Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

Michael Siegel
Universität Karlsruhe
Institut für Mikro- und Nanoelektronische Systeme
Hertzstraße 16
76128 Karlsruhe
m.siegel@ims.uni-karlsruhe.de

Overview of Invited Talks and Sessions

(lecture rooms HSZ 03, HSZ 105, HSZ 301, and HSZ 304; Poster P1A and P1B)

Invited Talks

TT 1.1	Mon	10:15–10:45	HSZ 03	**Strongly Correlated Fermionic Quantum Gases in Optical Lattices** — •Immanuel Bloch
TT 4.1	Mon	11:15–11:45	HSZ 105	**Stimulated Cooperative Dynamics in Complex Solids** — •Andrea Cavalleri
TT 13.1	Tue	9:30–10:00	HSZ 03	**Photons, Qubits and Computers - A Quantum Mechanics Lab on a Chip** — •Andreas Wallraff
TT 14.4	Tue	10:15–10:45	HSZ 105	**Evidence for a novel superconducting state in high magnetic fields** — •Joachim Wosnitza
TT 16.8	Tue	11:30–12:00	HSZ 304	**Two Dimensional Electron Gases at Oxide Interfaces** — •Jochen Mannhart
TT 21.1	Tue	14:00–14:30	HSZ 304	**Correlated charge detection in quantum dots** — •Klaus Ensslin
TT 22.1	Wed	9:30–10:00	HSZ 03	**Thermal expansion and magnetostriction close to quantum criticality** — •Markus Garst
TT 24.5	Wed	10:30–11:00	HSZ 301	**Theory of time-resolved optical and photoemission spectroscopy for correlated electron systems** — •Marcus Kollar
TT 26.1	Wed	14:00–14:30	HSZ 03	**Nanotube and Graphene ElectroMechanics** — •Adrian Bachtold
TT 28.1	Wed	15:15–15:45	HSZ 105	**Unconventional Superconductivity induced by Interfaces and Surfaces** — •Matthias Eschrig
TT 36.2	Thu	10:00–10:30	HSZ 03	**Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors** — •Andrey Chubukov
TT 37.8	Thu	11:30–12:00	HSZ 105	**Quantum dissipative spin ratchets** — •Milena Grifoni
TT 39.1	Thu	9:30–10:00	HSZ 304	**Electron spin resonance in Kondo systems** — •Peter Wölfle

Program of the Focussed Session "The Mott Transition in Model Systems"

TT 1.1	Mon	10:15–10:45	HSZ 03	**Strongly Correlated Fermionic Quantum Gases in Optical Lattices** — •Immanuel Bloch
TT 1.2	Mon	10:45–11:15	HSZ 03	**Mott transition and metastable superconductivity of repulsive Fermions in optical lattices** — •Achim Rosch
TT 1.3	Mon	11:15–11:45	HSZ 03	**Carrier dynamics of two-dimensional organic charge-transfer salts close to the Mott transition** — •Martin Dressel, Natalia Drichko, Michael Dumm, Jaime Merino
TT 1.4	Mon	12:00–12:30	HSZ 03	**Mott Transition in Frustrated Lattice Systems** — •Hirokazu Tsunetsugu
TT 1.5	Mon	12:30–13:00	HSZ 03	**Lattice Effects in Strongly Correlated π-electron Systems Close to the Mott Transition** — •M. de Souza, A. Bruehl, C. Strack, B. Wolf, R.S. Manna, J.A. Schlueter, D. Schweitzer, M. Lang

Program of the Focussed Session "Superconducting Quantum Circuits"

TT 13.1	Tue	9:30–10:00	HSZ 03	**Photons, Qubits and Computers - A Quantum Mechanics Lab on a Chip** — •Andreas Wallraff
TT 13.2	Tue	10:00–10:30	HSZ 03	**Two-photon probe of the Jaynes-Cummings model and controlled symmetry breaking in circuit QED** — Frank Deppe, Matteo Mariantoni, Edwin P. Menzel, •Achim Marx, Rudolf Gross, S. Saito, K. Kakuyanagi, H. Tanaka, K. Semba, T Meno, H. Takayanagi, E. Solano
TT 13.3	Tue	10:30–11:00	HSZ 03	**Landau-Zener Transitions in Qubit-Oscillator Settings** — •Sigmund Kohler
TT 13.4	Tue	11:15–11:45	HSZ 03	**Experiments on the quantum of heat conductance** — •Jukka Pekola, Matthias Meschke, Andrey Timofeev, Wiebke Guichard, Meri Helle, Mikko Möttönen
TT 13.5	Tue	11:45–12:15	HSZ 03	**Preparation of arbitrary quantum states in a microwave resonator** — •Max Hofheinz, Haohua Wang, Markus Ansmann, Radoslaw Bialczak, Erik Lucero, Matthew Neeley, Aaron O'Connell, Daniel Sank, James Wenner, John Martinis, Andrew Cleland
TT 13.6	Tue	12:15–12:30	HSZ 03	**Phase diffusion in single-qubit lasers** — •Stephan André, Valentina Brosco, Alexander Shnirman, Gerd Schön

Program of the Focussed Session "Superconductivity and Magnetism in Ferropnictides and Related Materials"

TT 36.1	Thu	9:30–10:00	HSZ 03	**Superconductivity and Magnetism in $LaO_{1-x}F_xFeAs$** — •Bernd Buechner, Hans-Joachim Grafe, Christian Hess, Ruediger Klingeler, Guenter Behr, Agnieszka Kondrat, Norman Leps, Guillaume Lang, Hans-Henning Klauss, Hubertus Luetkens
TT 36.2	Thu	10:00–10:30	HSZ 03	**Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors** — •Andrey Chubukov
TT 36.4	Thu	11:15–11:45	HSZ 03	**Relation of structure, magnetism, doping and pressure in AFe_2As_2** — •Helge Rosner, Deepa Kasinathan, Alim Ormeci, Katrin Koch, Miriam Schmitt, Walter Schnelle, Corneliu Miclea, Michael Nicklas, Manoj Kumar, Christoph Geibel, Ulrich Schwarz, Andreas Leithe-Jasper
TT 36.5	Thu	11:45–12:00	HSZ 03	**DFT studies of Iron-based Superconductors** — •Lilia Boeri, Oleg V. Dolgov, Alexander A. Golubov, Ole Krogh Andersen
TT 36.6	Thu	12:00–12:30	HSZ 03	**Quasiparticle renormalization effects in the normal-state optical properties of iron pnictides** — •Alexander Boris, N.N. Kovaleva, P. Popovich, Y. Matiks, C.T. Lin, R.K. Kremer, L. Boeri, O.V. Dolgov, I.I. Mazin, B. Keimer
TT 36.7	Thu	12:30–13:00	HSZ 03	**C-axis transport of pnictide single crystals** — •Paul Müller, Yuri Koval, Günter Behr, Bernd Büchner

Sessions

TT 1.1–1.5	Mon	10:15–13:00	HSZ 03	**Focussed Session: The Mott Transition in Model Systems**
TT 2.1–2.10	Mon	10:15–13:00	HSZ 301	**Transport: Nanoelectronics I - Quantum Dots and Wires, Point Contacts 1**
TT 3.1–3.10	Mon	10:15–13:00	HSZ 304	**Correlated Electrons: Spin Systems and Itinerant Magnets 1**
TT 4.1–4.6	Mon	11:15–13:00	HSZ 105	**Matter at Low Temperature: Cryotechnique, Cryodetectors and Measuring Devices**
TT 5.1–5.41	Mon	13:00–16:45	P1A	**Postersession Superconductivity: Materials - Fabrication and Properties**
TT 6.1–6.72	Mon	13:00–16:45	P1A	**Postersession Correlated Electrons: (General) Theory, Low-Dimensional Systems, Kondo Physics, Heavy Fermions, Quantum-Critical Phenomena**
TT 7.1–7.5	Mon	13:00–16:45	P1B	**Postersession Matter at Low Temperature: Materials**
TT 8.1–8.8	Mon	13:00–16:45	P1B	**Postersession Transport: Graphene and Carbon Nanotubes**
TT 9.1–9.10	Mon	14:00–16:45	HSZ 03	**Correlated Electrons: Metal-Insulator Transition 1**
TT 10.1–10.9	Mon	14:00–16:30	HSZ 105	**Superconductivity: Tunneling, Josephson Junctions, SQUIDs**

TT 11.1–11.10	Mon	14:00–16:45	HSZ 301	**Transport: Nanoelectronics I - Quantum Dots and Wires, Point Contacts 2**
TT 12.1–12.7	Mon	14:00–16:00	HSZ 304	**Correlated Electrons: Spin Systems and Itinerant Magnets 2**
TT 13.1–13.6	Tue	9:30–12:30	HSZ 03	**Focussed Session: Superconducting Quantum Circuits**
TT 14.1–14.9	Tue	9:30–12:15	HSZ 105	**Superconductivity: Non-Cuprate Non-Ferropnictide Superconductors**
TT 15.1–15.12	Tue	9:30–13:00	HSZ 301	**Correlated Electrons: Metal-Insulator Transition 2**
TT 16.1–16.12	Tue	9:30–13:00	HSZ 304	**Correlated Electrons: Low-dimensional Systems - Materials 1**
TT 17.1–17.8	Tue	14:00–16:15	HSZ 03	**Correlated Electrons: Quantum-Critical Phenomena 1**
TT 18.1–18.7	Tue	14:00–16:00	HSZ 105	**Superconductivity: Fabrication and Characterization**
TT 19.1–19.5	Tue	14:00–15:15	HSZ 301	**Correlated Electrons: Metal-Insulator Transition 3**
TT 20.1–20.4	Tue	15:30–16:30	HSZ 301	**Correlated Electrons: (General) Theory 1**
TT 21.1–21.7	Tue	14:00–16:15	HSZ 304	**Transport: Fluctuations and Noise**
TT 22.1–22.12	Wed	9:30–13:00	HSZ 03	**Correlated Electrons: Quantum-Critical Phenomena 2**
TT 23.1–23.11	Wed	9:30–12:30	HSZ 105	**Transport: Nanoelectronics III - Molecular Electronics**
TT 24.1–24.12	Wed	9:30–13:00	HSZ 301	**Correlated Electrons: (General) Theory 2**
TT 25.1–25.13	Wed	9:30–13:00	HSZ 304	**Superconductivity: Cuprate High-Temperature Superconductors 1**
TT 26.1–26.17	Wed	14:00–19:00	HSZ 03	**Transport: Graphene and Carbon Nanotubes**
TT 27.1–27.4	Wed	14:00–15:00	HSZ 105	**Superconductivity: Vortex Dynamics, Vortex Phases, Pinning**
TT 28.1–28.9	Wed	15:15–18:00	HSZ 105	**Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence**
TT 29.1–29.15	Wed	14:00–18:15	HSZ 301	**Correlated Electrons: Low-dimensional Systems - Materials 2**
TT 30.1–30.6	Wed	14:00–15:30	HSZ 304	**Superconductivity: Cuprate High-Temperature Superconductors 2**
TT 31.1–31.5	Wed	15:45–17:00	HSZ 304	**Matter at Low Temperature: Materials**
TT 32.1–32.36	Wed	14:00–18:00	P1A	**Postersession Superconductivity: Josephson Junctions, SQUIDs, Heterostructures, Andreev Scattering, Vortex Physics, Cryodetectors, Measuring Devices, Cryotechnique**
TT 33.1–33.26	Wed	14:00–18:00	P1A	**Postersession Correlated Electrons: Metal Insulator Transition, Spin Systems and Itinerant Magnets**
TT 34.1–34.7	Wed	14:00–18:00	P1A	**Postersession Matter at Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-Cold Atoms**
TT 35.1–35.33	Wed	14:00–18:00	P1A	**Postersession Transport: Nanoelectronics, Quantum Coherence and Quantum Information, Fluctuations and Noise**
TT 36.1–36.7	Thu	9:30–13:00	HSZ 03	**Focussed Session: Superconductivity and Magnetism in Ferropnictides and Related Materials**
TT 37.1–37.12	Thu	9:30–13:00	HSZ 105	**Transport: Nanoelectronics II - Spintronics and Magnetotransport**
TT 38.1–38.12	Thu	9:30–13:00	HSZ 301	**Correlated Electrons: Low-dimensional Systems - Models 1**
TT 39.1–39.12	Thu	9:30–13:00	HSZ 304	**Correlated Electrons: Heavy Fermions 1**
TT 40.1–40.18	Thu	14:00–19:00	HSZ 03	**Superconductivity: Ferropnictides 1**
TT 41.1–41.18	Thu	14:00–19:00	HSZ 105	**Matter at Low Temperature: Quantum Liquids, Bose-Einstein-Condensates, Ultra-cold Atoms**
TT 42.1–42.6	Thu	14:00–15:30	HSZ 301	**Correlated Electrons: Low-dimensional Systems - Models 2**
TT 43.1–43.11	Thu	15:45–18:45	HSZ 301	**Correlated Electrons: Heavy Fermions 2**
TT 44.1–44.18	Thu	14:00–19:15	HSZ 304	**Transport: Quantum Coherence and Quantum Information**
TT 45.1–45.9	Fri	10:15–12:45	HSZ 03	**Superconductivity: Ferropnictides 2**
TT 46.1–46.9	Fri	10:15–12:45	HSZ 301	**Correlated Electrons: Quantum Impurities, Kondo Physics**

The posters should be attached to the poster sites already during the morning sessions.

Annual General Meeting Low Temperature Physics Division

Donnerstag 19:30-20:30 Raum HSZ 304

TT 1: Focussed Session: The Mott Transition in Model Systems

Time: Monday 10:15–13:00 Location: HSZ 03

Invited Talk TT 1.1 Mon 10:15 HSZ 03

Strongly Correlated Fermionic Quantum Gases in Optical Lattices — •Immanuel Bloch — Institut für Physik, Johannes Gutenberg-Universität, Germany

Mixtures of ultracold quantum gases in optical lattices can act as novel fundamental model system, with which the physics of the Hubbard model can be experimentally tested in a versatile and highly tunable experimental setting. We present experiments on the static and dynamic properties of such strongly interacting fermions in optical lattices and compare these to state of the art calculations using e.g. Dynamical Mean Field Theory (DMFT) in three dimensions. For repulsive interacting degenerate quantum gas mixtures, we find that by increasing the interactions between the particles, the system can be tuned from a metal over a Mott insulator into a band insulator for increasing compression of the quantum gas. We have implemented a novel detection method that can directly measure the resulting compressibility of these interacting fermionic many-body systems. For increasingly attractive interactions, we find that beyond a critical interaction strength between the particles the gas expands rather than contracts. Such an anomalous spatial expansion is intimately linked to the formation of attractively bound fermion pairs in the system. Finally, novel experiments on the dynamical expansion of interacting fermions are presented. Such diffusion measurements should allow us to shed new light on the complex interplay of interacting fermions in disordered potentials in the future.

Topical Talk TT 1.2 Mon 10:45 HSZ 03

Mott transition and metastable superconductivity of repulsive Fermions in optical lattices — •Achim Rosch — Institute of Theoretical Physics, University of Cologne, 50937 Cologne

Cold atoms in optical lattices can be used to realize and control strongly correlated states of matter with unprecedented flexibility and precision. One can, for example, study the physics of the fermionic Mott transition by measuring [1] to what extent an atomic cloud in the Mott regime can be compressed. The experiments are well described by the dynamical mean field theory [1].

With cold atoms one can also realize novel non-equilbrium states. We show theoretically [2] that one can prepare an s-wave superfluid state when a dense clould of atoms described by the strongly repulsive Hubbard model is slowly expanded. Here we use that doubly occupied sites have an exponential large lifetime in the limit of strong repulsion. These pairs condense at a finite momentum which allows for a reliable detection of this exotic state of matter.

[1] U. Schneider, L. Hackermuller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, A. Rosch, preprint arXiv:0809.1464, accepted for publication in Science

[2] A. Rosch, D. Rasch, B. Binz, M. Vojta, preprint arXiv:0809.0505, accepted for publication in PRL

Topical Talk TT 1.3 Mon 11:15 HSZ 03

Carrier dynamics of two-dimensional organic charge-transfer salts close to the Mott transition — •Martin Dressel[1], Natalia Drichko[1], Michael Dumm[1], and Jaime Merino[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Departamento de Física Teórica de la Materia, Universidad Autónoma de Madrid, Spain

In recent years, it became clear that electronic interactions have a severe influence on the physics of two-dimensional electron systems [1-3]. Strong Coulomb repulsion drives a transition to a Mott-insulator in a half-filled meta, while in the case of a quarter-filled conduction band charge order is observed. Optical spectroscopy is the superior method to investigate the electronic properties. Our findings on organic crystals are compared with theoretical predictions.

Organic conductors serve as model systems to study physics in two-dimensions. The Mott transition can be tuned by decreasing the temperature or by increasing the effective electronic correlations. Physical and chemical pressure are proper tools to tune the bandwidth; doping or change of the stoichiometry allow for a variation of the carrier concentration. Close to the Mott transition but still on the metallic side, quasi-particles are observed in the 1/2-filled system κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]X only at temperatures well below 100 K, with a considerable growth of the Drude-like contribution. The itinerant carriers exhibit strong renormalization effects as the metal-insulator transition is approached.

[1] M. Dressel et al., Chem. Rev. **104** 5689 (2004).
[2] D. Faltermeier, et al., PRB **76**, 165113 (2007).
[3] J. Merino, et al., PRL **100**, 086404 (2008).

15 min. break

Topical Talk TT 1.4 Mon 12:00 HSZ 03

Mott Transition in Frustrated Lattice Systems — •Hirokazu Tsunetsugu — Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan

I will review in my talk our recent theoretical works on strongly correlated itinerant electrons on two typical frustrated lattices; Kagome and anisotropic triangular lattices. The main issues are how geometrical frustration modifies the Mott metal-insulator transition, one of the most interesting phenomena driven by strong correlation, and how magnetic correlations under frustration effects are related to coherence of electron dynamics, and also the possibility of new type of spin correlations near the transition point. To investigate these points, we have investigated a half-filled Hubbard model on these frustrated lattices by a cluster extension of dynamical mean field theory. In addition to the general trend of suppression of Mott transition, we found one-dimensional like spin correlations in the Kagome case and a reentrant insulator-metal-insulator crossover/transition in the anisotropic triangular lattice. The latter behavior is consistent with the phase diagram of κ-type ET salts experimentally determined by Kanoda group. Our results indicate that the interplay between large entropy inherent to spin frustration and short range antiferromagnetic correlation is responsible for this interesting reentrant behavior.

[1] T. Ohashi, N. Kawakami, and H. Tsunetsugu, Phys. Rev. Lett. **97**, 066401 (2006).
[2] T. Ohashi, T. Momoi, H. Tsunetsugu, and N. Kawakami, Phys. Rev. Lett. **100**, 076402 (2008).

Topical Talk TT 1.5 Mon 12:30 HSZ 03

Lattice Effects in Strongly Correlated π-electron Systems Close to the Mott Transition — •M. de Souza[1], A. Bruehl[1], C. Strack[1], B. Wolf[1], R.S. Manna[1], J.A. Schlueter[2], D. Schweitzer[3], and M. Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue Str. 1, SFB/TRR49, D-60438 Frankfurt (M), Germany — [2]Chem. and Mat. Science Divisions, Argonne NL, Argonne, IL 60439, USA — [3]Physikalisches Inst., Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany

Organic charge-transfer salts have been recognized as model systems for studying the interplay of strong electronic correlations and low dimensionality. Depending on the chemical composition and/or hydrostatic pressure, the materials show a rich variety of electronic phases including Mott insulating, spin- and charge-ordered, anomalous metallic, spin-liquid-like as well as superconducting states. By using ultrahigh-resolution thermal expansion measurements, we have explored the role of the lattice degrees of freedom for some of the above-mentioned phases. We will discuss the Mott transition in κ-(D8-BEDT-TTF)$_2$Cu[N(CN)$_2$]Br [1], the mysterious charge-order transition coinciding with ferroelectric order in (TMTTF)$_2$X [2] as well as the spin-liquid-like properties observed for κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ [3]. Our results highlight the intricate role of the lattice degrees of freedom for stabilizing the various ground states in these materials.

[1] M. de Souza *et al.*, Phys. Rev. Lett. **99**, 037003 (2007).
[2] M. de Souza *et al.*, Phys. Rev. Lett. **101**, 216403 (2008).
[3] S. Yamashita *et al.*, Nature Phys. **4**, 459 (2008).

TT 2: Transport: Nanoelectronics I - Quantum Dots and Wires, Point Contacts 1

Time: Monday 10:15–13:00 Location: HSZ 301

TT 2.1 Mon 10:15 HSZ 301

Friedel oscillations in quantum wires: interplay of interactions and non-equilibrium — Daniel F Urban[1] and •Andreas Komnik[2] — [1]Physikalisches Institut, Unversität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg i. Br. — [2]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg

We discuss the electron density oscillations in an interacting one-dimensional electron system with an impurity [1]. Under appropriate conditions the wave vector is given by different values $k_F = k_{L/R}$ on left/right side of the scatterer, leading to a Landauer dipole formation. While in the non-interacting system the Friedel oscillations possess only one periodicity related to the local k_L on the left side, the interplay of the interactions and non-equilibrium effects generates an additional peak in the spectrum of density oscillations at k_R. The position and shape of this spectral feature, which in coordinate space is observable as a beating pattern in the Friedel oscillations, reveals many important details about the nature of interactions. We believe that it has a potential to become an investigation tool in condensed matter physics.

[1] D.F.Urban and A.Komnik, Phys. Rev. Lett. **100**, 146602 (2008)

TT 2.2 Mon 10:30 HSZ 301

Scanning probe measurements and electromigration of metallic nanostructures under ultra-high vacuum conditions — •Dominik Stöffler[1], Shawn Fostner[2], Hilbert v. Löhneysen[1,3], Peter Grütter[2], and Regina Hoffmann[1] — [1]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Physics Department, McGill university, H3A-2T8 Montreal, Canada — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

Quantum effects play an important role in metal contacts of nanometer size. We use e-beam litho-graphy as well as shadow evaporation through a stencil mask to fabricate nanobridges made of gold and platinum. The bridges are subject to feedback-controlled electromigration in ultra-high vacuum (UHV). While investigating the e-beam fabricated platinum structures with the scanning tunneling microscope (STM) in UHV we discovered dense topographically higher features in regions of anteceding STM scans, suggesting deposition of additional material, possibly carbon, of up to 10 nm thickness. We imaged these regions with STM as well as with scanning electron microscopy (SEM). To avoid such a deposition on the metallic bridges we used atomic force microscopy to investigate the electromigration in UHV. The gold wires show no fundamental difference to electromigration under ambient conditions. Platinum wires need a higher voltage to start the electromigraton process compared to gold wires. We have obtained images with 3 nm resolution and have observed conductance plateaus related to the atomic structure of the resulting gold nanocontacts.

