study the influence of different surface layers on the transport properties of the Bi wires at temperatures below 1 K. Furthermore we are gathering additional data to decide if the observed behavior may be attributed to superconductivity.

TT 61.8 Fri 12:30 HSZ 304

Cotunneling in the 5/2 fractional quantum Hall regime — •Robert Zielke, Bernd Braunecker, and Daniel Loss — University of Basel

We consider two fractional quantum Hall samples weakly coupled via a quantum dot and investigate whether there are specific signatures for the $\nu = 5/2$ wave functions, especially the Moore-Read wave function, in the tunneling between the edge states through the quantum dot. The focus is specifically on the cotunneling regime, both elastic and inelastic.

TT 62: CE: Low-dimensional Systems - Models 2

Time: Friday 10:30–13:15 Location: HSZ 105

TT 62.1 Fri 10:30 HSZ 105

Entanglement Hamiltonian of quantum spin systems — •Vincenzo Alba, Masud Haque, and Andreas Lauchli — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We investigate the 'entanglement hamiltonian' of one-dimensional quantum spin systems, such as the XXZ chain and Heisenberg ladders. We analyze entanglement spectra obtained using exact diagonalization and DMRG. We provide physical insight into the main features of the spectra through perturbative calculations. In particular we show that the physics at the block boundaries plays a crucial role in determining the form of the entanglement spectrum and hence of the entanglement Hamiltonian.

TT 62.2 Fri 10:45 HSZ 105

Robustness of the toric code in an arbitrary magnetic field — Sébastien Dusuel[1], •Michael Kamfor[2], Román Orús[3], Kai Phillip Schmidt[2], and Julien Vidal[1] — [1]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [2]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Str. 4, TU Dortmund, 44221 Dortmund, Germany — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

We investigate the stability of the topological phase in the toric code model in the presence of an arbitrary uniform magnetic field by means of variational approach (iPEPS) and high order series expansion (PCUT). It is found that when this perturbation is strong enough, the anyonic gap closes and the system undergoes a phase transition whose nature depends on the field orientation. When this transition is of second order, it is in the Ising universality class except for a special line on which the critical exponent, driving the closure of the gap, varies continuously

TT 62.3 Fri 11:00 HSZ 105

Interaction-induced Fermi-surface renormalization in frustrated Hubbard models — •Luca F. Tocchio[1], Federico Becca[2], and Claudius Gros[1] — [1]Institute for Theoretical Physics, Frankfurt University, Max-von-Laue-Straße 1, D-60438 Frankfurt a.M., Germany — [2]CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy

We investigate the nature of the interaction-driven Mott-Hubbard transition for frustrated Hubbard models, using a variational Monte Carlo approach including a distance-dependent Jastrow factor and a novel-type of holon-doublon correlation, the so-called backflow correlations. They allow to treat the doublon-holon excitons correctly in the large-U limit and for an improved understanding of the Fermi-surface renormalization close to the Mott-Hubbard transition. Indeed, we find that the Fermi surface renormalizes to perfect nesting right at the Mott-Hubbard transition in the insulating state, with a first-order reorganization when crossing the transition into the metallic state. This result may potentially change our view of the Mott-Hubbard transition in finite dimensions, since it seems to be qualitatively different from its infinite-dimension analogon.

TT 62.4 Fri 11:15 HSZ 105

Excitations and spectral densities of the one-dimensional Ising model in a field — •Marc Daniel Schulz and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The one-dimensional quantum Ising model in a transverse field is a well-studied model in theoretical physics, which was solved exactly more than 40 years ago. 30 years ago, the prediction of the existence of a certain number of bound states at the critical point in the presence of an infinitesimal longitudinal field was made by integrable field theory. Here we study the excitation spectra and the spectral densities of the Ising model in a transverse and a longitudinal field, containing the physics of free and confined quasi-particles. To this end, we derive effective low-energy models for the low- and for the high-field case by means of perturbative and graph-based continuous unitary transformations. Our calculations are expected to be relevant for recent inelastic neutron scattering measurements on the quasi one-dimensional compound $CoNb_2O_6$ which is believed to be effectively described by an one-dimensional Ising model in a field.

TT 62.5 Fri 11:30 HSZ 105

Spin Correlations and Excitations in Small Antiferromagnetic Clusters — •Maren Gysler, Nikolaos P. Konstantinidis, and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

The importance of understanding correlations in small spin clusters has risen in recent years with the availability of magnetic systems such as single-molecule magnets and spins attached to surfaces, which consist of a dozen or so antiferromagnetically coupled metal centers with potentially large spin lengths. Strong correlations between neighboring spins are difficult to single out when the familiar product basis or irreducible tensor operator techniques are used. An efficient way to study ground-state correlations and low-energy spectra of small clusters is

the use of the valence bond basis, which defines a natural framework where strong short range correlations can directly be incorporated in the Hilbert space basis. Using the different bases we investigate the spin correlations and excitations in a number of generic spin systems, with particular emphasis on understanding the influence of the topology of the exchange couplings. Typical theoretical models would include the even and odd short chains with large spins and small wheels.