TT 2.3 Mon 10:45 HSZ 301

Non-equilibrium transport through coupled quantum dot–metallic island systems — •Marco G. Pala[1], Michele Governale[2], and Jürgen König[2] — [1]IMEP-LAHC, INP MINATEC, Centre National de la Recherche Scientifique, 38016 Grenoble, France — [2]Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

We study transport through a system composed of a single-level quantum dot tunnel-coupled to a metallic island. Such a system is of interest since it can be used to model transport trough a large island in series with charge trap centers [1]. A real-time diagrammatic technique [2,3], capable of accounting for non-equilibrium, Coulomb interaction and high-order tunneling processes, is employed to investigate transport in the resonant tunneling regime under the influence of a finite interaction strength between the dot and the island.

[1] M. Hofheinz et al., Eur. Phys. J. B **54**, 299 (2006).

[2] J. König, H. Schoeller, and G. Schön, Phys. Rev. Lett. **76**, 1715 (1996).

[3] H. Schoeller and G. Schön, Phys. Rev. B **50**, 18436 (1994).

TT 2.4 Mon 11:00 HSZ 301

Error Acconting in Electron Counting Experiments — •Michael Wulf and Alexander B. Zorin — Physikalisch Technische Bundeanstalt, Bundesallee 100, 38116 Braunschweig

Electron counting experiments attempt to provide a current of a known number of electrons per unit time. We propose architectures utilizing a few readily available electron-pumps or turnstiles with the typical error rates of 1 part per 10^4 with common sensitive electrometers to achieve the desirable accuracy of 1 part in 10^8. This is achieved not by counting all transferred electrons but by counting only the errors of individual devices; these are less frequent and therefore readily recognized and accounted for. We thereby ease the route towards quantum based standards for current and capacitance.

TT 2.5 Mon 11:15 HSZ 301

Interaction-induced harmonic frequency mixing in quantum dots — •Michael Thorwart[1], Reinhold Egger[2], and Alexander O. Gogolin[3] — [1]FRIAS, Universität Freiburg — [2]Universität Düsseldorf — [3]Imperial College London

We show [1] that harmonic frequency mixing in quantum dots coupled to two leads under the influence of time-dependent voltages of different frequency is dominated by interaction effects. This offers a unique and direct spectroscopic tool to access correlations, and holds promise for efficient frequency mixing in nano-devices. Explicit results are provided for an Anderson dot and for a molecular level with phonon-mediated interactions.

[1] M. Thorwart, R. Egger, and A.O. Gogolin, Phys. Rev. Lett. **101**, 036806 (2008)

15 min. break

TT 2.6 Mon 11:45 HSZ 301

Nonequilibrium Transport in the Interacting Resonant Level Model — •Peter Schmitteckert — Institut für Nanotechnologie, KIT, Karlsruhe, Germany

The Density Matrix Renormalization Group (DMRG) method is now a well established method to study interacting, low-dimensional quantum systems. In this talk I review the linear conductance calculations of the Kubo approach and the finite bias conductance calculations from real time simulations within DMRG. I will then discuss the finite bias conductance of the interacting resonant level model and compare to analytical calculations based on integrability in the continuum limit. The two approaches are in excellent agreement, and uncover among other things a power law decay of the current at large voltages when $U > 0$.

[1] Edouard Boulat, Hubert Saleur, and Peter Schmitteckert, Twofold Advance in the Theoretical Understanding of Far-From-Equilibrium Properties of Interacting Nanostructures, Phys. Rev. Lett. **101**, 140601 (2008).

TT 2.7 Mon 12:00 HSZ 301

Application of the weak-coupling CTQMC method to a Quantum Dot coupled to superconducting leads — •David J. Luitz and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

We apply the weak-coupling continuous time quantum Monte Carlo (CTQMC) method to the Anderson-model extended by a BCS term to describe a quantum dot coupled to s-wave superconducting leads. As the superconducting gap Δ grows, our data shows a phase transition from the 0- to π-junction regime of the Josephson current. By examining various spectral functions, we confirm the traditional interpretation that the Kondo-effect at small Δ corresponds to the 0-junction-regime, while the formation of a magnetic moment on the quantum dot leads to the π-phase-shift at large Δ. At constant Δ, the double occupancy as a function of U shows a jump, thereby signaling a first order transition between the singlet and local moment doublet regimes.

Within DMFT, this impurity problem provides a link to the periodic Anderson model (PAM) with superconducting conduction electrons. The signature of this first order transition in the impurity model in the PAM will be discussed.

TT 2.8 Mon 12:15 HSZ 301

Weak localization in a two-dimensional hole gas — •Viktor Krückl, Michael Wimmer, Inanc Adagideli, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

In several experiments the effect of weak localization is studied in two-dimensional hole gases but there are only few theoretical works which analyze the effects of the different hole types in a typical valence band structure. We investigate different materials modeled by the 4-band Luttinger Hamiltonian in a two-dimensional approximation. Transport properties in the diffusive regime as well as ballistic cavities are calculated in an effective tight-binding approximation by means of the Green function method. The influence of coupling between heavy holes and light holes leads to a decrease of the weak localization which is explained by the Berry curvature as well as a semiclassical description.

TT 2.9 Mon 12:30 HSZ 301

Tunneling through nanostructures: random matrix theory for the rate equation — •Carsten Timm — Institut für Theoretische Physik, Technische Universität Dresden

Under the conditions of weak hybridization and rapid dephasing, electronic tunneling through quantum dots or single molecules can be described by rate equations. Except for highly simplified models, one typically finds rather complex structures in the differential conductance. Random matrix theory has been used to describe statistical properties of the energy spectrum in such cases. Here, we follow a different approach: The rate equations for the probabilities P_n of states of the nanosystem can be written as $dP_m/dt = \sum_n A_{mn}P_n$. The eigenvalues of the stochastic matrix A describe the relaxational and oscillatory dynamics of the probabilities. We take A to be a random matrix. We discuss ensembles realized by these matrices and present results for the distribution and correlations of their eigenvalues.

TT 2.10 Mon 12:45 HSZ 301

Many-Body Effects in Quantum Heat Transport Through Nanostructures — •Haldun Sevinci, Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

Employing the nonequilibrium Green's function (NEGF) method at the atomistic level, we study the heat transport in nano-scale systems. Using diagramatic expansions of NEGFs we investigate the effects of anharmonic interactions in quantum thermal transport. The effects of nonlinear interactions on phononic transport are investigated. Specifically, the questions of thermal rectification and negative differential thermal resistance are addressed. Two possible schemes to control thermal rectification are discussed. The first one is by creating a mass gradient along the structure which is achieved experimentally by coating of a nanotube. The second one is modulating the width of the nanostructure along the transport direction which can be realized using graphene nanoribbons or Si nanowires.

TT 3: Correlated Electrons: Spin Systems and Itinerant Magnets 1

Time: Monday 10:15–13:00 Location: HSZ 304

TT 3.1 Mon 10:15 HSZ 304

Plaquette order in the J_1-J_2-J_3 model: a series expansion analysis — •Wolfram Brenig[1] and Marcelo Arlego[2] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, Germany — [2]Departamento de Física, Universidad Nacional de La Plata, Argentina

Series expansion based on the flow equation method is employed to study the zero temperature properties of the spin-1/2 J_1-J_2-J_3 antiferromagnet in two dimensions. Starting from the exact limit of decoupled plaquettes in a particular generalized J_1-J_2-J_3 model we analyze the evolution of the ground state energy and the elementary triplet excitations in powers of all three inter-plaquette couplings up to fifth order. We find the plaquette phase to remain stable over a wide range of exchange couplings and to connect adiabatically up to the case of the plain J_1-J_2-J_3 model, however not to the J_1-J_2 model at $J_3 = 0$. This corroborates other recent predictions. Additionally we estimate the extent of the plaquette phase by Dlog-Padé analysis of the critical lines that result from closure of the triplet gap.

TT 3.2 Mon 10:30 HSZ 304

DMRG Study of Anisotropic Triangular Heisenberg Lattice — •Andreas Weichselbaum[1,2] and Steven R. White[2] — [1]Ludwig-Maximilians-Universität, Lehrstuhl Jan von Delft, 80333 München — [2]University of California, Irvine, CA 92697, USA

The anisotropic antiferromagnetic two-dimensional triangular Heisenberg lattice for spin 1/2 describes certain classes of transition-metal oxides (TMOs) and chalcogenides (TMCs), clearly supported by experimental data. The understanding of the ground state properties of this kind of system from a theoretical point of view, however, has remained an extraordinary challenge. In the model under consideration, quasi-one-dimensional Heisenberg chains of uniform intrachain coupling strength J interact with their neighboring chains via the interchain coupling J'. By varying the anisotropy ratio $j \equiv J'/J$ from $j = 0$ (decoupled Heisenberg chains) to $j = 1$ (uniform triangular lattice with finite Neel order like local magnetization), it was pointed out in previous studies [1] that, indeed, there appears to exist spin liquid properties up to remarkably high values of j of about 0.85. We put these partially conjectured results under scrutiny by applying DMRG on finite systems with cylindrical boundary conditions specifically optimized to reduce finite size effects [2].

[1] S. Yunoki et al., PRB **74**, 014408 (2006).
[2] S. R. White et al., PRL **99**, 127004 (2007).

TT 3.3 Mon 10:45 HSZ 304

Effects of Dzyaloshinskii-Moriya interactions and non-magnetic impurities on the $S = 1/2$ Kagomé antiferromagnet — Ioannis Rousochatzakis[1], •Salvatore R. Manmana[1], Andreas M. Läuchli[2], Bruce Normand[3], and Frédéric Mila[1] — [1]Institute of Theoretical Physics (CTMC), EPF Lausanne, Schweiz — [2]MPI-PKS, Dresden, Germany — [3]Institute of Theoretical Physics, ETH Zürich, Schweiz

Motivated by recent NMR experiments[1] on $ZnCu_3(OH)_6Cl_2$, we present an exact diagonalization study of the combined effect of non-magnetic impurities and Dzyaloshinskii-Moriya (DM) interactions in the $S = 1/2$ Kagomé antiferromagnet. The magnetization response and the correlation matrix data reveal that the dimer freezing which occurs around the vacancy for $D = 0$ [2] (D is the magnitude of the DM vectors) persists up to $D/J \simeq 0.07$, above which a phase transition to the ($Q = 0$) semiclassical 120° state[3] takes place. Surprisingly however, the dimers next to the vacancy remain strong up to $D/J \sim 1-3$, i.e. well above the critical point. Implications for $ZnCu_3(OH)_6Cl_2$ will be discussed.

[1] A. Olariu, *et al.* , Phys. Rev. Lett. **100**, 087202 (2008).
[2] S. Dommange, *et al.*, Phys. Rev. B **68**, 224416 (2003);
A. Läuchli, *et al.*, Phys. Rev. B **76**, 144113 (2007).
[3] O. Cépas, *et al.*, Phys. Rev. B **78**, 140405 (2008).
[4] S. Miyahara, *et al.*, Phys. Rev. B **75**, 184402 (2007).

TT 3.4 Mon 11:00 HSZ 304

Dynamical properties of kagome lattice models with charge degrees of freedom — •Aroon O'Brien[1], Frank Pollmann[2], and Peter Fulde[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [2]University of California, Berkeley, CA94720, USA — [3]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Systems with frustrated interactions are typically characterized by a high density of low-lying excitations, leading to fascinating phenomena such as fractionalization. We study how charge degrees of freedom give rise to fractional charges in such systems.
For a spinless fermion model on a 2D checkerboard lattice, it is known that confined fractional charge excitations occur at certain filling factors. However, charge fractionalization, in the case of another 2D frustrated lattice, the kagome lattice, is not so thoroughly understood. We investigate, through the calculation of spectral functions, models of spinless fermions and hardcore bosons respectively, at 1/3 filling on finite kagome lattices. Of particular interest is the strongly correlated limit, where excitations carrying fractional charges can occur. We derive an effective model pertaining to this regime and present our findings in relation to a quantum dimer model on the hexagonal lattice. We find that the effective Hamiltonian is bipartite, allowing us to determine a gauge transformation which cures the negative sign problem. We discuss further results through the comparison of the

dynamical properties of the bosonic and fermionic models.

TT 3.5 Mon 11:15 HSZ 304

Numerical evidence of a U(1) liquid phase in the quantum dimer model on a diamond lattice — •Olga Sikora[1], Frank Pollmann[2], Nic Shannon[3], Karlo Penc[4], and Peter Fulde[1,5] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, CA94720, USA — [3]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [4]Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.B. 49, Hungary — [5]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Quantum dimer models (QDMs) are widely studied as effective models for many different condensed matter systems. Recently, it has been suggested that in the QDM on a bipartite lattice in 3D, a U(1) liquid extends for a finite range of parameters bordering the "Rokhsar-Kivelson" (RK) point [1,2]. We have used large-scale Green's function Monte Carlo simulations to establish the complete zero-temperature phase diagram for a QDM on a diamond lattice. Our results confirm explicitly the existence of the three phases conjectured for this model — a 16-sublattice ordered "R state" with cubic symmetry, a set of isolated states and, separating them, a U(1) liquid phase terminating at the RK point. Notably, our results for the liquid phase reproduce the energy spectra predicted by the corresponding U(1) theory.

[1] R. Moessner and S.L. Sondhi, Phys. Rev. B **68**, 184512 (2003).

[2] D.L. Bergman, G.A. Fiete, and L. Balents, Phys. Rev. B **73**, 134402 (2006).

15 min. break

TT 3.6 Mon 11:45 HSZ 304

Skyrmion Lattice in MnSi — Sebastian Mühlbauer[1,2], Benedikt Binz[3], Florian Jonietz[1], •Christian Pfleiderer[1], Achim Rosch[3], Andreas Neubauer[1], Robert Georgii[2], and Peter Böni[1] — [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]ITP, University of Cologne, Zülpicher Str. 77, D-50937 Cologne, Germany

Skyrmions represent topologically stable field configurations with particle-like properties. We use neutron scattering to observe the spontaneous formation of a two-dimensional lattice of skyrmion lines, a type of magnetic vortices, in the chiral itinerant-electron magnet MnSi. The skyrmion lattice stabilizes at the border between paramagnetism and long-range helimagnetic order perpendicular to a small applied magnetic field – regardless of the direction of the magnetic field relative to the atomic lattice. Our study experimentally establishes magnetic materials lacking inversion symmetry as an arena for new forms of crystalline order composed of topologically stable spin states.

TT 3.7 Mon 12:00 HSZ 304

Spin Torque Effects in a Helical Magnet — •Florian Jonietz[1], Sebastian Mühlbauer[1,2], Christian Pfleiderer[1], Rembert Duine[3], Benedikt Binz[4], Achim Rosch[4], Andreas Neubauer[1], Robert Ritz[1], Stefan Legl[1], Wolfgang Münzer[1], Robert Georgii[2], and Peter Böni[1] — [1]Physik Department E21, Technische Universität München — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz FRM II — [3]Institute for Theoretical Physics, Utrecht University — [4]ITP, University of Cologne

Spin torque interactions in soft ferromagnets are a promising route to novel spintronics devices. In these systems the spin torque is due to changes of the orientation of the spin-polarization of the conduction electrons in non-colinear spin structures, notably Bloch domain walls. A major constraint of these studies is the extrinsic nature of magnetic pinning in soft ferromagnets requiring very large current densities of order 10^{12} A/m^2. We report AC susceptibility and neutron scattering measurements in the A-Phase of MnSi, a two-dimensional skyrmion lattice [1], as a function of electric DC currents. The non-colinear spin structure is here intrinsic and due to Dzyaloshinsky-Moriya interactions, resulting in a very small pinning. We find distinct features that suggest spin torque effects at current densities that are 5 to 6 orders of magnitude smaller than those observed in soft ferromagnets. This identifies helical magnets as a new route to exploiting spin torque effects in novel spintronic applications.

[1] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, R. Georgii, P. Böni, in review (2008)

TT 3.8 Mon 12:15 HSZ 304

Skyrmion Lattice in $Fe_{1-x}Co_xSi$ — •Wolfgang Münzer[1], Christian Franz[1], Andreas Neubauer[1], Sebastian Mühlbauer[1], Tim Adams[1], Florian Jonietz[1], Christian Pfleiderer[1], Benedikt Binz[2], Achim Rosch[2], Robert Georgii[3], Peter Böni[1], Martin Schmid[4], and Juri Grin[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]ITP, University of Cologne, Zülpicher Str. 77, D-50937 Cologne, Germany — [4]Max Planck Institut für Chemische Physik fester Stoffe, 01187, Dresden, Germany

The recent identification of the A-phase in MnSi as a hexagonal lattice of anti-skyrmions raises the question, if skyrmion lattice ground states exist in further members of the series of B20 transition metal compounds. We have grown single crystals of selected compositions in the series $Fe_{1-x}Co_xSi$ by means of vapor transport and optical float zoning. Our samples are consistent with the previously reported temperature versus composition phase diagram. Comprehensive neutron scattering and magneto-transport measurements establish an extremely rich magnetic phase diagram of skyrmion phases as a function of magnetic field strength, temperature and direction.

TT 3.9 Mon 12:30 HSZ 304

Inelastic neutron scattering study of helimagnons in MnSi — •Marc Janoschek[1,2], Florian Jonietz[1], Sarah Dunsiger[1], Christian Pfleiderer[1], Peter Böni[1], Bertrand Roessli[2], Peter Link[3], and Achim Rosch[4] — [1]Physik Department E21, Technische Universität München, D-85748 Garching — [2]Paul Scherrer Institut, CH-5232 Villigen PSI — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), Technische Universität München, D-85748 Garching — [4]Institute of Theoretical Physics, Universität zu Köln, D-50937 Köln, Germany

In zero field the lack of inversion symmetry in MnSi results in a weak Dzyaloshinsky-Moriya interaction, that stabilises a spin spiral with a period of approximately 180Å below $T_c = 29.5$ K. Recent theoretical studies [1,3] predict a rich spectrum of Goldstone modes in the helical phase for wave vectors that are small compared to the helical propagation vector. These excitations, also referred to as helimagnons, are predicted to have a characteristic anisotropic dispersion relation with respect to the propagation direction of the spiral. We have performed extensive inelastic neutron scattering experiments by means of triple-axis spectroscopy in order to explore the nature of these excitations. The measurements have been carried out in the helical phase and in the A-phase where a skyrmion lattice has been observed recently[3].

[1] D. Belitz, T. R. Kirkpatrick and A. Rosch Phys. Rev. B 73, 054431 (2006).

[2] S. V. Maleyev, Phys. Rev. B 73, 174402 (2006).

[3] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, P. Böni, (2008).

TT 3.10 Mon 12:45 HSZ 304

Magnetic, electronic, and structural properties of the filled skutterudite $EuFe_4As_{12}$ — •Andreas Leithe-Jasper[1], Walter Schnelle[1], Helge Rosner[1], Yuri Prots[1], Yuri Grin[1], Walter Steiner[2], and Michael Reissner[2] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]TU Wien, Institut für Experimentalphysik, Wiedner Hauptstraße 8–10, 1040 Wien, Austria

The europium iron arsenide $EuFe_4As_{12}$ with filled skutterudite structure has been synthesized and its structural, electronic, magnetic and thermodynamic properties have been investigated. The Fe and Eu moments order ferrimagnetically at $T_C = 151$ K, the highest magnetic ordering temperature among filled skutterudite compounds. LDA band structure calculations confirm the observed magnetic polarizations and suggest that conduction electrons in $EuFe_4As_{12}$ have a large spin polarization, albeit lower than in isostructural $EuFe_4Sb_{12}$.

TT 4: Matter at Low Temperature: Cryotechnique, Cryodetectors and Measuring Devices

Time: Monday 11:15–13:00 Location: HSZ 105

Invited Talk TT 4.1 Mon 11:15 HSZ 105

Stimulated Cooperative Dynamics in Complex Solids — •Andrea Cavalleri — Max Planck Research Group for Structural Dynamics in CFEL - Hamburg — University of Hamburg

I will discuss some of our recent activities in the area of photo-control in solids with strongly correlated electrons. Control of a solid-state phase by impulsive electronic excitation in the near-infrared, and that of vibrational resonances at THz frequencies, extends the concepts of filling control and bandwidth control to the ultrafast timescale. These concepts are well known in slowly driven, conventional phase transitions, but are rather obscure in cases where one single degree of freedom is excited far away from equilibrium. Key to our endeavors are the new technological developments of ultrafast science, and the ability to generate ultrashort pulses that cover a spectral range between ˜THz frequencies (4.4 meV) and the hard x-rays (10 keV).

TT 4.2 Mon 11:45 HSZ 105

UHV Diffractometer for Soft X-Ray Diffraction at PETRA III — •Christian Schüssler-Langeheine — II. Physikalisches Institut, Universität zu Köln

Resonant diffraction in the soft x-ray range has recently shown to be a powerful technique to study nano-scale order phenomena like charge, orbital and spin order in strongly correlated electron systems.

The XUV beamline of the new synchrotron-radiation source PETRA III in Hamburg with its energy range from 200 eV up to 3 keV will cover the most important resonances of $3d$, $4d$ and $4f$ systems and will in addition to that provide a high coherent flux. For this beamline an UHV diffractometer suited for resonant and coherent soft x-ray scattering experiments is presently being set up. The experimental possibilities provided by the instrument at that beamline will be discussed with focus on the investigation of order phenomena in strongly correlated electron systems.

Funded by the BMBF through project 05KS7PK1.

TT 4.3 Mon 12:00 HSZ 105

Low Temperature Setup for Quenching Factor Measurements of $CaWO_4$ with Neutrons — •Christian Ciemniak[1], Chiara Coppi[1], Franz von Feilitzsch[1], Achim Gütlein[1], Christian Isaila[1], Jean-Côme Lanfranchi[1], Sebastian Pfister[1], Walter Potzel[1], Sabine Roth[1], and Wolfgang Westphal[1,2] — [1]Technische Universität München, Physik-Department E15, James-Franck-Str., D-85748 — [2]Deceased

CRESST is an experiment for the direct detection of dark matter (WIMPs) via nuclear recoil measurements on a $CaWO_4$ crystal. Different quenching factors for the nuclei allow the discrimination between background and a possible signal. To measure the quenching factors at low temperatures, a neutron scattering facility has been set up at the Maier-Leibnitz-Laboratory in Garching. In 2007 a cryostat has been installed and first measurements have been performed. For further optimization and to allow flight-time measurements at a fixed scattering angle, new electronic modules are presently being installed. We report on first results and ongoing upgrades. This work has been supported by funds of the DFG (SFB/Transregio 27: Neutrinos and Beyond), the Munich Cluster of Excellence (Origin and Structure of the Universe) and the Maier-Leibnitz-Laboratorium (Garching).

TT 4.4 Mon 12:15 HSZ 105

Progress in the micro-fabrication of high resolution magnetic calorimeters for x-ray spectroscopy — •Sönke Schäfer, Andreas Pabinger, Matias Rodrigues, Nadine Bleach, Thomas Wolf, Andreas Fleischmann, Loredana Fleischmann, and Christian Enss — KIP, Uni Heidelberg, INF 227, 69120 Heidelberg

Metallic magnetic calorimeters (MMC) are energy dispersive particle detectors with high energy resolution, that are operated at temperatures below 100 mK. MMCs consist of an absorber for the particles to be detected and a paramagnetic temperature sensor in tight thermal contact. The temperature rise upon the absorption of a particle, e.g. an x-ray photon, is detected via the change of the sensor's magnetization, being monitored by a low-noise high-bandwidth dc-SQUID. The thermodynamic properties of MMCs can be calculated with confidence, allowing for a prediction of the responsivity and the noise of detectors with given geometry and, consequently, a numerical optimization of MMCs for a given application. We studied two different types of fully micro-fabricated MMCs, that were optimized for the detection of x-ray photons with energies up to 10 keV. One of which made use of a cylindrical sensor positioned in the circular loop of a dc-SQUID residing in an external magnetic field. The second was based on a planar temperature sensor, that was read-out by a meander-shaped superconducting pick-up coil, transformer-coupled to a dc-SQUID. Both detectors were characterized at a number of operating temperatures and magnetic fields. We present data of both detectors and compare their performance with each other as well as with theoretical predictions.

TT 4.5 Mon 12:30 HSZ 105

Development and Characterization of a Micro-Hall Magnetometer and its Application to Molecular Nanomagnets — •A. Sundt, J. Dreiser, and O. Waldmann — Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany

Micro-Hall probes have been proven to be a simple and robust tool to measure magnetization curves $m(B)$ of small magnetic clusters at low temperatures with very high sensitivity [1,2]. We are currently building up such a micro-Hall magnetometer based on a GaAs/AlGaAs 2DEG to study magnetic molecules. Our design aims at extending the temperature range to studies from 1.5 K up to room temperature and obtaining an absolute measure of the samples' magnetization with high sensitivity. In order to achieve these goals geometric as well as Hall probe parameters are considered.

[1] M. Charalambous *et al.*, Phys. Rev. B **58**, 9510 (1998).
[2] H. M. Quddusi *et al.*, Rev. Sci. Instrum. **79**, 074703 (2008).

TT 4.6 Mon 12:45 HSZ 105

Mikroverdampfer für Hochleistungs-Kryoelektronik — •Gunter Kaiser und Jürgen Klier — ILK Dresden, Bertolt-Brecht-Allee 20, D-01309 Dresden

In einem Forschungsvorhaben wurden Mikroverdampfer zur Anwendung in der Hochleistungs-Kryoelektronik entwickelt. Die Leistungsgrenzen bezüglich des Verdampfungsprozesses in den Mikrokanälen sind durch das Gleichgewicht der Druckkräfte des Bernoulli-Effekt und der Oberflächenspannung gegeben. Es wurde der Einfluss der Quer- und Längs-Dimensionen der Struktur auf deren spezifischen Kälteleistung theoretisch untersucht und experimentell überprüft. Dazu wurde ein Mikroverdampfer, bestehend aus 21 Schlitzen mit einer Länge von 2 mm und einer Querdimension von 0.2 mm x 0.2 mm realisiert. Die Messungen zeigten einen flachen Verlauf der Arbeitstemperatur des Mikroverdampfers im Kälteleistungsbereich bis 10 W, gefolgt von einem steilen Anstieg der Arbeitstemperatur für höhere Kälteleistungen durch Austrocknung der Verdampferstruktur. Die Auslegungsrechnungen prognostizierten eine maximale Kälteleistung von 7.4 W. Der Mikroverdampfer lässt sich für verschiedene kryoelektronische Anwendungen, insbesondere für die Sensorkühlung in der zerstörungsfreien Werkstoffprüfung, für biomagnetische Anwendungen und zur Kühlung supraleitender Antennen und Hochfrequenzfilter einsetzen. Außerdem ist er geeignet unter Anwendung von Kohlendioxid im geschlossenen Kreisprozess auch Hochleistungs-Laserdioden für die Materialbearbeitung und für Schweißprozesse zu kühlen. Die Arbeiten wurden durch das BMBF (FKZ: 16SV1870) gefördert.

TT 5: Postersession Superconductivity: Materials - Fabrication and Properties

Time: Monday 13:00–16:45 Location: P1A

TT 5.1 Mon 13:00 P1A

Superconductivity in Ga-doped Germanium — •R. Skrotzki[1], T. Herrmannsdörfer[1], V. Heera[2], O. Ignatchik[1], M. Uhlarz[1], A. Mücklich[2], M. Posselt[2], H. Reuther[2], B. Schmidt[2], K.-H. Heinig[2], W. Skorupa[2], M. Voelskow[2], C. Wündisch[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf (FZD) — [2]Institut für Ionenstrahlphyik und Materialforschung, FZD

We report the first observation of superconductivity in heavily p-type doped germanium at ambient pressure conditions. Using Ga as dopant, we have produced a series of Ge:Ga samples by ion-beam implantation and subsequent short-term (msec) flash-lamp annealing. The combination of these techniques allows for Ga concentrations up to 6%, i.e., a doping level which is clearly larger than the solubility limit and not accessible to any other method so far. Transport measurements reveal superconducting transitions with T_c up to 0.5 K. In more detail, we observe a strong dependence of the superconducting critical parameters on the annealing conditions. Further, we find a strong anisotropy of the superconducting critical field reflecting the two-dimensional character of the superconducting state in the thin Ge:Ga layer having an effective depth of only 60 nm. We find critical magnetic in-plane fields even larger than the Pauli-Clogston limit. After its finding in Si [1] and diamond [2], our work reports another unexpected obervation of superconductivity in doped elemental semiconductors.

[1] E. Bustarret et al., Nature 444, 465 (2006).
[2] E. A. Ekimov et al., Nature 428, 542 (2004).

TT 5.2 Mon 13:00 P1A

Superconducting properties of boron-doped diamond — •M. Uhlarz[1], R. Skrotzki[1], T. Papageorgiou[1], J. Wosnitza[1,2], N. Dubrovinskaia[3,4], L. Dubrovinsky[5], N. Miyajima[5], A. Bosak[6], M. Krisch[6], H.F. Braun[7], and R. Wirth[8] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf — [2]Institut für Festkörperphysik, TU Dresden — [3]Institut für Geowissenschaften, Universität Heidelberg — [4]Lehrstuhl für Kristallographie, Physikalisches Institut, Universität Bayreuth — [5]Bayerisches Geoinstitut, Universität Bayreuth — [6]European Synchrotron Radiation Facility, Grenoble — [7]Physikalisches Institut, Universität Bayreuth — [8]GeoForschungsZentrum Potsdam

The question of the nature of superconductivity in boron-doped diamond (synthesized at high pressures and high temperatures) is still open. Here we present consistent measurements of resistivity and specific-heat on two samples containing pure ^{13}C and ^{12}C, revealing a 0.2 K shift of the superconducting transition temperature T_c. Hall-coefficient measurements confirm equal charge-carrier concentrations in both samples. The results are interpreted as a carbon-isotope effect more than two times larger than expected from the most simple BCS model for phonon-mediated superconductivity. Additional analyses of microstructure and exact boron content of the superconducting material show the presence of highly boron-enriched amorphous boundaries between the grains. For these investigations high-resolution transmission-electron microscopy and electron-energy-loss spectroscopy were used.

TT 5.3 Mon 13:00 P1A

Substitution and pressure effect on superconducting properties of $Na_{1-x}Ca_xAlSi$ — •Andreea Beleanu[1], Vadim Ksenofontov[1], Claudia Felser[1], and Petre Badica[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institute of Physics Johannes Gutenberg - University, 55099 Mainz

This work reports on the substitution of Na^+ with Ca^{2+} in the ternary alkali-metal silicide superconductor NaAlSi. The superconducting transition of NaAlSi takes place at a critical temperature T_c of 7 K. The superconducting properties of CaAlSi were reported to the distortion of the AlSi-layers. The Si bonding network thus plays an important role for the superconducting characteristics[1]. CaAlSi shows a superconducting transition at a T_c of 8.0 K [2]. Na^+ and Ca^{2+} cations have equal ionic radii but Ca provides an additional electron. The observation of the superconducting properties in dependence of electron-doping of $Na_{1-x}Ca_xAlSi$ is shown. The superconducting properties of $Na_{1-x}Ca_xAlSi$ were measured using SQUID magnetometry.

[1] S. Kuroiwa, H. Kawashima, H. Kinoshita, H. Okabe, J. Akimitsu, Physica C, 466, 11 (2007).
[2] M. Imai, K. Nishida, T. Kimura, H. Kitazawa, H. Abe, H. Kito, K. Yoshii, arXiv:cond-mat/0210692v1,(2002)

TT 5.4 Mon 13:00 P1A

Superconducting Properties of Niobium Thin Films grown by Pulsed Laser Deposition — Christian Pansow[1], •Veit Grosse[1], Alexander Steppke[2], Frank Schmidl[1], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena — [2]MPI für chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden

Niobium (Nb) as the element showing the highest critical temperature is the most commonly used material for superconducting applications. High quality thin films can be fabricated utilising electron beam evaporation or sputtering. However, special demands on the device fabrication process may favour other deposition techniques. Note, for example, the possibility for an *in situ* growth of multilayer systems, the realisation of new Josephson Junction concepts utilising carbon nanotubes or improving film quality by increasing ionisation of the evaporated material. In this framework pulsed laser deposition is a versatile technique to meet these demands.

Here we report on the superconducting properties of niobium thin films grown by pulsed laser deposition at room temperature. Depending on film thickness we achieved a critical temperature of 8.4 K and a critical current density of $3.0 \cdot 10^6$ A/cm^2 at 4.2 K. We compare the temperature dependence of the critical current and critical magnetic field with that of electron evaporated niobium films. Our samples showed a distinct ageing behaviour during several cooling cycles which can be attributed to oxygen diffusion into the fine grained structure of the films.

TT 5.5 Mon 13:00 P1A

Tunneling into Al doped MgB_2 thin films — •Rudolf Schneider, Alexander G. Zaitsev, and Jochen Geerk — Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe

Superconducting thin films with composition $Mg_{1-x}Al_xB_2$ ($0 \leq x < 0.6$) were prepared *insitu* by thermal sublimation of Mg combined with B rf and Al dc magnetron sputtering. The critical temperature, T_c, decreased linearly with a slope of -0.4 K per at% Al up to $x \approx 0.4$. For $0.4 < x < 0.5$ the formation of a plateau with a $T_c \approx 12$ K was observed. The plateau-like effect might be due to the formation of the superstructure $MgAlB_4$ with ordered alternating Mg and Al planes separated by B planes. Quasiparticle tunneling measurements were performed on sandwich-type crossed-strip tunnel junctions with artificial aluminum oxide barriers. Differential conductance measurements at low voltage allowed the determination of the small energy gap on the Fermi surface π sheet. The π gap decreased linearly with decreasing T_c of the films in agreement with a band filling model. Conductance measurements in the phonon region enabled the determination of the Eliashberg function α^2F for a low doping level $x \approx 0.1$ so far. Compared to the undoped MgB_2 a shift of the spectrum to higher energy was observed comparable to the renormalization of the phonon density of states measured on bulk samples with inelastic neutron scattering.

TT 5.6 Mon 13:00 P1A

Carbon Doping as an Effective Way to Enhance the Superconducting Properties of Mechanically alloyed in-situ MgB_2 — •Marko Herrmann[1], Wolfgang Hässler[1], Juliane Scheiter[1], Christian Rodig[1], Margitta Schubert[1], Ania Kario[1], Christine Mickel[1], Nadezda Kozlova[1], Konstantin Nenkov[1], Manfred Ritschel[1], Wolfgang Gruner[1], Ludwig Schultz[1,2], and Bernhard Holzapfel[1,2] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, P.O.Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Department of Physics, 01062 Dresden, Germany

Up to now, carbon doping is the only reliable way to enhance the superconducting properties of Mg_2 significantly. Due to the substitution of carbon on boron sites of the lattice, increased impurity scattering results in an enhanced upper critical field. Subsequently, an improved high field j_c-performance of carbon-doped MgB_2 is observed. Among the plethora of carbon-containing compounds studied so far, nanos-

tructured carbon and carbon nanotubes (CNT) are potentially the most promising materials. Especially the elongated microstructural features of CNTs may additionally function as artificial pinning centers. In this work, the impact different carbon sources has on the structural and superconducting properties of nanocrystalline MgB_2 bulk samples and tapes is discussed. Precursor powders of carbon-doped MgB_2 were produced by mechanical alloying. In order to preserve the microstructural features of the CNTs, the standard processing procedure was modified.

TT 5.7 Mon 13:00 P1A

A mechanism of superconductivity in non-centrosymmetric system — •TETSUYA TAKIMOTO and PETER THALMEIER — max planck institute for chemical physics of solids, dresden

Unconventional superconductivity in non-centrosymmetric compounds like $CePt_3Si$, $CeRhSi_3$, and $CeIrSi_3$ attracts much attention. The most exotic feature of these compounds is a quite large upper critical field of superconductivity, which exceeds the Pauli limiting field. Therefore, it is considered that the possibility of spin-triplet superconductivity is not excluded in the non-centrosymmetric system. In addition, the Sigrist group has suggested that the d-vector of possible triplet superconductivity in non-centrosymmetric systems is parallel to the Rashba field, by which the inversion symmetry is broken. Based on a Hubbard model including the Rashba field, we study the superconductivity with an assumption suggested by the Sigrist group. The superconductivity is induced by spin fluctuations including anomalous spin fluctuations, which vanish in centrosymmetric systems. We will also discuss property of the superconducting state.

TT 5.8 Mon 13:00 P1A

Response and transport in non–centrosymmetric superconductors — •LUDWIG KLAM[1], DIETRICH EINZEL[2], and DIRK MANSKE[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

We formulate a kinetic theory for non–centrosymmetric superconductors (NCS) at low temperatures in the clean limit. The transport equations are solved quite generally in spin– and particle–hole (Nambu) space by performing first a transformation into the so–called helicity–band basis and second a Bogoliubov transformation to the quasiparticle–quasihole phase space. Our result is a particle–hole–symmetric, gauge–invariant and charge conserving description, which is valid in the whole quasiclassical regime ($|q| \ll k_F$ and $\omega \ll E_F$). Including the long–range Coulomb interaction, we calculate the Lindhard, the dielectric, and the Raman response function.

For the Raman case, we present within this framework our recent results for the polarization–dependence of the electronic (pair–breaking) Raman response for NCS at zero temperature. Furthermore, we use a Green's function approach in order to calculate the dynamic spin susceptibility for the β-band of $CePt_3Si$ where the 3D band–structure can be obtained from recent ARPES measurements. Finally, we identify the relevant wave vectors for Cooper–pairing mediated by the spin susceptibility.

TT 5.9 Mon 13:00 P1A

Angular dependence of the upper critical field H_{c2} for $CeCu_2Si_2$ — •HUGO A. VIEYRA[1], NIELS OESCHLER[1], JEEVAN S. HIRALE[1,2], CHRISTOPH GEIBEL[1], and FRANK STEGLICH[1] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]I. Physik. Institut, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Unconventional superconductivity is one of the most important and fascinating topics within solid state physics. It plays a major role in the study of high-T_c and heavy-fermion superconductors. Nevertheless, the underlying physical mechanism of unconventional superconductivity is still not completely understood. A clear example of this paradigm is $CeCu_2Si_2$, the first unconventional superconductor discovered almost three decades ago. Angular dependent measurements have already proven to be powerful techniques to study the properties of the unconventional superconducting state. In this work, we present angular-dependent resistivity measurements on single-crystalline $CeCu_2Si_2$ samples with antiferromagnetic order below 800 mK and a superconducting transition around 600 mK. From the angular dependence of the upper critical field H_{c2}, no anisotropy is observed within the basal plane, whereas a large anisotropy is observed when the magnetic field rotates out of plane ($\mathbf{H}//\mathbf{a}$) towards the crystallographic c-axis ($\mathbf{H}//\mathbf{c}$). As the angular dependence deviates from the prediction based on the anisotropic mass model, strong Pauli paramagnetic limiting seems to dominate the upper critical field at low temperatures.

TT 5.10 Mon 13:00 P1A

Deviations from the conventional BCS behavior in the penetration depth of lutetium-nickel-borocarbide films at terahertz frequencies — •T. FISCHER[1], A. V. PRONIN[1], J. WOSNITZA[1], T. NIEMEIER[2], and B. HOLZAPFEL[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]IFW Dresden, 01171 Dresden, Germany

We have measured the temperature and frequency-dependant transmission and phase shift through $LuNi_2B_2C$ thin films on MgO substrates at terahertz frequencies. From the measured data, we could accurately determine the complex dielectric constant, $\hat{\epsilon}$, the complex optical conductivity, $\hat{\sigma}$, and the penetration depth, λ. Comparing our measured results with theory, we find strong deviations from the standard one-band BCS predictions. These deviations can be attributed to the multiband nature of the superconducting state in $LuNi_2B_2C$.

TT 5.11 Mon 13:00 P1A

Quantum Oscillations in the superconducting state of $LuNi_2B_2C$ — •B. BERGK[1], O. IGNATCHIK[1], M. BARTKOWIAK[1], T. MANIV[2], V. ZHURAVLEV[2], P.C. CANFIELD[3], and J. WOSNITZA[1] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Dresden, Germany — [2]The Schulich Faculty of Chemistry, Technion Israel Institute of Technology, Haifa, Israel — [3]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, USA

We have studied the de Haas-van Alphen (dHvA) effect of the borocarbide superconductor $LuNi_2B_2C$ both in the normal and in the superconducting state by use of the field-modulation method in high magnetic fields up to 15 T and at low temperatures down to 0.5 K. In the superconducting state we observed an additional damping of the dHvA oscillation amplitudes compared to the normal state for different dHvA frequencies. This is due to the opening of the superconducting gap and, therefore, enables us to determine the magnetic-field-dependent gap for different bands from this experiment. The possibility to perform the measurements at various crystal orientations in the magnetic field allows to examine the angular dependence of the superconducting gap parameter.

TT 5.12 Mon 13:00 P1A

Multiband superconductivity in YNi_2B_2C single crystals studied by use of specific-heat measurements — •A. BEKKALI[1,2], J. WOSNITZA[1,2], M. UHLARZ[1], R. BEYER[1], M. SCHNEIDER[3], G. BEHR[3], S.-L. DRECHSLER[3], and G. FUCHS[3] — [1]Institut Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]TU Dresden, Institut für Festkörperphysik, D-01062 Dresden, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01171 Dresden, Germany

We present new specific-heat data for two different YNi_2B_2C single crystals grown by a zone-melting method. The two samples ($T_{c,A} = 15.26(4)$ K, $T_{c,B} = 15.6(1)$ K) were studied in magnetic fields up to $B = 9$ T in the temperature range from $T = 0.35 \ldots 20$ K, using both a relaxation and a heat-pulse method. In the superconducting state ($B = 0$) we find an uncommon dependence of the electronic contribution to the specific heat, $C_{el}(T)$, strengthening the assumption of a multiband nature of the superconducting state of YNi_2B_2C. A quantitative analysis of $C_{el}(T)$ evidences multiple electronic contributions from electrons with very different electron-phonon coupling strengths, thus exhibiting several different superconducting energy gaps $\Delta(T, B = 0)$. This feature is in agreement with recent de Haas – van Alphen results [1] and point-contact spectroscopy data [2].

[1] B. Bergk et al., PRL **100** (2008) 257004.
[2] P. Raychaudhuri et al., Physica C **460-462** (2007) 95.

TT 5.13 Mon 13:00 P1A

Organic Superconductors Revisited: STM imaging and DFT calculations of the bc plane of κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ — JOHANNES M. BÜTTNER[1], •CARSTEN L. ROHR[1], FLORIAN A. PALITSCHKA[1], NATASCHA D. KUSHCH[2], MARK V. KARTSOVNIK[3], WERNER BIBERACHER[3], and BIANCA A. HERMANN[1] — [1]Dept. of Physics / CeNS, LMU Munich and Walther-Meissner-Institute (WMI), Munich, Germany — [2]Institute of Problems of Chemical Physics, Russian Academy of Science, Chemogolovka, Moscow-region, 142432 Rus-

sia — [3]Walther-Meissner-Institute (WMI) and TU Munich, Munich, Germany

Organic superconductors of the BEDT-TTF family are of a layered nature and show a pseudogap. Because of that, these materials are of high interest for the understanding of the physics of high-temperature superconductors. Due to the fragility of organic superconductor crystals caused by the weak charge-transfer bonding, we conducted a study on single crystals of drastically different age[1]:The surfaces of a ten years aged crystal and a freshly prepared κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ crystal were imaged by scanning tunneling microscopy. The molecularly-resolved STM images of the bc plane of the crystals agree well with each other. The variation in brightness at the various positions of the molecules matches a new Density-Functional-Theory (DFT) simulation (Perdew-Wang91 gradient-corrected exchange-correlation functional) of the cationic layer, based on a crystal structure of [2]. Hence, we attribute this symmetry breaking of the BEDT-TTF dimers to intrinsic surface electronic states.

TT 5.14 Mon 13:00 P1A

Inducing Superconductivity with Picosecond Pressure Pulses in a Quasi-2D Organic Salt — •Julia Stähler, Arzhang Ardavan, and Andrea Cavalleri — University of Oxford, Department of Physics, Clarendon Laboratory, Parks Rd, Oxford OX1 3PU, UK

The quasi-2D organic compounds of the BEDT-TTF family are prototype materials for unconventional superconductivity. In particular, the κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl exhibits a very rich phase diagram including a pressure-driven antiferromagnetic insulating to superconducting (AF-SC) phase transition below 13 K. So far, all studies of organic superconductors focused on the equilibrium properties of these materials, i.e. the system's response to slow adiabatic changes of the environment. The present work, however, aims at investigating the dynamic formation of the SC phase after excitation of a picosecond pressure transient using femtosecond laser pulses: The laser intensity is absorbed and leads to a significant local temperature increase at constant volume. As a direct consequence, a pressure pulse is launched in the material. This coherent acoustic pulse traverses through the sample at the speed of sound and is expected to induce the AF-SC phase transition. This phase transition will lead to noticeable changes of the sample's conductivity and therefore affect the dielectric function $\epsilon(\omega)$ of the material. In particular, at low energies in the region of the superconducting gap, a significant variation of reflectivity is anticipated. Thus, we employ THz radiation(1 THz = 4 meV) as a probe of the superconducting state. Picosecond time resolution is realized by tuning the time delay between pump laser pulse and THz pulse.