15 min. break

TT 62.6 Fri 12:00 HSZ 105

Real-Space Renormalization Yields Finite Correlations — Thomas Barthel, •Martin Kliesch, and Jens Eisert — Potsdam University

Real-space renormalization approaches for quantum lattice systems generate certain hierarchical classes of states that are subsumed by the multiscale entanglement renormalization Ansatz (MERA). It is shown that, with the exception of one spatial dimension, MERA states are actually states with finite correlations, i.e., projected entangled pair states (PEPS) with a bond dimension independent of the system size [1]. Hence, real-space renormalization generates states which can be encoded with local effective degrees of freedom, and MERA states form an efficiently contractible class of PEPS that obey the area law for the entanglement entropy.
[1] Phys. Rev. Lett. 105, 010502 (2010)

TT 62.7 Fri 12:15 HSZ 105

The 1-D t-J model in and out of equilibrium — •Alexander Moreno and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart, Germany

On the basis of the density matrix renormalization group (DMRG) we study the ground-state phase diagram of the model and the excitation content of each phase. As a first step, we determine the transition lines between a repulsive Luttinger liquid (LL) phase, an attractive LL phase, a spin-gap (Luther-Emery - LE) phase, and phase-separation. In particular, we resolve a controversy about the extension of the LE phase, and show evidence for real-space pairing deep in that phase. By switching an electric field after the creation of an electron in the system, we aim at identifying the charge of the fractionalized elementary excitations that result from the electron. A previous quantum Monte Carlo simulation of the model [1] revealed that the spectral content of the electron addition spectrum could be accounted for by a spinon, a holon, and an antiholon, as in the supersymmetric $1/r^2$ t-J model [2]. These excitations have respectively $S = 1/2$, $Q = 0$; $S = 0$, $Q = -e$; and $S = 0$, $Q = 2e$, where e is the charge of the electron.
[1] C. Lavalle, M. Arikawa, S. Capponi, F. F. Assaad, and A. Muramatsu, Phys. Rev. Lett. **90**, 216401 (2003).
[2] M. Arikawa, Y. Saiga, and Y. Kuramoto, Phys. Rev. Lett. **86**, 3096 (2001).

TT 62.8 Fri 12:30 HSZ 105

Relaxation dynamics of an exactly solvable electron-phonon model — •Dante Marvin Kennes and Volker Meden — Institut für Theoretische Physik A and JARA-Fundamentals of Future Information Technology, RWTH Aachen University, 52056 Aachen, Germany

We address the question whether observables of an exactly solvable model of electrons coupled to (optical) phonons relax into large time stationary state values and investigate if the asymptotic expectation values can be computed using a stationary density matrix. A sudden quench of the electron-phonon coupling, starting from the noninteracting canonical equilibrium at temperature T in the electron as well as in the phonon subsystems is considered as well as a setup being given by the product of the phonon vacuum and the filled Fermi sea supplemented by a highly excited additional electron. In accordance with earlier studies of such type of models we find that expectation values which become stationary can be described by the density matrix of a generalized Gibbs ensemble which differs from that of a canonical ensemble.

TT 62.9 Fri 12:45 HSZ 105

Local density of states of a quarter-filled 1D Mott insulator with a boundary — •Dirk Schuricht — Institut für Theorie der Statistischen Physik, RWTH Aachen — JARA-Fundamentals of Future Information Technology

We determine the local density of states (LDOS) of a quarter-filled one-dimensional Mott insulator in the presence of a strong impurity potential, which is modeled by a boundary. To this end we calculate the Green function in the low-energy limit using field theory techniques. The Fourier transform of the LDOS shows signatures of a pinning of the spin density wave at the imprity as well as several dispersing features at frequencies above the charge gap, which can be interpreted as propagating spin and charge degrees of freedom. Finally, we discuss the effect of bound states localized at the impurity.

TT 62.10 Fri 13:00 HSZ 105

Correlation effects in quantum spin Hall states: a Quantum Monte Carlo study — Martin Hohenadler, •Thomas C. Lang, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We consider a quantum spin hall insulator as realized by the Kane-Mele model with spin orbit coupling λ supplemented by a Hubbard U term. On the basis of projective auxiliary field quantum Monte Carlo simulations on lattice sizes up to 12×12, we map out the magnetic phase diagram. Beyond a critical value of $U > U_c$ the quantum spin Hall insulating state is unstable towards magnetic ordering. At $U < U_c$ we study the spin, charge and single particle dyanmics of the helical edge state by retaining the Hubbard interactions only on the edge of a ribbon. As U_c is approached we observe a substantial depletion of low-lying spectral weight in the dynamical charge structure factor, and a robust signature of the helical edge state in the single particle spectral function.