TT 5.15 Mon 13:00 P1A

$Na_{1-x}CoO_2$ bulk preparation by sol-gel and solid state routes — •Sandra Heinz[1], Ingo Fritsch[2], Claudia Fasel[1], Philipp Komissinskiy[1], Jose Kurian[1], Hanns-Ulrich Habermeier[2], and Lambert Alff[1] — [1]Department of Materials Science, TU Darmstadt, Germany — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany

For the investigation of unconventional superconductivity thin films are advantageous for Josephson junctions and tunneling devices. In case of the possible p-wave superconductor water intercalated sodium cobaltate, high quality thin films showing superconductivity have been obtained [1,2]. The first step of thin film preparation by pulsed laser deposition is a reproducible, phase pure bulk target. Here we report on sodium cobaltate target fabrication by a sol-gel and by a solid state route. Two preparation routes are described to receive high quality, stable targets without parasitic phases. The targets were characterized by X-ray diffraction, high resolution scanning electron microscopy, energy dispersive X-ray analysis, thermal gravimetric analysis and magnetometry. $Na_{1-x}CoO_2$ targets can be obtained for x between 0.3 and 0. Textured targets can be realized with grain sizes down to the nanometer range by the sol-gel method.

[1] Y. Krockenberger, I. Fritsch, G. Cristiani, A. Matveev, L. Alff, H.-U. Habermeier, and B. Keimer, Appl. Phys. Lett. 86, 191913 (2005).

[2] Y. Krockenberger, I. Fritsch, G. Cristiani, H.-U. Habermeier, Li Yu, C. Bernhard, B. Keimer, and L. Alff, Appl. Phys. Lett. 88, 162501 (2006).

TT 5.16 Mon 13:00 P1A

Electron-Phonon Interaction and Phonon Renormalization in the Lamellar Cobaltate Na_xCoO_2 — •Johannes Knolle[1], Alexander Donkov[1], Ilya Eremin[1,2], and Maxim Korshunov[1,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Institute für Mathematische und Theoretische Physik, TU Braunschweig, 38106 Braunschweig, Germany — [3]Siberian Branch of Russian Academy of Sciences, L.V. Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

We study theoretically the electron-phonon interaction in Na_xCoO_2. For the A_{1g} and E_{1g} phonon modes found in Raman experiments, we calculate the matrix elements of the electron-phonon interaction. Analyzing the feedback effect of the conduction electrons on the phonon frequency ω, we investigate the doping dependence of these two phonon modes. Due to the momentum dependence of the electron-phonon interaction, we find the strongest renormalization of the E_{1g} mode around the Brillouin zone boundary which should be observed in the neutron scattering. At the same time, the A_{1g} mode shows the strongest coupling to the conducting electrons around the Γ point and reveals its doping dependence in the Raman experiments. Our results shed light on the possible importance of the electron-phonon interaction in the lamellar sodium cobaltates.

TT 5.17 Mon 13:00 P1A

Superconductivity and magnetism in electrochemically doped oxides — •Andreia Ioana Popa[1], Hemke Maeter[2], Christine Täschner[1], Ingo Hellmann[1], Rüdiger Klingeler[1], Bernd Büchner[1], and Hans-Henning Klauss[2] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany — [2]IFP, TU Dresden, Germany

We study the magnetic and electronic properties of transition metal oxides in which the valency of the metal ions is modified electrochemically by Li intercalation/deintercalation. The electrochemical doping strongly affects the electronic and magnetic properties. One example is the evolution of superconductivity in the CuO_2 planes of $Li_xSr_2CuO_2Br_2$. Electron doping is realized by Li-intercalation and superconductivity is found below 9K. Electrochemical treatment hence allows studying the electronic phase diagram of this new electron doped cuprate superconductor. Another relevant class of materials under study are mixed valent vanadium-oxide multiwall nanotubes which represent a technologically relevant material for lithium-ion batteries. Upon electron doping of VO_x-NTs, our data confirm a higher number of magnetic V^{4+} sites. Interestingly, room temperature ferromagnetism evolves after electrochemical intercalation of Li making VO_x-NTs a novel type of self-assembled nanoscaled magnets.

TT 5.18 Mon 13:00 P1A

Masked ion beam patterning of nano-size regions of high-T_c superconducting thin films — •Marius Bodea[1], Khurram Siraj[1], Johannes Pedarnig[1], Dieter Bäuerle[1], Wolfgang Lang[2], Herbert Richter[2], Markus Marksteiner[2], Christine Hasenfuss[1], Leopold Palmetshofer[1], Renata Kolarova[1], Peter Bauer[1], and Costas Grigoropoulos[3] — [1]Technical and Natural Science Faculty, Johannes Kepler University, A-4040 Linz, Austria — [2]Faculty of Physics, University of Vienna, A-1090 Vienna, Austria — [3]Department of Mechanical Engineering, University of California, Berkeley, CA 94720-1740, USA

Ion-beam irradiation of the high-temperature superconductor (HTS) $YBa_2Cu_3O_7$ (Y-123) creates different types of defects depending on ion mass, energy and dose. Irradiation with Helium ions of moderate energy (75 keV) primarily creates point defects by displacement of oxygen atoms in Y-123. The He ions penetrate thin films of Y-123 (thickness 100 nm) producing defects that are distributed homogeneously in the HTS layer. The collision cascades show small lateral straggle. This allows for patterning of nanostructures by directing a low divergence ion beam onto a HTS thin film sample through a mask. The modification of electrical transport properties of Y-123 thin films by He ion irradiation, the variation of thin film resistivity and critical temperature with ion dose and the patterning of features about 200 nm in size by masked ion beam irradiation are presented. Computer simulations indicate that nano-patterning of Y-123 thin films with 10 nm lateral resolution is achievable.

TT 5.19 Mon 13:00 P1A

A new experimental setup for the preparation of oxide thin film - nanoparticle heterostructures — •Maria Sparing, Elke Backen, Ruben Hühne, Sebastian Fähler, Bernd Rellinghaus, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, IMW, P.O. Box 270116, D-01171 Dresden, Germany

The application of superconducting $YBa_2Cu_3O_{7-x}$ (YBCO) thin

films in external magnetic fields is limited by their critical current density J_c. Since J_c strongly depends on the density and structure of pinning defects in the material, it can be improved by the introduction of artificial pinning centers, as e.g. created by nanoparticles. Although the influence of nanoparticles has been widely studied, a direct correlation between particle properties, defect structure and superconducting properties is still lacking, mainly because the control of the particle properties is not straight forward. Well controlled size distributions and areal densities of nanaoparticles with mean diameters between 3 nm and 20 nm can be obtained by DC magnetron sputtering in an inert gas atmosphere. We have already shown that, when implemented in YBCO thin film structures, such particles clearly influence J_c [1]. Here, we present a new experimental setup, which combines the inert gas condensation of nanoparticles with the preparation of oxide thin films by pulsed laser deposition in one chamber. This setup allows for the preparation of novel particle - thin film heterostructures, which yield the potential for a better understanding of the correlation between particle properties, defect structure and J_c.

[1] M. Sparing et *al.*, Supercond. Sci. Technol. **20**, 239 (2007)

TT 5.20 Mon 13:00 P1A

An influence of gamma irradiation on oxygen mobility in $YBa_2Cu_3O_{7-\delta}$ — •Anis Saad[1], Mikalai Kalanda[2], and Sergey Demyanov[2] — [1]Al-Balqua Applied University, Salt, Jordan — [2]Scientific-Practical Materials Research Centre NAS of Belarus, Minsk, Belarus

It is known, that in the process of irradiation, physical-chemical properties of $YBa_2Cu_3O_{7-\delta}$ considerably change due to the formation of radiation defects of various kind.

The most effective way of investigation of the Co^{60} isotope gamma ray irradiation effect on oxygen exchange dynamics and anions redistribution in CuO_x crystal structure planes of HTS $YBa_2Cu_3O_{7-\delta}$ compound is a plotting of superconducting critical temperature T_c, the superconducting transition temperature width ΔT_c and crystal lattice parameters difference $\Delta(b-a)$ dependences on irradiation dose.

In this way, as a result of comparison of T_c and ΔT_c values for irradiated high-density sample and non-irradiated high-density sample, respectively, it was determined that the gamma irradiation with energy 1.25 MeV, subsequent annealing at temperature 770 K and oxygen partial pressure pO_2 = 5 x 10^5 Pa during 12 h, leads to the T_c and $\Delta(b-a)$ values rise and decrease of ΔT_c value.

One can suppose that during the Co^{60} isotope gamma ray irradiation, radiation defects are formed which promote ionization of oxygen atoms. This process promotes redistribution of anions in CuO_x chained layers and stimulates oxygen sorption-desorption processes in the studied structures.

TT 5.21 Mon 13:00 P1A

A check on the checkerboard-like STM patterns of the Bi-cuprates — •Lars Schumachenko, Olaf Lübben, Hendrik Glowatzki, Lenart Dudy, Alica Krapf, Christoph Janowitz, and Recardo Manzke — Humboldt Universität zu Berlin

Topological scanning tunneling microscopy (STM) patterns of the high-temperature superconducting Bi-cuprates are long known to have beside the atomic grid an incoherent background (see, e.g., [1,2]). Measuring the Bi-cuprate Bi2212 at low bias and temperatures below the pseudogap-temperature [3], this background is ordered with a typical periodicity of $4a_0$ x $4a_0$ (here a_0 is the inplane Cu-O-Cu-length). We will present STM-measurements of the Bi-cuprates La-Bi2201 and Bi2212 and show thereby that at room temperature and relative high bias the background is already ordered. In our interpretation, this ordered background is preferentially caused by the extra Oxygen present in these materials. How these findings would challenge the interpretation of the 4x4 order as the revelation of the hidden checkerboard order [4] will be discussed.

[1] S. H. Pan et al., Nature 413, 282 (2001).
[2] Ø. Fischer et al., Rev. Mod. Phys. 79, 353 (2007).
[3] M. Vershinin et al., Science 303, 1995 (2004).
[4] T. Hanaguri et al., Nature 430, 1001 (2004).

TT 5.22 Mon 13:00 P1A

Evidence for static, site centered stripe order by photoemission on $Bi_2Sr_{1,2}La_{0,8}CuO_6$ — •Valentina Scherer[1], Christoph Janowitz[1], Beate Müller[1], Lenart Dudy[1], Alica Krapf[1], Helmut Dwelk[1], Recardo Manzke[1], Taichi Okuda[2], and Akito Kakizaki[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institute for Solid State Physics (ISSP),University of Tokyo, Japan

$Bi_2Sr_{1,2}La_{0,8}CuO_6$ single crystals with a single CuO_2-layer per unit cell, a nominal hole doping around $n_H = 0,1$ and, vanishing T_C were grown and characterized. High resolution photoemission revealed an electronic structure decisively different from any hitherto reported one on Bi-cuprates. While no spectral weight, dispersion, or Fermi surface crossings along the nodal line could be detected, a strong buildup of spectral weight around the antinodal M-point occured. By comparison to spectral functions, dispersions, and Fermi surfaces from different calculations it will be shown that for this doping level indeed the site centered stripe model is realized.

TT 5.23 Mon 13:00 P1A

Checking the band structure of $Bi_2Sr_2CaCu_2O_{8+\delta}$ on polarization dependencies via angle resolved photoemission spectroscopy — •Hendrik Vita, Beate Müller, Lenart Dudy, Stephan Thürmer, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

High resolution angle resolved photoemission spectroscopy (ARPES) has been performed on $Bi_2Sr_2CaCu_2O_{8+\delta}$, a classical representative of cuprate superconducters. With this approach the complex electronic structure of valence electrons in solids gets accessible. The excitation is generated by a high flux He-I_α ultaviolett source. Measuring the emitted electrons near zone boundary point M in reciprocal space, we focus on structures near the Fermi suface and around 1 eV binding energy. In particular linear polarized light is used, which is realized by a new monochromator equipped with a stage to rotate the orientation of the polarization. We assume that different excitations in the energy distribution curves show similar dependence on polarization. Especially for related systems like the single layer $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, phenomena measured in different polarization planes were already observed [1]. There the splitting of the superconducting peak up in two seperate excitations is reported. These measured structures are strongly correlated in respect to polarization.

[1] R. Manzke et. al., Phys. Rev. B **63**, R100504 (2001)

TT 5.24 Mon 13:00 P1A

Valence-bond stripes in cuprates: ARPES and inter-layer tunneling — •Alexander Wollny and Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

The effect of stripe formation in the underdoped cuprates has been a much discussed topic for more than ten years. Motivated by recent neutron scattering and STM experiments we develop a phenomenological mean-field model for valence-bond stripes dominated by local singlet formation.

We explore the electronic spectrum for valence-bond stripes and its interplay with d-wave superconductivity. The results are compatible with ARPES data for $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$. Further we derive the effect of long ranged stripe order (with and without magnetic ordering) on the interlayer tunneling between two CuO_2-layers, giving an alternative mechanism, besides the anti-phase SC scenario, for effective layer decoupling in $La_{1.875}Ba_{0.125}CuO_4$.

TT 5.25 Mon 13:00 P1A

Optical sum rule anomalies in high-temperature superconductors — •Alessandro Toschi[1], Giorgio Sangiovanni[1], Karsten Held[1], Massimo Capone[2,3], and Claudio Castellani[2] — [1]Institut für Festkörperphysik, Technische Universität Wien, Austria — [2]Dipartimento di Fisica, Università "La Sapienza", Roma, Italy — [3]SMC, CNR-INFM, Roma, Italy

Many unusual features recently observed in the optical spectroscopy experiments in the cuprates can be simply understood[1] as arising from the vicinity to the Mott transition, without invoking more involved and exotic mechanisms. Specifically, we compare calculations based on the Dynamical Mean Field Theory (DMFT) of the Hubbard model with the optical spectral weight W_{opt} of different cuprates, explaining most of the anomalies found in the optical sum rules with respect to normal metals, including the existence of two different energy scales for the doping- and the T-dependence of W_{opt}. A further support to this result is provided by the analysis of the optical conductivity in a typical case of the Mott-Hubbard metal-insulator transition, namely the V_2O_3[2].

[1] A.Toschi, M. Capone, M. Ortolani, P. Calvani, S. Lupi, and C. Castellani, Phys. Rev. Lett. 95, 097002 (2005); A.Toschi, and M. Capone, Phys. Rev. B 77, 014518 (2008).
[2] L. Baldassarre , A. Perucchi, D. Nicoletti, A.Toschi, G. San-

giovanni, K.Held M. Capone, M. Ortolani, L. Malavasi, M. Marsi, P. Metcalf, P. Postorino, and S. Lupi, Phys. Rev. B 77, 113107 (2008).

TT 5.26 Mon 13:00 P1A

Superconductivity at the interfaces of oriented graphite crystalline regions? — Jose Barzola-Quiquia and •Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig

Magnetotransport measurements in bulk graphite as well as in mesoscopic multigraphene samples show a behaviour compatible with granular superconductivity with critical temperatures above 20 K [1]. Transmission electron microscope characterization and the thickness dependence of the transport behaviour suggest that the superconducting regions are located at the interfaces between crystalline graphite regions.

[1] P. Esquinazi et al., Phys. Rev. B **78**, 134516 (2008).

TT 5.27 Mon 13:00 P1A

The Superconducting Phase Diagram of $Ba_{1-x}K_xFeAs$ Single Crystals — •M. Bartkowiak[1], G.L. Sun[2], C.T. Lin[2], B. Keimer[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, Postfach 510119, 01314 Dresden — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

The discovery of superconductivity in iron pnictides has opened up a new class of high-T_c superconductors. It is quite remarkable that superconductivity is induced in layers of FeAs. These layers are separated by either rare-earth oxides or barium, which when doped act as charge-carrier reservoir. Single crystals of the (122) phase are currently available. We have determined the temperature dependence of the critical field H_{c2}, for various single crystals of K-doped $BaFe_2As_2$ using ac-transport measurements.

The experiments were done at the pulsed-field facility in Dresden in fields up to 60 T applied parallel and perpendicular to the superconducting planes. The obtained phase diagram serves as an excellent benchmark for theoretical models of the order parameter.

TT 5.28 Mon 13:00 P1A

Crystal growth and selected properties of alkali/alkaline earth metal iron arsenides by flux growth and floating zone melting — •Andreea Claudia Budea[1], Igor Morozov[2], Norman Leps[1], Agnieszka Joanna Kondrat[1], Jorge Enrique Hamann-Borrero[1], Christian Hess[1], Rüdiger Klingeler[1], Günter Behr[1], and Bernd Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Inorganic Chemistry Department, Moscow State University, Moscow, Russia

Large high quality crystals of various classes of novel alkali/alkaline earth metal-iron arsenides were grown by flux or by high pressure floating zone (FZ) methods. Careful selection and handling of high-purity starting materials and the control of oxygen impurities during the whole preparation process is required. The process parameters crucially depend on solution temperature and the solidification mode of the compound from tin flux. The relatively small partial pressures of arsenic in this class of compounds and the nearly congruent melting behavior enable the melting and crystallization in a high pressure floating zone facility under argon pressures above 40 bar. The characterization and selected physical properties of $Li_{1-x}FeAs$, $Ba_{1-x}K_xFe_2As_2$, $Ba(Fe_{1-x}Co_x)_2As_2$ are reported.

TT 5.29 Mon 13:00 P1A

Crystal growth and sample-dependent physical properties of new superconducting $SrFe_{2-x}M_xAs_2$ (M = transition metal) compounds — •Andreas Leithe-Jasper, Walter Schnelle, Helge Rosner, and Ulrich Burkhardt — MPI für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

We have recently reported about superconductivity with T_c up to 20 K in Co-substituted $SrFe_2As_2$ polycrystalline samples [1]. Here, electron-doping of the FeAs layers was accomplished by direct substitution of the transition metal. It was found that sample preparation and distribution of impurity phases influences the observed physical properties in a subtle way. The temperature dependence of the electrical conductivity as well magnetic susceptibility (superconducting parameters, magnetic secondary phases, homogeneity) and specific heat capacity will be presented and discussed. Crystals have been grown by a modified self-flux technique and the distribution of transition-metal dopants has been investigated by electron microprobe analysis. A comparison of the observed features with polycrystalline samples will be given. In addition, the possibility of complementary direct hole-doping has been explored.

[1] A. Leithe-Jasper, W. Schnelle, C. Geibel, H. Rosner, Phys. Rev. Lett. 101, 207004 (2008).

TT 5.30 Mon 13:00 P1A

Thermal expansion studies on $RFeAsO_{1-x}F_x$ (R=La, Ce, Pr, Sm, Gd) — •L. Wang, N. Leps, U. Köhler, G. Behr, R. Klingeler, C. Hess, and B. Büchner — Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany

We present thermal expansion α and magnetostriction data of $RFeAsO_{1-x}F_x$ with R=La, Ce, Pr, Sm, Gd. The undoped compounds, with $x = 0$, exhibit thermal expansion anomalies at both the spin ordering transition T_N and the structural phase transition T_S. A negative anomaly of α at T_N clearly implies the negative pressure dependence of magnetic ordering. In addition, we find a large regime of structural fluctuations above T_S which exhibit a positive pressure dependence. While no qualitative changes occur for different R-ions at higher temperature, the presence of magnetic R-sites yields antiferromagnetic order of 4f-moments. A finite magnetostriction far above the 4f-ordering temperatures indicates magnetic fluctuations. Upon doping, superconductivity evolves while both features indicating T_N and T_S disappear. The thermodynamic properties at the superconducting transitions are discussed.

TT 5.31 Mon 13:00 P1A

Superconductivity and magnetism in the oxypnictides: high field ESR and μSR studies of (La,Gd)$FeAsO_{1-x}F_x$ compounds — •Ferenc Murányi[1,2], Alexey Alfonsov[2], Vladislav Kataev[2], Anke Köhler[2], Jochen Werner[2], Günter Behr[2], Norman Leps[2], Rüdiger Klingeler[2], Agnieszka Kondrat[2], Christian Hess[2], Bernd Büchner[2], Rustem Khasanov[3], Hubertus Luetkens[3], and Hans-Henning Klaus[4] — [1]Physics Institute, University of Zürich, Winterthurerstr. 190, 8057 Zürich, Switzerland — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]IFP, TU Dresden, D-01069 Dresden, Germany

The discovery of a new class of superconducting materials, $ReFeAsO_{1-x}F_x$, stirred up the scientific community. Here we report the Gd^{3+} high field ESR study of differently doped (La,Gd)$FeAsO_{1-x}F_x$ compounds. In lightly Gd-doped LaFeAsO samples the SDW transition yields line-broadening at the transition temperature, the SDW transition is then suppressed upon F-doping. In the dense compound, GdFeAsO, with SDW transition around 140 K, the Gd-ESR was also studied. With 15% F-doping superconductivity appears at $\sim$ 21 K. The SDW and SC transitions are clearly seen in ESR and in μSR as well. Surprisingly the reminiscence of the SDW transition of the undoped material (GdFeAsO) was identified in the doped (15% F) compound at lower temperature ($\sim$ 80 K). This indicates the importance of the the interplay between superconductivity and magnetism in oxypnictides.

TT 5.32 Mon 13:00 P1A

Magnetism, structure, thermodynamics and transport of $RO_{1-x}F_xFeAs$ (R=La, Ce, Sm, Gd) superconductors — J. E. Hamann-Borrero[1], A. Kondrat[1], N. Leps[1], L. Wang[1], A. Alfonsov[1], F. Hammerath[1], A. Narduzzo[1], H. Grafe[1], G. Lang[1], D. Paar[1], J. Werner[1], G. Behr[1], V. Kataev[1], •C. Hess[1], R. Klingeler[1], B. Büchner[1], H. Luetkens[2], H.-H. Klauss[3], S. Kimber[4], R. Feyerherm[4], D. Argyriou[4], M. Kosmala[5], O. Schumann[5], and M. Braden[5] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, PSI, CH-5232 Villigen, Switzerland — [3]Institut für Festkörperphysik, TU Dresden, D-01069 Dresden, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), 14109 Berlin, Germany — [5]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We discuss magnetism, structure, thermodynamics and transport properties of the new oxypnictide superconductors $RO_{1-x}F_xFeAs$ (R=La, Ce, Sm, Gd). At zero fluorine doping we observe a close link between electronic, structural and magnetic degrees of freedom at the structural and the magnetic phase transitions $T_S \approx 160$ K and $T_N \approx 138$ K. F-doping leads to the suppression of these transitions and the emergence of superconductivity. The superconducting doping levels exhibits an interesting interplay between magnetism and

superconductivity. We discuss the influence of different R-ions on the physical properties.

TT 5.33 Mon 13:00 P1A

Electronic phase separation and magnetic order in the cobalt doped $RFe_{2-x}Co_xAs_2$ (R=Sr, Eu) iron pnictide superconductors — A. Kwadrin[1], H. Maeter[1], H.-H. Klauss[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], •M. Kraken[3], J. Litterst[3], A. Jesche[4], A. Leite-Jasper[4], H. Rosner[4], W. Schnelle[4], and C. Geibel[4] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Institut für Physik der Kondensierten Materie, TU Braunschweig — [4]Max-Planck-Institut für Chemische Physik fester Stoffe Dresden

We have investigated the magnetic and superconducting properties of $RFe_{2-x}Co_xAs_2$ with R=Sr, Eu and $0 \leq x \leq 0.4$ by means of muon spin relaxation (μ^+SR) and Mössbauer spectroscopy. Under ambient pressure the antiferromagntic ordering temperature, T_N of $SrFe_{2-x}Co_xAs_2$ decreases with increasing Co-doping. However, T_N remains finite even as superconductivity appears as a function of doping. This shows that electronic phase separation plays a role in this system. High pressure experiments show a reduction the magnetic ordering temperature by pressure. On the contrary, $EuFe_{2-x}Co_xAs_2$ does not show superconductivity under ambient pressure but a peculiar interplay of the rare earth and iron magnetic order as a function of the Co-doping level.

TT 5.34 Mon 13:00 P1A

Electronic phase diagram of the $LaO_{1-x}F_xFeAs$ superconductor: A muon spin relaxation study — •H. Luetkens[1], H.-H. Klauss[2], F.J. Litterst[3], T. Dellmann[3], R. Klingeler[4], C. Hess[4], R. Khasanov[1], A. Amato[1], C. Baines[1], M. Kosmala[5], O.J. Schumann[5], M. Braden[5], J. Hamann-Borrero[4], N. Leps[4], A. Kondrat[4], G. Behr[4], J. Werner[4], and B. Büchner[4] — [1]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Institut für Festkörperphysik, TU Dresden — [3]Institut für Physik der Kondensierten Materie, TU Braunschweig — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden — [5]II. Physikalisches Institut, Universität zu Köln

The structural and electronic phase diagram of $LaO_{1-x}F_xFeAs$ and, in particular, the exact nature of the change from the magnetically ordered to the superconducting state that was determined by means of x-ray scattering, muSR and Mössbauer spectroscopy will be presented [1-3]. A discontinuous first-order-like change of the Néel temperature, the superconducting transition temperature, the sublattice magnetisation and the superfluid density is found between x=0.04 and x=0.05. While these results strongly question the relevance of quantum critical behaviour in iron pnictides they prove an important role of the structural orthorhombic distortion disappearing exactly at the SDW magnetism and superconductivity phase boundary.

[1] H. Luetkens et al., Phys. Rev. Lett. 101, 097009 (2008).
[2] H.-H. Klauss et al., Phys. Rev. Lett. 101, 077005 (2008).
[3] H. Luetkens et al., arXiv:0806.3533 (2008).

TT 5.35 Mon 13:00 P1A

Electronic structure studies of $BaFe_2As_2$ by angle-resolved photoemission spectroscopy — •Thirupathaiah Setti[1], Jörg Fink[1,2], Ruslan Ovsyannikov[1], Hermann Andreas Dürr[1], Cludia Felser[3], Shafagh Dastjani Farahani[3], Dirt Johrendt[4], Marianne Rotter[4], Yingkai Huang[5], Sanne de Jong[5], and Mark Golden[5] — [1]Helmholtz Zentrum, Berlin — [2]IFW, Dresden — [3]Inst.für Anorg. Chemie und Anal. Chemie, Johannes Gutenberg-Universität, Mainz — [4]Department Chemie und Biochemie, LMU München, München — [5]Vander Waals-Zeeman Institute, University of Amsterdam, Amsterdam, The Netherlands

We report high resolution angle-resolved photoemission spectroscopy (ARPES) studies of the electronic structure of $BaFe_2As_2$, which is one of the parent compounds of the Fe-pnictide superconductors. ARPES measurements have been performed at 20 K and 300 K, corresponding to the orthorhombic antiferromagnetic phase and the tetragonal paramagnetic phase, respectively. Photon energies between 30 and 175 eV and polarizations parallel and perpendicular to the scattering plane have been used.Changes in spectral weights at the Fermi level upon variation of the polarization of the incident photons yield important information on the orbital character of the states near the Fermi level. Only small differences in the electronic structure are observed between 20 and 300 K. The results are compared with LAPW calculations for the tetragonal paramagnetic phase and the orthorhombic antiferromagnetic state. Finally, the photon energy dependence of the spectra provides information on the kz dispersion of the bands.

TT 5.36 Mon 13:00 P1A

NMR studies on the new iron arsenide superconductors including the superconducting state — •Hans-Joachim Grafe[1], Guillaume Lang[1], Franziska Hammerath[1], Dalibor Paar[1,2], Katarina Manthey[1], Nicholas Curro[3], Günther Behr[1], Jochen Werner[1], and Bernd Büchner[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Dept. of Physics, Faculty of Science, Univ. of Zagreb, P. O. Box 331, — [3]Dept. of Physics, Univ. of California, Davis, CA 95616, USA

We summarize our Nuclear Magnetic Resonance (NMR) and Nuclear Quadrupole Resonance (NQR) results on the new iron arsenide superconductor $LaO_{1-x}F_xFeAs$ in the normal state [1,2], and show new NMR data in the superconducting state. Beyond early evidence of nodes and spin-singlet pairing [2], we find evidence of a deviation of the T^3 behaviour of the spin lattice relaxation rate, $1/T_1$, at temperatures significantly below T_c, which would agree with the suggested extended s-wave symmetry [3]. The deviation of the T^3 behaviour is induced by the pair breaking effect of impurities. Different amounts of impurities would lead to different temperature dependences of $1/T_1$, which would allow to differentiate between d-wave and extended s-wave symmetries.

[1] H.-J. Grafe et al., arXiv:0811.4508
[2] H.-J. Grafe et al., PRL 101, 047003 (2008)
[3] A. Chubukov et al., PRB 78, 134512 (2008)

TT 5.37 Mon 13:00 P1A

High pressure study of $CaFe_2As_2$ and $BaFe_2As_2$ — •William Duncan[1], Oliver Welzel[2], Xian-hui Chen[3], Malte Grosche[2], and Philipp Niklowitz[1] — [1]Royal Holloway, University of London, Egham, UK — [2]Cavendish Laboratory, Cambridge, UK — [3]Dept. of Physics, University of Science and Technology of China, Hefei, People's Republic of China

The high pressure behaviour of the stoichiometric 1-2-2 iron arsenide compounds has been controversial. We investigate high quality stoichiometric single crystals grown from FeAs self-flux. Measurements on $CaFe_2As_2$ in a piston-cylinder pressure cell indicate a very low critical pressure of about 2 kbar for the onset of superconductivity. The pressure range in which full resistive transitions can be observed is exceedingly narrow, much less than one kbar, supporting suggestions in the literature that pressure-induced superconductivity is not a bulk phenomenon in $CaFe_2As_2$.

$BaFe_2As_2$ has been investigated up to 30 kbar in a piston-cylinder cell, and at higher pressures using anvil cell techniques, with both solid and liquid pressure media. Our data show a gradual suppression of the spin density wave/structural transition with pressure, falling below 100 K above 50 kbar. Low temperature anomalies in the resistivity below about 25 K suggest the onset of filamentary superconductivity.

We continue to explore the phase diagram of both systems to higher pressure, in order to investigate, in particular, the vicinity of the expected quantum critical point in $BaFe_2As_2$.

TT 5.38 Mon 13:00 P1A

Raman spectroscopic studies on single crystals of the iron-based superconductor $SmFeAsO_{1-x}F_x$ — •Ivan Jursic[1], Joachim Schoenes[1], Zbigniew Bukowski[2], and Janusz Karpinski[2] — [1]Technische Universität Braunschweig, Institut für Physik der Kondensierten Materie, 38106 Braunschweig, Germany — [2]ETH Zürich, Laboratorium fuer Festkörperphysik, 8093 Zürich, Switzerland

The recent discovery of superconductivity in iron-based oxypnctides has led to a great interest in this new class of non-cuprate high-T_c superconductors. Though theoretical work predicts a small electron-phonon coupling, which means that this should not be the driving mechanism for the observerd T_c's in this class of material, the exact coupling mechanism is still under debate.

We present Raman studies on superconducting $SmFeAsO_{1-x}F_x$ single crystals where the T_c was determined by SQUID magnetometric measurements to be 34 K. At room temperature polarized measurements were performed to assign the phonon modes. Furthermore studies at different temperatures reaching from 5K to 300K were done to investigate the phonon behavior. The phonon frequencies shift with temperature and we investigate this shift in terms of electron-phonon coupling.

TT 5.39 Mon 13:00 P1A

Multi-orbital Dynamical Correlations in Iron Pnictides — •L. Craco — Max-Planck-Institut fuer Chemische Physik fester Stoffe

In view of the importance of dynamical correlations associated with electron interactions in Fe-pnictides, we will discuss our recent LDA+DMFT results for the correlated electronic structure of Sm- and La-based compounds [1,2]. We will show why multi-orbital electronic correlations are necessary for a concrete description of key physical responses found in their normal state. We present theory-experiment comparison of the one- and two-particle spectral functions. Such a comparison is required for deciding whether a given system is correlated, and if so, how strongly. Our study supports the view that superconductivity in Fe-pnictides arises from a bad metallic, incoherent normal state that is proximate to a Mott-Hubbard insulator.

[1] L. Craco, M. S. Laad, S. Leoni, and H. Rosner, Phys. Rev. B **78**, 134511 (2008); and, Virtual Journal of Applications of Superconductivity **15**, Issue 8 (2008).

[2] M.S. Laad, L. Craco, S. Leoni, and H. Rosner, arXiv:0810.1607.

TT 5.40 Mon 13:00 P1A

Feedback spin resonance in the Fe-pnictide superconductors — •Alireza Akbari[1], Peter Thalmeier[2], Ilya Eremin[1], and Peter Fulde[1] — [1]Max Planck Institute for the Physcis of Complex Systems, D-01187 Dresden, Germany — [2]Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

The superconducting feedback resonance in inelastic neutron scattering has been found in numerous unconventional superconductors of the cuprate, heavy fermion type and recently in the FeAs class. This collective spin excitation in the 3d FeAs superconducting layers appears below T_c at an energy $\omega_r < 2\Delta_0$ and momentum transfer $\mathbf{Q}$ $[\Delta(\mathbf{k}+\mathbf{Q}) = -\Delta(\mathbf{k})]$. This resonance has been found in some Fe_2As_2 type superconductors and may be a more general phenomenon. An indirect evidence for enhanced Fe 3d spin dynamics in the superconducting state was recently observed in $CeFeAsO_{1-x}F_x$. The crystalline electric field (CEF) excitations of localized Ce 4f- states at 20 meV were found to couple weakly to the spin excitations in the FeAs layers leading to characteristic frequency shift and broadening effects. The temperature dependence of CEF excitations is studied within a RPA approximation. The experimental decrease of CEF excitation energy with temperature in the normal state is explained. Below T_c the feedback effect leads to an enhanced 3d spin response around 20 meV at $\mathbf{Q} = (\pi, \pi)$. The spectral shape and its temperature dependence of 3d and total 4f-3d spin dynamics are calculated. We compare the results to similar examples in the unconventional heavy fermion superconductors.

TT 5.41 Mon 13:00 P1A

Pecularities of the superconducting gaps and the fermion-boson interaction in $TmNi_2B_2C$ as seen by point-contact spectroscopy — •Oksana Kvitnitskaya[1,2], Yurii Naidyuk[1], Lidiya Tiutrina[1], Igor Yanson[1], Günter Fuchs[2], Konstantin Nenkov[2], Günter Behr[2], and Stefan-Ludwig Drechsler[2] — [1]ILT Kharkiv, Ukraine — [2]IFW Dresden

Point-contact (PC) investigations on the title compound in the normal and superconducting (SC) state ($T_c \simeq 10.6$ K) are presented. The T-dependence of two SC gaps in $TmNi_2B_2C$ determined by Andreev-reflection spectroscopy deviates from the BCS behavior in displaying a maximum at about $T_c/2$. Additional evidence for the presence of a 2nd gap half as large as the main gap is given. For the first time "reentrant" features were found in the Andreev-reflection spectra measured in magnetic fields. The PC spectroscopy of the fermion-boson interaction in $TmNi_2B_2C$ reveals a pronounced phonon maximum at 9.5 meV and a more smeared one around 15 meV, while at higher energies the PC spectra are almost featureless. Additionally, the intense peak slightly above 3 meV observed in the PC spectra of $TmNi_2B_2C$, is presumably caused by crystalline-electric-field excitations. The peak near 1 meV detected for some spectra is connected with a modification of the crystal electric field probably due to boron or carbon vacancies.

TT 6: Postersession Correlated Electrons: (General) Theory, Low-Dimensional Systems, Kondo Physics, Heavy Fermions, Quantum-Critical Phenomena

Time: Monday 13:00–16:45 Location: P1A

TT 6.1 Mon 13:00 P1A

Magnetic and electronic properties of double perovskites $La_{2-x}Sr_xCoIrO_6 (0 \leq x \leq 1)$ — •Narendirakumar Narayanan[1,2], Robert Laskowski[3], Daria Mikhailova[1,2], Anatoly Senyshin[1], Peter Blaha[3], Karlheinz Schwarz[3], Helmut Ehrenberg[1,2], and Hartmut Fuess[1] — [1]Darmstadt University of Technology, Department of Materials Science — [2]IFW Dresden, Institute for Complex Materials — [3]Vienna University of Technology, Institute of Materials Chemistry

Double Perovskites (DP) $A_2BB'O_6$ with 3d transition metals at B-site and 4d or 5d transition metals at B'-site have been extensively studied due to their interesting physical properties, that could be tuned by the partial substitution of the ions involved[1-2]. The ability of Iridium to display different oxidation states and structural constraints (distortion of bond angles) on 5d orbitals, which are generally considered more extended in nature compared to the 3d or 4d ones promise interesting physical properties. We discuss the composition La_2CoIrO_6 in terms of density functional theory (DFT). We focus mainly on two open aspects. The first one concerns the realization of an insulating state in this material. We show that insulating state can develop only, if we apply LDA/GGA+U method for both B and B' atoms. The second aspect concerns the magnetic properties. Calculations indicate that this DP has a non-collinear magnetic structure.

[1] K.-I. Kobayashi, T. Kimura, H. Sawada, K. Terakura and Y. Tokura, Nature 395, 677 (1998).

[2] H. Kato, T. Okuda, Y. Okimoto, Y. Tomioka, K. Oikawa, T. Kamiyama, and Y. Tokura, Phys. Rev. B 65, 144404 (2002).

TT 6.2 Mon 13:00 P1A

Novel unitary transformations to treat systems with quasiparticles of finite lifetime — Tim Fischer[1], •Nils Drescher[1], Sebastian Duffe[1], and Götz S. Uhrig[1,2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

The method of self-similar continuous unitary transformations maps a given Hamiltonian to an effective Hamiltonian whose final structure depends on the generator of the unitary transformation. The aim is to derive an effective Hamiltonian simpler than the original Hamiltonian without losing its physics. One route is to disentangle sectors of different number of quasiparticles which is achieved by the MKU generator [1,2]. But this route fails if the elementary excitations have a finite lifetime due to hybridization with continua which is a common situation in physics.

We propose variants of the MKU generator and prove that they lead to converging flow equations. The new unitary transformations are tested and illustrated for one-dimensional spin models.

[1] A. Mielke, Eur. Phys. J. B 5, 605 (1998)

[2] C. Knetter, G.S. Uhrig, Eur. Phys. J. B 13, 209 (2000)

TT 6.3 Mon 13:00 P1A

Nonequilibrium steady-state density of states of the Falicov-Kimball model in the presence of a large electric field — •Alexander Joura[1] and Jim Freericks[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Georgetown University, Washington, DC 20057, U.S.A.

The electronic density of states (DOS) of the Falicov-Kimball model in a constant uniform electric field E is calculated using a Kadanoff-Baym-Keldysh nonequilibrium Green's function technique and dynamical mean-field theory. When the electron-electron interaction U vanishes, the DOS is the Wannier-Stark ladder of delta functions spaced by the Bloch frequency. If U is increased, the delta function peaks initially broaden due to the scattering, but ultimately evolve into a continuous structure for large U's. As E is increased from small values, where linear response theory can be used and we see broadened Wannier-Stark peaks, the DOS develops a shape with large peaks at

miniband edges, separated in energy by U. We verify the accuracy of our calculations by checking the DOS against frequency-moment sum rules, and an independent transient-response calculation of the Green's functions at long times. While our formalism has been applied to the Falicov-Kimball model, it can also be directly extended to other models like the Hubbard or periodic Anderson model, by using more complicated impurity problem solvers.

TT 6.4 Mon 13:00 P1A

Charge transport in classical geometrically frustrated systems — •David Leipold and Erich Runge — TU-Ilmenau, Institut für Physik, D-98693 Ilmenau

The quantum mechanics of geometrically frustrated systems has been studied intensively in recent years [1,2]. Here, we study classical charge transport on the criss-crossed checkerboard lattice, which is the two-dimensional counterpart of the pyrochlore lattice. We present results obtained by Monte Carlo simulations in a wide range of particle densities, applied voltages and temperatures. Furthermore, we discuss analytical models which reproduce the simulated behavior in various limits. Our simulations confirm the existence of a number of structures, which are classical analogues of quantum mechanical quasi-particles. These were predicted earlier [3] to carry fractional charge. Due to their high mobility, they contribute substantially to charge transport.

[1] E. Runge and P. Fulde, Phys. Rev. B **70**, 245113 (2004)

[2] F. Pollmann, P. Fulde, E. Runge, Phys. Rev. B **73**, 125121 (2006)

[3] F. Pollmann, J.J. Betouras, E. Runge, Phys. Rev. B **73**, 174417 (2006)

TT 6.5 Mon 13:00 P1A

Matrix product state calculation of the correlation density matrix: an unbiased analysis of long-range correlations — •Wolfgang Münder[1], Andreas Weichselbaum[1], Jan von Delft[1], and Christopher Henley[2] — [1]Department of Physics and Center for NanoScience, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilans-Universität, Theresienstrasse 37, 80333 Munich — [2]LASSP, Clark Hall, Cornell University, Ithaca, NY 14853-2501

A useful concept for determining the dominant correlations of the ground state wave function of a lattice model, in an unbiased fashion without prior knowledge, is the correlation density matrix (CDM) [1]. For two disjoint, separated clusters A and B, it is defined to be the density matrix of their union, minus the direct product of their respective density matrices, $\rho_{AB}^{CDM} = \rho_{A\cup B} - \rho_A \otimes \rho_B$. It encodes all possible correlations between the clusters A and B and has block-diagonal form, dictated by the symmetries of the Hamiltonian. We analyse it for a family of interacting spinless fermion models on a ladder [1], which has nontrivial mappings to free fermions in certain limits [2]. We use the density matrix renormalization group (implementing Abelian symmetries explicitly) to calculate the ground state in the form of a matrix product state, from which the correlation density matrix can straightforwardly be obtained. We also discuss methods for extracting the Luttinger liquid scaling exponents from the correlation density matrix.

[1] S.-A. Cheong and C.L. Henley, arXiv:0809.0075v1 (2008).

[2] S.-A. Cheong, PhD thesis, Cornell Univ., (2007), http://people.ccmr.cornell.edu/~clh/Theses/cheong-habis.pdf

TT 6.6 Mon 13:00 P1A

A fast impurity solver based on merging the equation of motion method and genetic algorithms — •Qingguo Feng, Yuzhong Zhang, and Harald O. Jeschke — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The successful application of LDA+DMFT to strongly correlated systems generates increasing interest in the development of fast impurity solvers for DMFT. By using the equation of motion method with a suitable decoupling scheme, a new fast impurity solver is established. An efficient way to find self-consistent solutions of the closed set of integral equations is found in a combination of iteration and genetic algorithms. This new impurity solver can work directly on the real frequency axis and yields the Green's function for all temperatures. The successful description of various physical properties of Hubbard and periodic Anderson models demonstrates the power of our method in understanding strongly correlated systems.

TT 6.7 Mon 13:00 P1A

CDMFT and DCA with Lanczos solver — •giorgio sangiovanni[1], erik koch[2], and olle gunnarsson[3] — [1]Vienna University of Technology — [2]Forschungszentrum Jülich — [3]Max-Planck Institut Stuttgart

Quantum cluster methods are among the most powerful tools to study strongly correlated systems. While a huge variety of impurity-solver are available nowadays for single-site Dynamical Mean Field Theory, for Cellular Dynamical Mean Field Theory (CDMFT) and Dynamical Cluster Approximation (DCA) only Quantum Monte Carlo-based solvers are usually employed. Exact Diagonalization has been hitherto used only for extremely small clusters. We introduce Hamiltonian-based solver using Lanczos at T=0 exploiting the cluster point symmetry. This implies symmetries of the hybridization, which can substantially reduce the number of independent parameters to fit the bath Green function. We review these symmetries and derive general sum-rules for the hybridizations, which (i) allow to check the quality of a fit using a finite set of bath sites and (ii) imply what hybridizations vanish. Such rationalization of the Lanczos solver is a necessary step towards a more efficient algorithm which may eventually allow us to treat larger systems.

TT 6.8 Mon 13:00 P1A

Superconductivity in the two-dimensional extended periodic Anderson model — •Nham Phan Van[1,2] and Klaus W Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Max-Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

The two-dimensional periodic Anderson model with an additional local Coulomb repulsion U_{fc} between localized f and conduction electrons is investigated by the use of the projector-based renormalization method. When the f-level energy ϵ_f is close to the Fermi level, the valence transition becomes sharper by increasing U_{fc}. We start from an Hamiltonian which includes small gauge symmetry breaking fields and derive self-consistent equations for the order parameters. Our numerical results show that the d-wave superconducting order is dominant close to the sharp valence transition regime. This affirms that the valence fluctuations might lead to superconductivity in the Ce based heavy-fermion systems under high pressure.

TT 6.9 Mon 13:00 P1A

Thermodynamics and transport properties of the single-band Hubbard model — •Ken Lichtner and Wolfgang Nolting — Institut für Physik, Humboldt-Universität, Newtonstraße 15, 12489 Berlin, Germany

We study the possibility and stability of band-ferromagnetism in the single-band Hubbard model, focusing on thermodynamics as well as transport properties calculated fully self-consistently within our "local modified perturbation theory". The obtained self energy fulfills the first four spectral moments, therewith guaranteeing the correct high-energy behaviour, and is exact up to second order perturbation theory. Results are presented for f.c.c. as well as s.c. lattices. Phase diagrams are shown for ferromagnetic and paramagnetic solutions presented in terms of finite T and n. An overall comparison with the dynamical mean-field theory for infinite-dimensional lattices (DMFT) and the simple mean field theory (Stoner) is drawn.

TT 6.10 Mon 13:00 P1A

Slyanin isomorphism and a correspondence between coordinate and functional Bethe ansatz — •Andreas Osterloh — Institut für theoretische Physik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany.

We focus on the Sklyanin functional Bethe ansatz (FBA) from a different point of view, interpreting it as a coordinate Bethe ansatz (CBA) tailored from algebraic insight. This perspective sheds light on the Sklyanin isomorphism and establishes a direct access to the eigenstates. The isomorphism unveils the meaning of the Sklyanin Q-functions and shows that the resulting T-Q recursion relations can be extended at the best convenience to outside the Sklyanin FBA lattice.

TT 6.11 Mon 13:00 P1A

Antiferroquadrupolar phases in $\mathbf{U(Pd_{1-x}Pt_x)_3}$, $x \leq 0.01$ — •Markus Schäpers[1], Matthias Bleckmann[1], Dirk Schulze Grachtrup[1], Stefan Süllow[1], and Keith McEwen[2] — [1]Technsiche Universität Braunschweig, Braunschweig, Deutschland — [2]University College London, London, England

The double hexagonal compound UPd_3 has been shown to undergo several successive phase transitions below 8 K. These low temperature

phases are antiferroquadrupolar ordered ones with different AFQ order parameters. In-field measurements on UPd_3 reveal a complex response of these phases on magnetic fields, leading to a very rich magnetic phase diagram [1-3].

Here, for the first time we present resistivity measurements and a magnetic phase diagram for single crystalline lowly doped samples $U(Pd_{1-x}Pt_x)_3$, $x \leq 0.01$, and compare these measurements to pure UPd_3. We find that doping leads to reduced ordering temperatures but leaves the underlying physics of the AFQ ordered phases unaffected

[1] Y. Tokiwa, K. Sugiyama, T. Takeuchi, M. Nakashima, R. Settai, Y. Inada, Y. Haga, E. Yamamoto, K. Kindo, H. Harima and Y. Onuki, J. Phys. Soc. Jpn. 70 (2001) 1731

[2] D. F. McMorrow, K. A. McEwen, U. Steigenberger, H. M. Rønnow and F. Yakhou, Phys. Rev. Lett. 87 (2001) 057201

[3] H. C. Walker, K. A. McEwen, D. F. McMorrow, S. B. Wilkins, F. Wastin, E. Colineau and D. Fort, Phys. Rev. Lett. 97 (2006) 137203

TT 6.12 Mon 13:00 P1A

Structural relaxation due to electronic correlations in the paramagnetic insulator $KCuF_3$ — •Ivan Leonov[1], Nadia Binggeli[2,3], Dmitry Korotin[4], Vladimir I. Anisimov[4], Natasa Stojic[5,3], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Abdus Salam International Center for Theoretical Physics, 34014 Trieste, Italy — [3]INFM-CNR Democritos, 34014 Trieste, Italy — [4]Institute of Metal Physics, 620219 Yekaterinburg GSP-170, Russia — [5]International School for Advanced Studies, SISSA, 34014 Trieste, Italy

We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations [1]. It combines *ab initio* band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. Results obtained for paramagnetic $KCuF_3$, namely an equilibrium Jahn-Teller distortion of 4.2% and antiferro-orbital ordering, agree well with experiment. The electronic correlations are also found to be responsible for a considerable enhancement of the orbital polarization. The GGA+DMFT scheme presented here opens the way for fully microscopic investigations of the structural properties of strongly correlated electron materials such as lattice instabilities observed at correlation induced metal-insulator transitions.

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

TT 6.13 Mon 13:00 P1A

Phonon renormalization from local and transitive electron-lattice couplings in strongly correlated systems — •Ernst von Oelsen[1], Andrea Di Ciolo[2,3], Jose Lorenzana[2,3,4], Marco Grilli[2,3], and Götz Seibold[1] — [1]Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany — [2]Dipartimento di Fisica, Università di Roma "La Sapienza", P. Aldo Moro 2, 00185 Roma, Italy — [3]SMC-Istituto Nazionale di Fisica della Materia — [4]ISC-Consiglio Nazionale delle Ricerche

Within the time-dependent Gutzwiller approximation (TDGA) applied to Holstein- and SSH-Hubbard models we study the influence of electron correlations on the phonon self-energy. For the local Holstein coupling we find that the phonon frequency renormalization gets weakened upon increasing the onsite interaction U for all momenta. In contrast, correlations can enhance the phonon frequency shift for small wave-vectors in the SSH-Hubbard model. Moreover the TDGA applied to the latter model provides a mechanism which leads to phonon frequency corrections at intermediate momenta due to the coupling with double occupancy fluctuations. Both models display a shift of the nesting-induced to a $q = 0$ instability when the onsite interaction becomes sufficiently strong and thus establishing phase separation as a generic phenomenon of strongly correlated electron-phonon coupled systems.

TT 6.14 Mon 13:00 P1A

Calculation of thermoelectric properties by LDA+DMFT — •Philipp Wissgott, Philipp Hansmann, Nico Parragh, Alessandro Toschi, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

Strongly correlated electron systems were recently found to show impressive thermoelectric properties. For example the transition metal oxides Na_xCoO_2 [1] and $LiRh_2O_4$ [2] have a thermopower of almost 100 μV/K. As bandstructure and electronic correlations can play an important role for the thermopower, we investigate these materials with the combination of density functional theory and dynamical mean field theory. Following [3], effects of Na disorder, which lead to stronger correlations, are taken into account by a binary distribution. In comparison to experiment, we present results for the thermopower, the resistivity, and the thermal conductivity at various temperatures.

[1] I. Terasaki, Y. Sasago and K. Uchinokura, Phys. Rev. B **56**, R12685 (1997).

[2] Y. Okamoto *et al.*,Phys. Rev. Lett. **101** 086404 (2008).

[3] C.A. Marianetti and G. Kotliar, Phys. Rev. Lett. **98** 176405 (2007).

TT 6.15 Mon 13:00 P1A

Electronic structure of the low-dimensional transition metal oxyhalide VOCl — •Sebastian Glawion[1], Markus Scholz[1], Karin Goss[1], Michael Sing[1], Harald Jeschke[2], Tanusri Saha-Dasgupta[3], Roser Valenti[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Institut für Theoretische Physik, Universität Frankfurt — [3]S.N. Bose National Centre for Basic Sciences, Kolkata, India

In the quest for RVB-like superconductivity, layered oxyhalides of the form MOX (M=Ti,V; X=Cl,Br) have been discussed some fifteen years ago as possible candidates. This was due to their low-dimensional crystal structure involving frustrated triangular lattice planes. While no superconducting state in these Mott insulators was observed yet, other interesting phenomena, e.g. an unconventional spin-Peierls transition, have been found in TiOX. The isostructural material VOCl has a $3d^2$ configuration and shows antiferromagnetic ordering below 150K; magnetic susceptibility measurements show an anisotropy along the a-axis. Electronically, however, the degree of one-dimensionality observed by photoemission is reduced compared to the well-studied $3d^1$ TiOX systems. LDA+U calculations indicate that VOCl is a Mott insulator despite its two $3d$ electrons. Upon n-doping with alkali metals new states appear in the gap without having quasi-particle character, i.e. no evidence for a metallic phase is found. A comparison between VOCl and TiOX is expected to yield new insights into the importance of one-dimensionality and multi-band Mott-Hubbard physics in the oxyhalides.

TT 6.16 Mon 13:00 P1A

Electronic properties of Fe, Mn, and Ni impurities in MgO thin films — T. Haupricht[1], •Y.-Y. Chin[1,2], R. Gierth[1], J. Weinen[1], S. G. Altendorf[1], A. Hendricks[1], Z. Hu[1], J. Gegner[1], H. Fujiwara[1], D. Regesch[1], H. H. Hsieh[3], H.-J. Lin[2], C. T. Chen[2], and L. H. Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

Transition metal ions in MgO can serve as model systems for various (usually more complicated) d^n systems in octahedral symmetry. Going from bulk crystals to impurity systems the core level and valence band photoemission (PES) and soft x-ray absorption (XAS) spectra can change significantly e.g. due to the absence of non-local screening effects [v. Veenendaal et al., PRL 70 (1993)]. Here, we present our core level and valence band PES and XAS data of Fe, Mn, and Ni impurities in MgO thin films grown on metal substrates in-situ by means of molecular beam epitaxy (MBE). Compared to the bulk compounds FeO, MnO, and NiO, remarkable differences are observed in the spectra. In order to understand these differences we have simulated the spectra using configuration interaction cluster calculations. Ab-initio oriented approaches such as LDA+DMFT are highly desired to obtain parameter free explanations.

TT 6.17 Mon 13:00 P1A

Ultrasonic investigation of the quasi-2D quantum antiferromagnet Cs_2CuCl_4 — •A. Sytcheva[1], S. Zherlitsyn[1], J. Wosnitza[1], O. Chiatti[1], A. A. Zvyagin[2,3], and R. Coldea[4] — [1]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Germany — [2]MPI für Physik komplexer Systeme, Dresden, Germany — [3]Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine — [4]Wills Physics Laboratory, University of Bristol, United Kingdom

We report on results of sound-velocity and sound-attenuation measurements in the triangular-lattice quasi-2D spin-1/2 antiferromagnet (AFM) Cs_2CuCl_4 ($T_N = 0.6$ K), in magnetic fields up to 18 T applied along the a axis and at low temperatures from 5 down to 0.3 K. Be-

low T_N this material displays a 3D incommensurate spiral long-range AFM order, which is stable up to $B_s \approx 8.5$ T for fields applied along the a axis. Above this field all spins are polarized. For the AFM phase a possibility for the Bose-Einstein condensation of magnons has been suggested whereas beyond the AFM phase at low temperatures a proximity to the spin liquid (SL) state is considered in this compound. The longitudinal c_{11} acoustic mode, which has a propagation direction along the a axis, shows pronounced anomalies in sound velocity and attenuation in discussed temperature and field range indicating spin-strain interaction. It also demonstrates frequency-dependent effects indicating the presence of relaxation processes. The ultrasonic results are analyzed with a theory based on exchange-striction coupling. There is a good qualitative agreement between theory and experiment.

TT 6.18 Mon 13:00 P1A

Effects of structural modulations on the quasiparticle distribution in 2H-TaSe$_2$ — •Torben Hänke[1], Alexander Kordyuk[1], Volodymyr Zabolotnyy[1], Daniil Evtushinsky[1], Paul Sass[1], Christian Hess[1], Sergey Borisenko[1], Helmut Berger[2], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institut de Physique Appliquée, EPF, 1015 Lausanne, Switzerland

We report on a temperature dependent scanning tunneling microscopy (STM) and angle resolved photoemission (ARPES) study of the Cu intercalated dichalcogenide 2H-TaSe$_2$. The Cu intercalation leads not only to a lowering of the transition temperature into the commensurate charge-density wave state (CDW) but also to the formation of a $\sqrt{13} \times \sqrt{13}$ superstructure, previously observed for the 1T polytype only [1]. The origin, spectroscopic appearance, and influence of these superstructures on the electronic properties of 2H-TaSe$_2$ will be discussed.

[1] D. Stoltz *et al.*, Phys. Rev. B **76** 073410 (2007).

TT 6.19 Mon 13:00 P1A

Low temperature magnetism of La$_{1-x}$Sr$_x$CoO$_3$ ($x \sim 0.002$) — •V. Kataev[1], A. Alfonsov[1], E. Vavilova[1,2], B. Büchner[1], A. Podlesnyak[3], M. Russina[3], A. Furrer[4], Th. Strässle[4], E. Pomjakushina[4,5], K. Conder[5], and D.I. Khomskii[6] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Hahn–Meitner–Institut, D-14109 Berlin, Germany — [4]Laboratory for Neutron Scattering, ETH Zürich & PSI, CH-5232 Villigen PSI, Switzerland — [5]Laboratory for Developments and Methods, PSI, CH-5232 Villigen PSI, Switzerland — [6]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

We present results of electron spin- (ESR), nuclear magnetic resonance (NMR) and inelastic neutron scattering (INS) studies of single crystals of La$_{1-x}$Sr$_x$CoO$_3$. In contrast to LaCoO$_3$, which is nonmagnetic at $T \lesssim 30$ K, a very small Sr^{2+} doping ($x \sim 0.002$) yields a strong magnetization already at low T. ^{59}Co NMR measurements indicate the formation of extended magnetic clusters in this temperature regime. ESR spectroscopy reveals multiple gapped resonance excitations with different g-factor values suggesting that magnetic clusters have a large spin multiplicity and substantial spin-orbital coupling. The Q-dependence of the INS intensity gives evidence that the cluster comprises 7 magnetic Co ions. We argue that the doped hole couples these ions ferromagnetically yielding a spin-state polaron with a huge local magnetic moment.

TT 6.20 Mon 13:00 P1A

Collective two-particle excitations in cuprates and manganites: Resonant inelastic x-ray scattering and electron energy loss spectroscopy — •Jochen Geck[1], Roberto Krauss[1], Roman Schuster[1], Martin Knupfer[1], Patrick Ribeiro[1], Bernd Büchner[1], Pieter Glatzel[2], Javier Herrero-Martin[2], Joaquin Garcia-Ruiz[3], Diego Casa[4], Thomas Gog[4], Hiroki Wadati[5], and George A. Sawatzky[5] — [1]IFW Dresden, Germany — [2]European Synchrotron Radiation Facility, France — [3]Universidad de Zaragoza, Spain — [4]Advanced Photon Source, USA — [5]University of British Columbia, Canada

The two-particle charge excitations of Sr_2CuO_3, which contains one-dimensional corner-sharing CuO_2-chains, were studied by Resonant Inelastic X-ray Scattering (RIXS) at the Cu K-edge. At the center of the Brillouin zone, the dependence of the various charge-transfer excitations on the incident photon energy E_i was studied in detail. The different charge transfer excitations resonate for different intermediate states, i.e., different E_i, which allows to draw conclusions about the symmetry of the created excitations. Further, the RIXS results are discussed in comparison to previous Electron Energy Loss Spectroscopy (EELS) studies. A similar approach was then used to investigate the two-particle excitations (La,Sr)$_2$MnO$_4$. Surprisingly, the excitations observed for the doped manganite materials share similar traits with the ones observed for the doped cuprates.

TT 6.21 Mon 13:00 P1A

Specific heat of a Cu$_3$ spin tube — •Juergen Schnack[1] and Roman Schnalle[2] — [1]Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld — [2]Universität Osnabrück, Fachbereich Physik, D-49069 Osnabrück

[(CuCl$_2$tachH)$_3$Cl]Cl$_2$ is a frustrated three-leg spin tube of antiferromagnetically coupled Cu spins with $s = 1/2$ [1,2]. The $T = 0$ phase diagram (gaps, plateaus) was discussed in e.g. [3,4]. Here we report on the specific heat of the spin tube which was determined experimentally. For low temperatures the specific heat is linear in temperature – reminiscent of a one-dimensional gapless spin chain – followed by a pronounced peak at higher temperatures. This behavior is discussed theoretically.

[1] J. Schnack *et al.*, Phys. Rev. B **70**, 174420 (2004).
[2] J. Schnack, C. R. Chimie **10**, 15 (2007).
[3] A. Lüscher *et al.*, Phys. Rev. B **70**, 060405(R) (2004).
[4] J.-B. Fouet *et al.*, Phys. Rev. B **73**, 014409 (2006).

TT 6.22 Mon 13:00 P1A

High Magnetic Field Measurements on single crystalline (5-MAP)$_2$CuBr$_4$ — •Daniela Rauch[1], Jan Kreitlow[1], Yurii Skourski[2], Mark M. Turnbull[3], and Stefan Süllow[1] — [1]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Braunschweig — [2]Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, Dresden — [3]Carlson School of Chemistry and Biochemistry, Clark University, Worcester, USA

(2-amino-5-methylpyridinium)$_2$CuBr$_4$, abbreviated as (5-MAP)$_2$CuBr$_4$, has been characterized as a square S=1/2 Heisenberg antiferromagnetic lattice [1,2]. The compound consists of two-dimensional sheets of highly distorted CuBr$_4$ tetrahedra separated by the organic cations. The magnetic coupling constants are 6.5 K for the intra-sheet coupling, 1.5 K for a residual inter-sheet coupling, with both interactions in effect resulting in an antiferromagnetic transition occurring at T$_N$=3.8 K.

Here we report a single crystal high magnetic field study on (5-MAP)$_2$CuBr$_4$, with magnetic fields up to 40 T at temperatures down to 1.5 K. From the data additional information on local anisotropies such as of the g-factor can be obtained and will be discussed.

[1] H. Place, R. Willett, Acta Cryst. **C43** (1987) 1050.
[2] F.M. Woodward, A.S. Albrecht, C.M. Wynn, C.P. Landee, M.M. Turnbull, Phys. Rev. B **65** (2002) 144412

TT 6.23 Mon 13:00 P1A

Specific heat of the highly anisotropic antiferromagnet [Cu(pyz)$_2$(HF$_2$)]PF$_6$ — •R. Beyer[1], M. Uhlarz[1], J. Wosnitza[1], and J.A. Schlueter[2] — [1]Hochfeld-Magnetlabor (HLD), Forschungszentrum Dresden-Rossendorf (FZD), Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, USA

The metal-organic compound [Cu(pyz)$_2$(HF$_2$)]X with X = PF$_6$ exhibits a quasi-cubic lattice of copper ions (S = $\frac{1}{2}$), but the magnetic properties show a predominantly two-dimensional (2D) nature due to a large anisotropy in the exchange couplings. The magnetic entropy and the antiferromagnetic ordering, eventually occurring at about 4.4 K, were investigated by specific-heat measurements. For this we established a continuous relaxation-time technique, using a single relaxation process to get specific heat data over a wide temperature range. The calorimetric investigations, performed between 2 and 100 K and in magnetic fields up to 14 T, have revealed a non-monotonic field dependence of the ordering temperature. The results are as expected from the model for a S = $\frac{1}{2}$ 2D square-lattice quantum Heisenberg antiferromagnet with an additional weak interlayer exchange (via Cu-F-H-F-Cu bonds).

In comparison to the X = BF$_4$ compound, the antiferromagnetically ordered phase extends to much higher temperatures. In a more detailed analysis, we can extract all exchange interactions with an interlayer coupling ten times larger than in X = BF$_4$. Thus, the 2D character is significantly reduced in X = PF$_6$.

TT 6.24 Mon 13:00 P1A

From solid to cluster – a computational study on the model compound Li_2CuO_2 — •Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and Helge Rosner[2] — [1]IFW Dresden, PF 270116, 01171 Dresden — [2]MPI CPfS Dresden, Nöthnitzer Str. 40, 01187 Dresden

The treatment of strong electron correlations is one of the major challenges in modern solid state physics and chemistry. Two standard approaches tackle the problem from opposite directions: In principle, quantum chemistry can deal with strong correlations exactly, but only for small clusters. Thus, finite size effects and the embedding of the clusters have to be controlled. 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 widely used LSDA+U method. Using the 1D model compound Li_2CuO_2 as an example, we present a computational study on the DFT level, aiming to a controlled, smooth transition from a 3D system to a cluster while preserving the most relevant physics of the system. Step by step, the structural complexity of the system is reduced, controlling the leading interactions by a tight binding procedure. Our study shall provide deeper insight into the implications caused by the different levels of approximations.

TT 6.25 Mon 13:00 P1A

Magnetic properties of the new low dimensional S=1/2 system: $Cu(NO_3)_2{\cdot}H_2O$ — M. Yehia[1], E. Vavilova[1,2], •V. Kataev[1], R. Klingeler[1], O. Volkova[3,4], E. Lapsheva[4], V. Shutov[4], O. Savelieva[4], A.N. Vasiliev[4], and B. Büchner[1] — [1]Institute for Solid State Physics, IFW Dresden, 01171 Dresden, Germany. — [2]Kazan Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia. — [3]Institute of Radiotechnics and Electronics, 125009 Moscow, Russia. — [4]Moscow State University, 119991 Moscow, Russia.

The new low dimensional S=1/2 system $Cu(NO_3)_2{\cdot}H_2O$ is studied by ESR (9.5 GHz), magnetic susceptibility $\chi(T)$, specific heat $Cp(T)$ and NMR. The anisotropy of the ESR measureables reveals a two dimensional nature of the $Cu^{2+}(S = 1/2)$ layers in this material. The T-dependence of the ESR response for different field directions indicates a substantial magnetic anisotropy and occurrence of different exchange paths in the Cu layers. A phase transition of antiferromagnetic nature at $T_N \sim 3.4$ K can be identified in the $\chi(T)$ data. This is consistent with the specific heat measurements which exhibit a peak at 3.4 K in zero magnetic field. However, an application of an external field of 3 T strongly suppresses this peak. In addition, a broad anomaly has been observed at low temperatures in the $Cp(T)$ data. On the basis of our experimental data we discuss the interplay between the structure and magnetism of this novel compound.

TT 6.26 Mon 13:00 P1A

Surface studies of charge-ordering transition metal oxides by means of scanning tunneling microscopy — Paul Sass[1], •Dirk Bombor[1], Grzegorz Urbanik[1], Torben Hänke[1], Christian Hess[1], Bernd Büchner[1], Pascal Reutler[2], and Alexandre Revcolevschi[2] — [1]Leibniz Institute for Solid State and Materials Research, IFW-Dresden, Germany — [2]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, France

The surface of the transition metal oxides $La_{5/3}Sr_{1/3}NiO_4$ and $La_{0.5}Sr_{1.5}MnO_4$ was studied by means of scanning tunneling microscopy (STM). Both materials are model systems for charge ordering phenomena. Despite the insulating nature of these materials we achieved atomic resolution on cleaved surfaces of $La_{5/3}Sr_{1/3}NiO_4$ and $La_{0.5}Sr_{1.5}MnO_4$. Topogrophic images of both compounds reveal periodic modulations, which can be interpreted as signature of short range surface charge ordering. Nevertheless, no direct evidence of charge ordering structures which appear in the volume was found on the surface of our samples. Spectroscopic investigations of the manganite $La_{0,5}Sr_{1,5}MnO_4$ reveal changes in density of states at the fermi level with decreasing temperature, especially an enhacement of the energy gap at the charge ordering temperature.

TT 6.27 Mon 13:00 P1A

Coupled spin S = 1 /2 dimer-systems based on nitronyl-nitroxide biradicals — Cong T. Pham[1], Katarina Removic-Langer[1], •Bernd Wolf[1], Yulia D. Borzdina[2], Evgeny A. Mostovich[2], Martin Baumgarten[2], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, SFB/TR49, 60438 Frankfurt(M) — [2]Max-Planck-Institut für Polymerforschung, SFB/TR49, 55128 Mainz

Due to the collective behaviour of their magnetic excitations, arrays of coupled S = 1/2 spin-dimers in magnetic fields are of general interest in solid state physics as they can be considered as a gas of interacting bosons. Depending on whether the repulsion or the hopping of magnetic excitations dominates, the magnons (triplons) may form superlattices or undergo Bose-Einstein condensation (BEC). The investigation of BEC under various conditions, especially the comparison between field- and pressure-induced condensation, as well as the influence of dimensionality is a subject of current interest. In this contribution we will present a new class of coupled spin-dimer systems based on purely organic building blocks. We will show magnetic susceptibility and magnetization data of various nitronyl-nitroxide biradicals from which we extract the influence of the bridging ligands on the intra-dimer coupling constant J. The target materials show moderate values of their intra-dimer exchange coupling and indications for significant inter-dimer couplings. In addition, due to the huge variety of possible bridging ligands and their chemical modification, the magnetic exchange in nitronyl-nitroxide biradicals can be fine tuned.

TT 6.28 Mon 13:00 P1A

Capacitive dilatometry under Helium-gas pressure — •Christian Balz, Andreas Brühl, Rudra Sekhar Manna, Bernd Wolf, and Michael Lang — Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany

Important interaction parameters of organic conductors can be tuned by applying moderate external pressure. For the κ-$(ET)_2X$ salts, for instance, many interesting regions of the phase diagram can be traversed by applying pressure of only a few hundred bars (e.g., paramagnetic Mott insulator, antiferromagnetic Mott insulator, superconductor or paramagnetic metal), see, e.g., [1]. Furthermore, thermal expansion measurements have been particularly suitable for exploring phase transitions such as the Mott metal-insulator transition [2], so it is highly desirable to combine the two techniques. In a pilot study, we have performed ultra-high resolution thermal expansion measurements at room temperature and under pressures up to 4 bar by combining capacitive dilatometry with the Helium-gas pressure technique. In a first step, we were able to accurately reproduce the expected pressure-induced changes in the dielectric constant of Helium. In addition, we are assembling a cryostat, where the same type of capacitive dilatometer cell that was used in our pilot experiment will be located inside a pressure cell. With this setup, we target at performing ultra-high resolution thermal expansion ($\Delta l/l \geq 10^{-10}$) measurements over wide ranges of temperatures and hydrostatic Helium-gas pressures up to 2.5 kbar.

[1] S. Lefebvre *et al.*, Phys. Rev. Lett. **85**, 5420 (2000)
[2] M. de Souza *et al.*, Phys. Rev. Lett. **99**, 037003 (2007)

TT 6.29 Mon 13:00 P1A

Magnetic-field dependence of the T^*-anomaly in quasi-2D organic superconductors — Jens Brandenburg[1], •Pintu Das[1], Jens Müller[1,2], Michael Lang[2], Franziska Weickert[1,3], Marek Bartkowiak[3] und Jochen Wosnitza[3] — [1]Max–Planck–Institut für Chemische Physik fester Stoffe, Dresden — [2]Johann–Wolfgang–von–Goethe Universität, SFB/TR49, Frankfurt am Main — [3]Hochfeld–Magnetlabor Dresden, Forschunszentrum Dresden–Rossendorf, Dresden

The family of quasi-2D superconductors $\kappa-(BEDT-TTF)_2X$ are model systems for strongly correlated low–dimensional metals. Recently, the unusual normal–conducting state — characterized by a line of anomalies T^* (in the order of 40 K) — has attracted considerable attention: a "pseudo-gap"behavior in analogy to the high-T_c cuprates, a crossover from an incoherent "bad"metal to a coherent Fermi–liquid regime, and a density–wave–type phase transition have been suggested as possible scenarios. To investigate the possibility of a magnetic origin we carried out detailed transport measurements in pulsed magnetic fields up to 60 T. For two different compounds, X = $Cu[N(CN)_2]Br$ and $Cu(NCS)_2$, we observed a maximum in the relative magnetoresistance change right around T^*. This indicates the significance of magnetic degrees of freedom which are coupled to the transport properties. Also, for the first time we were able to determine the magnetic–field dependence of T^* showing a small negative shift with increasing field. We discuss the implications of our experimental data for possible models explaining the anomalous normal–conducting state.

TT 6.30 Mon 13:00 P1A

Multi-frequency ESR studies on $(TMTTF)_2X$: evidence of the anisotropic Zeeman interaction in the charge ordered

state — •S. Yasin[1,2], B. Salameh[2], M. Dumm[2], and M. Dressel[2] — [1]Institut Hochfeld-Magnetlabor Dresden, Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

We studied the charge ordered (CO) state of the quasi 1-D $S = 1/2$ quantum spin chains $(TMTTF)_2X$ (X=SbF_6 and AsF_6) by comprehensive W-Band (95 GHz), Q-band (34 GHz) and X-Band (9.5 GHz) ESR experiments between 4 and 300 K in order to explore the nature of the exchange interaction in the CO state. At high temperatures, both compounds show a linear decrease of the linewidth with decreasing temperature; this behavior does not depend on the applied microwave frequency as well as the anisotropy of both, linewidth and g-value. Below T_{CO}, the breaking of the inversion symmetry of the $(TMTTF)_2$-dimers results in additional contributions ΔH_{CO} to the ESR linewidth. While the linewidth is frequency independent along the three principle magnetic axes a, b', and $c*$, it is substantially enhanced for the Q- and W-band measurements along the diagonal of $a - b'$ plane. The enhanced linewidth along 45^o in the $a - b'$ plane below T_{CO} shows a quadratic frequency dependence which is characteristic for anisotropic Zeeman interaction. From this finding we can conclude that the charge order leads to two inequivalent magnetic sites. We will compare this result to one obtained on anion-ordered TMTTF salts where a different charge-order pattern was proposed.

TT 6.31 Mon 13:00 P1A

Quantum-Phase-Transition within Density Functional Theory using exact Exchange-Correlation Potentials — •Martin Moch[1] and Peter Schmitteckert[1,2] — [1]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76021 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

Density Functional Theory (DFT) is one of the most widely used numerical tools to study properties of interacting Fermi systems. In our work we consider the question whether DFT is able to describe the quantum phase transitions based on the interplay of disorder and interaction. To this end we calculate exact Kohn-Sham potentials for disordered, interacting, half-filled, one-dimensional Fermi systems from the local densities obtained from the Density Matrix Renormalization Group (DMRG) calculations. In the framework of Anderson localization one-dimensional systems are always localized. However, for attractive interaction the real system undergoes a phase transition to a metallic phase at a finite interaction. Here we report on the manifestation of this phase transition in the effective non-interacting DFT description.

TT 6.32 Mon 13:00 P1A

Comparison of dynamics in quantum impurity models with bosonic and fermionic baths — •David Roosen[1], Karyn Le Hur[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main, Germany — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Equivalence relations between quantum impurity models with bosonic and fermionic baths can be derived using the bosonization technique [1]. We focused on the well-known mapping between the anisotropic Kondo and the spin boson model (for a recent review on this model see [2]) and investigated, to which degree this equivalence holds for general local observables, and whether it extends to nonequilibrium dynamics.

The dynamics of the two models are investigated using a time-dependent Numerical Renormalization Group (NRG) algorithm [3] developed recently. A detailed study of the time-dependent entanglement entropy, a measure of increasing importance due to its prominent role in numerous fields of physics ranging from quantum information science to quantum phase transitions in condensed matter systems [4], has been carried out.

[1] S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982).
[2] K. Le Hur, Annals of Physics **323**, 9, 2208, (2008).
[3] F. Anders, and A. Schiller, Phys. Rev. Lett. **95**, 196801 (2005).
[4] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).

TT 6.33 Mon 13:00 P1A

Dynamical correlation functions in the Ising model with a boundary — •Dirk Schuricht and Fabian H. L. Essler — The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

Using scanning tunneling microscopy one can measure the local density of states in the vicinity of impurities. In one-dimensional systems, like stripes in high-temperature superconductors or carbon nanotubes, an impurity is equivalent to a boundary. This motivates the study of correlation functions in models with boundaries. In particular, the low-energy properties of strongly correlated systems are typically described by boundary field theories. We have calculated the dynamical correlation functions in the semi-infinite quantum Ising chain in the presence of a boundary magnetic field [1]. The used form-factor expansion is found to be fastly convergent for $M|R| > 0.1$, where R is the distance from the boundary and $1/M$ the correlation length. At sufficiently late times we observe oscillatory behaviour of the correlations arbitrarily far away from the boundary. We investigate the effects of the boundary bound state that is present for a range of boundary magnetic fields.

[1] D. Schuricht and F. H. L. Essler, J. Stat. Mech.: Theor. Exp. P11004 (2007).

TT 6.34 Mon 13:00 P1A

Quantum Monte Carlo results on phonon softening in the two-dimensional Holstein model — •Prabuddha Chakraborty[1,2], Richard Scalettar[2], and Warren Pickett[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]University of California, Davis, CA 95616, USA

In this poster, we present new observations on the phonon spectral density in the two dimensional Holstein model. The numerical method we use is Determinant quantum Monte Carlo, combined with Maximum Entropy which is used to extract the real frequency spectral density of the phonons. We highlight one of our most surprising observations: the presence of a ubiquitous softening of the phonon at the center of the Brillouin zone, in direct contradiction to established results in this problem. We summarize the behaviour of the softening across a wide range of electron densities, phonon frequencies and electron-phonon interaction strengths.

TT 6.35 Mon 13:00 P1A

Huge thermomagnetic and thermoelectric effects in Luttinger liquids and spin chains — •David Rasch[1], Arti Garg[2], Achim Rosch[1], and Efrat Shimshoni[3] — [1]University of Cologne, Germany — [2]Technion, Haifa, Israel — [3]Bar-Ilan University, Ramat-Gan, Israel

The interplay of Umklapp scattering and weak disorder in Luttinger liquids and spin chains leads to strong effects in the field and doping dependence of transport quantities. We show that the thermal conductivity of spin chains as a function of a magnetic field B displays a pronounced dip for $B \sim T$. In metallic systems, we predict large violations of the Wiedemann Franz law. Depending on the doping, the Wiedemann Franz ratio $\kappa/(\sigma T)$ can become either very large or very small.

TT 6.36 Mon 13:00 P1A

Quantum dots coupled to Luttinger liquid leads - conductance and charging — •Peter Wächter[1], Volker Meden[2], and Kurt Schönhammer[1] — [1]Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen

The theoretical description and experimental realization of quantum dots is a very active field in condensed matter physics. In our work, we model quantum dots as non-degenerate energy levels coupled to Luttinger liquid leads, i.e. we couple the zero-dimensional dot to leads of dimension one in order to study how the Luttinger liquid physics in the leads affects the physics of the dot. In particular we identify universal power law scaling in the charging of a single quantum dot and comment on the conductance through such a system. Furthermore we explore the conductance through parallel quantum dots coupled to Luttinger liquid leads.

TT 6.37 Mon 13:00 P1A

Optical signatures of Kondo effect in quantum dots — Hakan E. Türeci[1], Atac Imamoglu[1], Andreas Weichselbaum[2], •Markus Hanl[2], Theresa Hecht[2], and Jan von Delft[2] — [1]Institute of Quantum Electronics, ETH-Zürich, CH-8093 Zürich, Switzerland — [2]Arnold Sommerfeld Center for Theoretical Physics, LMU München, D-80333 München, Germany

We analyze the optical signatures of many body interactions between an optically excited QD electron and an adjacent fermionic reservoir.

The optical absorption lineshapes are calculated using the numerical renormalization group, following [1]. The resulting optical lineshape is highly nontrivial: at zero magnetic field, it has a power-law singularity of the form $I(\omega) \sim (\omega - \omega_{th})^{-\sigma}$ with exponent σ showing two distinct cross-overs, which can be understood analytically in terms of the fixed points of the RG flow of the symmetric Anderson model. We also analyze the dependence of the optical response on external magnetic field and finite temperature.

[1] R. Helmes et al., Phys. Rev. B, **72**, 125301 (2005)

TT 6.38 Mon 13:00 P1A

Superperturbation solver for quantum impurity models — •Christoph Jung[1], Hartmut Hafermann[1], Sergey Brener[1], Mikhail Katsnelson[2], Alexei Rubtsov[3], and Alexander Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University of Nijmegen, 6525 AJ Nijmegen, The Netherlands — [3]Department of Physics, Moscow State University, 119992 Moscow, Russia

We present a very efficient solver for the general Anderson impurity problem. It is based on the perturbation around a solution obtained from exact diagonalization using a small number of bath sites. We formulate a perturbation theory which is valid for both weak and strong coupling and interpolates between these limits. Good agreement with numerically exact quantum Monte-Carlo results is found for a single bath site over a wide range of parameters. In particular, the Kondo resonance in the intermediate coupling regime is well reproduced for a single bath site and the lowest order correction. The method works directly on the real axis and thus allows to access the density of states without the need of analytical continuation of imaginary time data.

TT 6.39 Mon 13:00 P1A

Comparison between NRG and DMRG as impurity solver — •Robert Peters, Piet Dargel, and Thomas Pruschke — Friedrich Hund Platz 1, 37077 Goettingen

Impurity models like the Anderson model play an important part in strong correlation physics. They model the situation of localized, partially filled f- or d-shells in metals and artificially produced quantum dots or Qubits. Also strongly correlated lattice models, like e.g. the Hubbard model, can be mapped via dynamical mean field theory on a self-consistency calculation of an impurity model. In recent years the Density Matrix Renormalization Group (DMRG) was introduced as novel method to solve such impurity problems. We here compare results for static and dynamic properties of quantum impurities obtained with DMRG to those from the well-established Numerical Renormalization Group (NRG). Special emphasis will be put on the possible application of DMRG to systems with multiple orbitals or multiple impurities.

TT 6.40 Mon 13:00 P1A

Kondo model in and out of equilibrium: Functional RG at strong coupling — •Holger Schmidt and Peter Wölfle — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We apply the functional renormalization group (RG) method to calculate the conductance of a quantum dot in the Kondo regime in and out of equilibrium. The local spin 1/2 operator is described in pseudofermion representation. The set of of coupled RG equations for the pseudofermion self-energy and vertex functions in Keldysh space is derived and analyzed. Neglecting three-particle and higher vertex functions the equations are solved. It is found that the imaginary part of the self energy limits the growth of the two-particle vertex function at low temperatures and voltages $T, V \ll T_K$ (Kondo temperature), providing a semiquantitative description down into the strong coupling regime. In the regime $\max(T, V) \gg T_K$ we recover the results of [1].

[1] A. Rosch *et al.*, Phys. Rev. Lett. **90**, 076804 (2003).
[2] J. Paaske *et al.*, Phys. Rev. B, **70**, 1553041 (2004).

TT 6.41 Mon 13:00 P1A

Correlation effects in the two-site Anderson model (TIAM) — •Torben Jabben — TU-Darmstadt, Darmstadt, Hessen

Within the framework of the enhanced non-crossing approximation (ENCA), an approximative solution of the TIAM is obtained, which is applicable to any finite value of the Coulomb repulsion U.

One-particle spectra and thermodynamic properties are presented and discussed. Especially the competition between two independent Kondo effects at each impurity and the non-local singlet or triplet formation between both impurities is discussed.

TT 6.42 Mon 13:00 P1A

Variational local moment approach to Kondo effect in the multi-orbital Anderson impurity model — •Anna Kauch[1] and Krzysztof Byczuk[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Theoretical Physics, Faculty of Physics, Warsaw University, Hoza 69, PL-00-681 Warszawa, Poland

The recently developed [1,2] variational local moment approach (VLMA) to the single impurity Anderson model is presented. We focus on the application of the method to the multi-orbital impurity model in various regions of parameters where different types of Kondo effects can occur. The application of VLMA to the multi-orbital Hubbard model as an impurity solver of the dynamical mean-field theory equations is also addressed.

The method is based on assuming the existence of local moments – following the single orbital local moment approach of D. Logan [3]. The values of the local moments are obtained within VLMA by minimizing the ground state energy of the system.

[1] A. Kauch and K. Byczuk, Physica B 378-380, 297 (2006).
[2] A. Kauch and K. Byczuk, Quantum Magnetism, Proceedings of the NATO Advanced Study Institute on Quantum Magnetism, Les Houches, France, pp. 85-95 (Springer, 2008).
[3] D. Logan and M.T. Glossop, J. Phys. Condens. Matter 12, 985 (2000).

TT 6.43 Mon 13:00 P1A

Kondo screening cloud in the Anderson impurity model — •Andreas Holzner[1,2], Fabian Heidrich-Meisner[1], Ian McCulloch[3], Ulrich Schollwöck[1], and Jan von Delft[2] — [1]Institut für Theoretische Physik C, RWTH Aachen University, D-52056 Aachen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [3]School of Physical Sciences, University of Queensland, QLD 4072, Australia

A magnetic moment in a metal or in a quantum dot is, at low temperatures, screened by the conduction electrons by the mechanism of the Kondo effect. This gives rise to spin-spin correlations between the magnetic moment and the conduction electrons, which can have a substantial spatial extension. We study this phenomenon, the so-called Kondo cloud, by means of the density matrix renormalization group method for the case of the single-impurity Anderson model. Our goal is to elucidate whether the Kondo screening length, typically assumed to be proportional to the inverse Kondo temperature, can be extracted from the spin correlations. For several mechanisms that destroy the Kondo effect, we investigate the induced behavior of the screening cloud.

TT 6.44 Mon 13:00 P1A

The chaotic Kondo box: mean-field approach — •Sebastien Burdin[1], Rainer Bedrich[2], and Martina Hentschel[2] — [1]Institute of Theoretical Physics, Cologne University — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

We study the low temperature physical properties of a mesoscopic bath of electrons (E.g., a big quantum dot), coupled to a local Kondo impurity (E.g., a small quantum dot, or a magnetic ion). Here, a crucial difference with the Kondo effect occuring in a bulk material results from a finite mean level spacing. This low energy scale can generate deviations from the universal behavior which would be expected for a bulk system. Using a mean-field approximation for the Kondo interaction, we consider as a first step a "clean system", where the non-interacting energy levels are characterized by a constant distribution. Then, a more realistic situation is considered, for which the energy levels are distributed randomly. This is realized within the random matrix theory. In both cases, we study the local magnetic susceptibility, the conductance, and the local density of electronic states as a function of the temperature, the mean level spacing, the Kondo coupling, and the number of electrons on the dot.

TT 6.45 Mon 13:00 P1A

Periodic time dependent Kondo model — Markus Heyl and •Stefan Kehrein — Arnold-Sommerfeld-Center for Theoretical Physics, Ludwigs-Maximilians-Universität München

In this work we study a nonequilibrium steady state in the Kondo model generated by periodic switching of the interaction. As has been shown in Ref. [1], at the Toulouse point the Kondo model can be mapped onto a noninteracting resonant level model even for nonequilibrium interaction quenches. Since the resonant level model is exactly solvable, we are therefore able to investigate the real-time dynamics on all time scales, especially the buildup of the steady state. We characterize this steady state by calculating the spin-spin correlation function.

[1] D. Lobaskin and S. Kehrein, J. Stat. Phys. **123**, 301-313 (2006).

TT 6.46 Mon 13:00 P1A

Continuous-Time Quantum Monte Carlo Approach to Strongly Correlated Nonlinear Transport — •Andreas Dirks[1], Thomas Pruschke[1], and Philipp Werner[2] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Institut für Theoretische Physik, ETH Zürich

The tremendous progress in nano structuring made a broad variety of physical phenomena of quantum impurity systems experimentally accessible through transport measurements. However, computational methods for a reliable description of strongly correlated transport are still rare. We investigate the application of continuous-time Quantum Monte Carlo algorithms to the imaginary-time formalism introduced by Han and Heary [1].

[1] J. E. Han, and R. J. Heary, Phys. Rev. Lett. **99**, 236808 (2007)

TT 6.47 Mon 13:00 P1A

Uniaxial pressure effects on the superconductivity of $CeCoIn_5$ — •Kai Grube[1], Sebastian Zaum[1,2], Roland Schäfer[1], Eric D. Bauer[3], Christoph Meingast[1], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The heavy-fermion superconductor $CeCoIn_5$ shows strongly anisotropy thermodynamic and transport properties due to its tetragonal crystal structure. A comparison with its cubic parent compound $CeIn_3$, with an order of magnitude smaller transition temperature T_c, suggests the importance of anisotropy for the superconducting pairing mechanism in these alloys. We have performed thermal expansion and magnetostriction measurements along the a- and c-axes of $CeCoIn_5$ single crystals. From measurements transverse and longitudinal to magnetic fields up to $B = 14\,\mathrm{T}$, it has been possible to calculate the uniaxial pressure effects on the superconductivity, dT_c/dp_i ($i = a$, c) and dB_{c2}/dp_i, and the Grüneisen parameters, $\Gamma_a(T, B)$ and $\Gamma_c(T, B)$. We will discuss the stress and strain dependences of the characteristic energy scales and relate them to the effects of hydrostatic pressure, magnetic field, and doping.

TT 6.48 Mon 13:00 P1A

Coexistence of antiferromagnetism and superconductivity in Cd-doped $CeCoIn_5$ — •O. Stockert[1], U. Witte[2,3], M. Nicklas[1], R. Schedler[3], K. Kiefer[3], J. D. Thompson[4], A. D. Bianchi[5], Z. Fisk[5], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Los Alamos National Laboratory, Los Alamos NM, USA — [5]University of California, Irvine CA, USA

Starting from the heavy-fermion superconductor $CeCoIn_5$ with a superconducting $T_c = 2.3\,\mathrm{K}$, doping with cadmium induces antiferromagnetic order in $CeCo(In_{1-x}Cd_x)_5$ above a critical Cd concentration $x_c \approx 0.005$ with a subtle interplay between magnetism and antiferromagnetism. We report on elastic neutron scattering experiments of the heavy-fermion alloy $CeCo(In_{1-x}Cd_x)_5$ with $x = 0.0075$ to study the magnetic structure and the influence of superconductivity on the antiferromagnetism. Below $T_N = 2.4\,\mathrm{K}$ and down to lowest temperatures $T < 100\,\mathrm{mK}$ commensurate antiferromagnetic order with a propagation vector $\tau = (1/2\ 1/2\ 1/2)$ was detected. The transition into the superconducting state at $T_c = 1.7\,\mathrm{K}$ is accompanied by a kink in the magnetic intensity followed by a saturation towards lower temperatures at a reduced value. These results indicate a coexistence of antiferromagnetism and superconductivity, but reveal at the same time a strong influence of the superconducting state on the magnetic order. Our results will be discussed in comparison to other heavy-fermion superconductors.

TT 6.49 Mon 13:00 P1A

Scanning Tunneling Spectroscopy studies on heavy fermion superconductors — •Stefan Ernst[1], Steffen Wirth[1], Hirale Jeevan[1], Christoph Geibel[1], Frank Steglich[1], and Zachary Fisk[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Department of Physics and Astronomy, UC Irvine, USA

Scanning Tunneling Spectroscopy (STS) is a powerful tool for mapping the local electronic density of states (DOS) of sample surfaces. Of particular interest are experiments with superconducting (SC) materials, as information about the SC energy gap can directly be obtained. The application of STS to heavy fermion (HF) superconductors might be a valuable contribution to the understanding of this class of materials. Fundamental properties such as the symmetry of the SC order parameter or excitations due to the SC pairing interaction might be revealed.

This work reports on STM measurements carried out at low temperatures and under ultra-high vacuum (UHV) conditions with the possibility of applying a magnetic field. For the materials investigated here, spectroscopic features in the order of a few hundred μeV are expected. The sufficiently high resolution of our STM, in particular with respect to energy, has been verified. Due to the short SC coherence length of HF materials, a clean tunnel junction is required to investigate the SC gap by means of STS. Methods were developed to prepare clean surfaces of single crystals *in situ*. Preliminary STM and STS measurements were conducted on single crystalline samples of the HF superconductors $CeCoIn_5$, $CeIrIn_5$, and $CeCu_2Si_2$.

TT 6.50 Mon 13:00 P1A

Magnetic field dependency of the spin wave excitation gap in UPt_2Si_2 — •Dirk Schulze Grachtrup[1], Matthias Bleckmann[1], Stefan Süllow[1], and John A. Mydosh[2] — [1]TU Braunschweig, Institute for Physics of Condensed Matter, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [2]University Cologne, II. Physikalisches Institut, Zülpicher Str. 77, 50937 Cologne, Germany

Tetragonal UPt_2Si_2 has recently been characterized as moderately mass enhanced antiferromagnetic compound, which in various physical properties reveals a resemblance to the hidden order material URu_2Si_2 [1,2].

To further characterize this resemblance we have examined UPt_2Si_2 with resistivity measurements in magnetic fields. In particular, we find the antiferromagnetic phase transition at T_N=32 K in zero field to shift slightly downwards to 31 K at B = 9 T // c-axis. Further, the temperature dependence of the resistivity in the range up to 20K can be described by an opening of a spin wave excitation gap. In contrast to T_N this gap displays a much larger reduction by about 30% with increasing magnetic field up to 9T. We discuss the relationship between spin excitation gap and magnetic ordering, this in particular with respect to the difference in field response.

[1] S. Süllow, A. Otop, A. Loose, J. Klenke, O. Prokhnenko, R. Feyerherm, R.W.A. Hendrikx, J.A. Mydosh, H. Amitsuka, J. Phys. Soc. Jpn. **77** (2008) 024708
[2] N. Johannsen, S. Süllow, A.V. Sologubenko, T. Lorenz, J.A. Mydosh, Phys. Rev. B **78** (2008) 121103

TT 6.51 Mon 13:00 P1A

Interplay between crystal-field splitting and Kondo-effect in $CeNi_9Ge_{4-x}Si_x$. — Christian Gold[1], Ludwig Peyker[1], •Ernst-Wilhelm Scheidt[1], Wolfgang Scherer[1], and Herwig Michor[2] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria

$CeNi_9Ge_4$ exhibits a Kondo lattice behavior with unusual single-ion non-Fermi-lquid features and with the largest ever recorded value of the electronic specific heat $\Delta C/T \approx 5.5\,\mathrm{J/mol\,K^2}$ without showing any trace of magnetic order. An entropy calculation yielding $S = Rln4$ at $T < 20\,\mathrm{K}$ suggests that in $CeNi_9Ge_4$ a crystal electrical field (CEF) ground state quasi quartet of Ce^{3+} splits into two doublets leading to an interplay between Kondo effect and CEF splitting on the same energy scale. $CeNi_9Si_4$ is a Kondo lattice system with an enhanced Sommerfeld coefficient of $\gamma \approx 155\,\mathrm{mJ/mol\,K^2}$ which can be well described by the degenerate Coqblin-Schrieffer model ($J = 5/2$). Here we report on specific heat, susceptibility and resistivity measurements of the substitution series $CeNi_9Ge_{4-x}Si_x$ which *i*) exhibits a continuous crossover from a four-folder CEF ground state to a two folder one in present of Kondo screening for $x = 0.5$ - 4 and which *ii*) follows a reduction of the Kondo temperature T_K with decreasing lattice volume between $x = 0$ and 0.1, which is in contrast to the compressible Kondo lattice model.

TT 6.52 Mon 13:00 P1A

Polarization dependent XAS on $CeMIn_5$ (M=Co, Rh and Ir) and $CePt_3Si$ determines crystal-field ground state and sequence of states. — •T. Willers[1], A. Severing[1], Z. Hu[1], N. Hollmann[1], P.O. Körner[1], H.-J. Lin[2], C.T. Chen[2], D. Schmitz[3], E.D. Bauer[4], B. Fak[5], G. Lapertot[5], and L.H. Tjeng[1] — [1]Institute of Physics II, University of Cologne — [2]NSRRC, Taiwan — [3]BESSY, Berlin — [4]Los Alamos Nat. Lab., Los Alamos, NM, USA — [5]CEA, SPSMS, Grenoble, France

The tetragonal compounds $CeMIn_5$ (P4/mmm) are of interest since the interplay between the antiferromagnetic behaviour of the Ce local moments, an unconventional normal state, and superconducting behaviour of the heavy electrons can be studied [1 and references therein]. The non-centro symmetric system $CePt_3Si$ is also tetragonal (P4/mm), becomes antiferromagnetic at 1K and superconducting below 0.7K [2]. In all these compounds the knowledge of the crystal-field potential is crucial for the description of the low temperature properties. Here linear polarized soft X ray absorption data at the Ce-M_{45} edges of $CeMIn_5$ with M=Co, Rh and Ir and $CePt_3Si$ will be presented with the view to elucidate the crystal field schemes of these compounds. Not only the ground state symmetry, but also the sequence of states could be obtained from the temperature dependence of the XAS data. Furthermore the influence of the Kondo effect on the Ce-M_{45} edges of these compounds will be discussed.

[1] J.L. Sarrao and J.D. Thompson, J. Phys. Soc. Japan **76,** 051013 (2007). [2] E. Bauer et al., Physica B **359,** 360 (2005).

TT 6.53 Mon 13:00 P1A

Ge based filled skutterudites MPt_4Ge_{12}: a ^{195}Pt NMR study. — •M. Baenitz, R. Sarkar, R. Gumenik, A. Leithe-Jasper, W. Schnelle, H. Rosner, U. Burkhardt, M. Schmidt, U. Schwarz, Yu. Grin, and F. Steglich — Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Filled skutterudites MT_4X_{12}(M: alkaline or rare earth metals, T: Fe, Ru, Os, X: P, As, Sb) show a wide variety of strongly correlated electron physics from heavy fermions to Kondo insulators to unconventional superconductors. The new type of skutterudites, the Ge based system MPt_4Ge_{12} form with M = Ba, Sr, La, Ce, Pr, Sm, Eu[1,2]. They exhibit metallic behaviour and show, with the exception of the systems with Ce, Sm and Eu, superconductivity at low temperature (T_c < 10 K)[1,2]. Here we present a temperature dependent ^{195}Pt NMR study on the whole series of MPt_4Ge_{12} compounds with special attention on the magnetic systems with Ce, Sm and Eu. Here shift ^{195}K(T) and spin lattice relaxation rate are discussed in the context of a dense Kondo system with a mixed valence state of Ce as well as for Sm. Especially the pronounced maximum observed in ^{195}K(T) provides very strong evidence for a mixed valence behavior for this new class of material.

[1] Phys. Rev. Lett. 100, 017002 (2008).
[2] Phys. Rev. Lett. 99, 217001 (2007).

TT 6.54 Mon 13:00 P1A

Possible crystal electrical field shift in the system $CeNi_{9-x}Cu_xGe_4$. — •Ernst-Wilhelm Scheidt[1], Ludwig Peyker[1], Christian Gold[1], Wolfgang Scherer[1], Ernst Bauer[2], Herwig Michor[2], Tobias Unruh[3], and Peter Link[3] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040 Wien, Austria — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz, Technische Universität München, 85747 Garching, Germany

Crystal structure, specific heat, magnetic susceptibility, electrical resistivity and inelastic neutron studies on the heavy fermion system $CeNi_{9-x}Cu_xGe_4$ ($0 \le x \le 1$) reveal a continuous tuning of the ground state by Ni/Cu substitution from an effectively fourfold degenerate non-magnetic Kondo ground state of $CeNi_9Ge_4$ with pronounced non-Fermi-liquid (nFL) features towards a magnetically ordered, effectively twofold degenerate ground state in $CeNi_8CuGe_4$ with T_N = 0.18 K. NFL behavior, $C/T \propto \chi \propto -\ln T$ and $\rho \propto T$, is observed for $x \cong 0.4$. Hitherto, this is the first example where a substitution driven quantum phase transition is connected not only with changes of the relative strength of Kondo effect and RKKY interaction, but also with a reduction of the effective crystal field ground state degeneracy.

TT 6.55 Mon 13:00 P1A

Low-temperature specific heat of the heavy-fermion superconductor $CeCu_2Si_2$ — •Julia Arndt[1], Oliver Stockert[1], Robert Borth[1], Thomas Lühmann[1], Hirale Jeevan[1,2], Christoph Geibel[1], Michael Loewenhaupt[3], and Frank Steglich[1] — [1]Max-Planck-Institut f. Chem. Physik fester Stoffe, Dresden — [2]I. Physikal. Inst., U Göttingen — [3]Inst. f. Festkörperphysik, TU Dresden

$CeCu_2Si_2$, the first heavy-fermion superconductor to be discovered, exhibits a complex interplay of antiferromagnetism and superconductivity (SC). In very subtle dependence on the exact stoichiometry its ground state is either antiferromagnetically ordered (A-type), superconducting (S-type), or both (A/S-type). Recent neutron scattering experiments on S-type $CeCu_2Si_2$ ($T_c \approx 600$ mK) [1] and their theoretical interpretation [2] give indications of magnetically mediated SC with an order parameter of $d_{x^2-y^2}$ symmetry. Different order parameter symmetries cause characteristic temperature dependences of the specific heat well below T_c. We performed measurements of the specific heat at temperatures from 50 mK to 4 K and magnetic fields up to 8 T on large single crystals of A-, S- and A/S-type $CeCu_2Si_2$ as well as on 2% and 10% Ge doped $CeCu_2Si_2$ using an adapted quasi-adiabatic heat-pulse method with background heating. The results are compared with each other, with special focus given to the analysis of the low-temperature specific heat of S-type $CeCu_2Si_2$ in order to be able to draw conclusions as to the nature of SC in the system.

[1] O. Stockert *et al.*, Physica B **403**, 973 (2008)
[2] I. Eremin *et al.*, Phys. Rev. Lett. **101**, 187001 (2008)

TT 6.56 Mon 13:00 P1A

Boron-induced change of valence state of Eu and structural phase transition in $EuPd_3B_x$ ($0 \le x \le 0.55$) — •Roman Gumeniuk, Claire Loison, Walter Schnelle, Wilder Carrillo-Cabrera, Paul Simon, Ulrich Burkhardt, Marcus Schmidt, Miriam Schmitt, Ulrich Schwarz, Helge Rosner, and Andreas Leithe-Jasper — MPI für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

A detailed experimental and theoretical study of the solubility of B in $EuPd_3$ ($AuCu_3$ structure type) and its influence on the physical properties is presented. Theoretical calculations (LDA + U + CPA method) predict in $EuPd_3B_x$ a change of non-magnetic $4f^6$ Eu to magnetic $4f^7$ Eu for a $x > 0.2$ together with an anomaly in the unit cell volume. At 950 °C the incorporation of B in $EuPd_3B_x$ is possible up to $x = 0.55$, as can be concluded from the lattice parameters, WDXS and chemical analyses. Transmission electron microscopy investigations show the existence of a superstructure for $Eu_2Pd_6B_y$ in the region of $0.7 \le y \le 1$ (Ti_2Rh_6B structure type [1], space group $Fm\bar{3}m$, a = 8.3096(2)-8.3730(2) Å). From Eu L_{III} XAS studies as well as from magnetic susceptibility data it can be deduced that the Eu species in $EuPd_3$ and in $EuPd_3B_x$ ($0 \le x \le 0.2$) exhibit a $4f^6$ state, while for $EuPd_3B_x$ ($0.2 \le x \le 0.35$) and $Eu_2Pd_6B_y$ ($0.7 \le y \le 1$) they are in an intermediate valence state. Our findings are discussed with respect to previously published studies [2,3].

[1] B. Fowka *et al.* Z. Krist. 221 (2006) 445.
[2] B. Darshan *et al.* Phys. Rev. B, 30 (1984) 4031.
[3] S.K. Dhar *et al.* Phys. Rev. B, 29 (1984) 5953.

TT 6.57 Mon 13:00 P1A

^{11}B NMR study of the low dimensional Kondo lattice $YbNiB_4$ — •Rajib Sarkar[1], Michael Baenitz[1], Arpana Prasad[2], Zakir Hossain[2], Frank Steglich[1], and Cristoph Geibel[1] — [1]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology, Kanpur 208016, India

$YbNiB_4$ deserves special attention because of its interesting physical properties. Recently we reported $YbNiB_4$ being a Kondo system with a strong 2D character, which makes this compound unique among the Yb-based systems. Two antiferromagnetic transitions show up at 5.4 K and 4.0 K [1]. Furthermore the structural homologue $YbAlB_4$ is proposed to be a heavy Fermion system showing superconductivity at T_c=80 mK and quantum criticality without external tuning [2]. Here we present for the first time ^{11}B NMR results on $YbNiB_4$ as a function of temperature (2-295 K) and field. ^{11}B NMR spectra are typical powder pattern with pronounce first order quadrupolar splitting. By lowering the temperature spectra is shifted and broadened. The observed small negative shift indicates the relevance of conduction electron polarization by the Yb $4f^{13}$ moments. Further analysis of shift as well as the spin-lattice relaxation is in progress.

[1] A. Prasad et. al., to be published,
[2] Nature Physics 4, 603(2008).

TT 6.58 Mon 13:00 P1A

Strong electron correlations in $FeSb_2$: An optical investi-

gation and comparison with $RuSb_2$ — •Alexander Herzog[1], Michael Marutzky[1], Jörg Sichelschmidt[1], Anders Bentien[1], Frank Steglich[1], Shin-Ichi Kimura[2], Simon Johnsen[3], and Bo Iversen[3] — [1]MPI Chemical Physics of Solids, 01187 Dresden, Germany — [2]UVSOR, Institute for Molecular Science, Okazaki 444-8585, Japan — [3]Dep. of Chemistry, University of Aarhus, 8000 Aarhus, Denmark

We investigated the far-infrared optical conductivity of $FeSb_2$, being a possible d electron Kondo semiconductor, and its non magnetic homologue $RuSb_2$. For $FeSb_2$ we found an indirect gap of 30 meV and semiconducting behavior for all crystal axes. Another gap feature at 6 meV, appearing below $T = 100$ K, possibly corresponds to the colossal Seebeck coefficient [1] and may therefore be related to strong electronic correlations. However, we found a clear decrease of the reflectivity around 6 meV upon applying a magnetic field which demonstrates contradictory behavior to a common Kondo semiconductor scenario. We propose multiple absorptions due to disordered Fe atoms to be the origin of this gap feature. Furthermore, we discuss a possible relation of an anomalous change in the phonon spectrum of $RuSb_2$ below 100 K to the opening of a 6 meV gap in the isostructural $FeSb_2$. Nevertheless, strong electronic correlations are indicated by a temperature dependent spectral weight redistribution up to energies as large as 1 eV.

[1] A. Bentien et al., Europhys. Lett. **80**, 39901 (2007).

TT 6.59 Mon 13:00 P1A

^{121,123}Sb magnetic resonance as a local probe for gap formation in $FeSb_2$ — •Michael Baenitz[1], Andrei Gippius[2], Simon Johnsen[3], Bo Iversen[3], and Frank Steglich[3] — [1]Max-Planck Institut for Chemical Physics of Solids, Dresden, Germany — [2]Faculty of Physics, Moscow State University, Moscow, Russia — [3]Department of Chemistry, University of Aarhus, Denmark

There is a revived interest on $FeSb_2$ after classifying this system as the second Fe containing Kondo insulator after FeSi. The formation of a spin and charge gap out of an enhanced density of states $N(E_F)$ is one of the key features of these materials. Furthermore $FeSb_2$ surprisingly shows a colossal Seebeck coefficient around 10 K. Here we report on a comparative study on $FeSb_2$ and its structural homologue $RuSb_2$. For both compounds we found two regimes in the temperature dependence of $^{123}(1/T_1)$. Above 40 K (HT) a conventional activated behavior (with D/k_B @ 450 K for $FeSb_2$) dominates in $1/T_1$. Below 40 K (LT) in both systems an unconventional $1/T_1$ behavior with a smooth maximum at 10 K is observed. To analyze this behavior we propose the presence of T-dependent in-gap states forming a narrow band of localized spins with $S = 1/2$ near the bottom of the conduction band. This model enables us to fit the $^{123}(1/T_1)$ data in the entire temperature range (LT + HT) for $FeSb_2$. Furthermore the relevance of these in-gap states for the colossal Seebeck effect is discussed.

TT 6.60 Mon 13:00 P1A

Quantum phase transition of the sub-Ohmic spin-boson model — •André Winter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

Quantum dissipation plays a highly interesting role in several fields of physics, like the decoherence of qubits or charge transfer in donor-acceptor systems. Therefore, we study these quantum-dissipative effects via the spin-boson model, which describes a two-level system coupled to a bosonic bath with a spectral density $J(\omega) \propto \omega^\sigma$. We use an advanced Monte Carlo cluster algorithm to explore the quantum phase transition between localized and delocalized phase of this model in the sub-Ohmic regime ($0 < \sigma < 1$). The applied method, which based on the path integral approach to Quantum Monte-Carlo computations, works without discretization and uses cluster updates of continuous worldline-segments to investigate the quantum critical point effectively. We compute the critical exponents of the phase transition and their dependence on the bath exponent characterizing the low frequency behaviour of the spectral function of the bosonic bath.

TT 6.61 Mon 13:00 P1A

Longitudinal magnon decay near a quantum critical point — •Lucas Hollender and Matthias Vojta — Institut für theoretische Physik, Universiät zu Köln, Köln, Deutschland

A spin dimer system shows a zero-field magnetic order-disorder transition at a critical ratio of the inter-dimer to intra-dimer couplings. We investigate the decay process of the longitudinal magnon in the antiferromagnetic phase, which has been observed in neutron scattering experiments, as function of the distance to the quantum phase transition. We employ a perturbative analysis within a modified bond operator formalism to compute the lifetime of the longitudinal mode and compare the results to recent neutron scattering measurements on $TlCuCl_3$.

TT 6.62 Mon 13:00 P1A

A 'hidden disorder' scenario for the low-temperature phase transitions in heavy-fermion compounds — •Tanja Rindler-Daller and Matthias Vojta — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

In the study of the low-temperature phase transitions in heavy-fermion compounds, one encounters a complex variety of ordering phenomena. In particular, the nature of the so-called 'hidden order' transition in URu_2Si_2, which is characterized by severe thermodynamical signatures, is not yet fully understood. We adopt an effective theory with 2 competing fields in order to explore the idea of 'hidden disorder'. By performing a scaling analysis and studying a simple model, we can show that the proposed scenario is able to account for the observed anomalies in the specific heat, and serves thus as a rationale for a more detailed microscopic analysis, which is under way.

TT 6.63 Mon 13:00 P1A

Quantum Criticality of the Pomeranchuk Instability: Interplay of Multiple Dynamical Exponents — •Mario Zacharias[1], Markus Garst[1], Achim Rosch[1], and Peter Wölfle[2] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe

We consider the Pomeranchuk instability of an isotropic Fermi liquid in two dimensions, $d = 2$. The effective Ginzburg-Landau theory contains two critical modes with different dynamics. There is a ballistic mode with dynamical exponent $z = 2$ and a Landau-damped mode with $z = 3$. While the $z = 3$ mode dominates thermodynamics at $T > 0$ the $T = 0$ quantum dynamics is governed by the $z = 2$ mode. As the $T = 0$ theory is at its upper critical dimension we use the renormalization group (RG) to analyse the leading logarithmic singularities. The resulting universality class is found to be distinct from the Ising- as well as from the XY-model.

At finite temperatures, there is an intricate interplay between the two modes. At criticality, the length scales $\xi_T \sim T^{-1/z}$ separates the quantum from the classical regime. The different dynamical exponents yield an overlap regime where the ballistic mode still has its quantum character while the damped mode is already classical. We find that this regime dominates the properties at finite T. In particular, we argue that the usual separation of quantum and classical dynamics at $T > 0$ is not valid, implying a breakdown of "dimensional reduction". Further, this interplay leads to a universal T dependence of the correlation length at criticality.

TT 6.64 Mon 13:00 P1A

Emergent Lorentz symmetry with vanishing velocity in a critical two-subband quantum wire — •Matthias Sitte[1], Achim Rosch[1], Julia S. Meyer[2], Konstantin A. Matveev[3], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We consider a quantum wire with two subbands of spin-polarized electrons in the presence of strong interactions. We focus on the quantum phase transition when the second subbands starts to get filled. Performing a one-loop renormalization group (RG) analysis of the effective Hamiltonian, we identify the critical theory as a conformal field theory (CFT) of three Majorana fields having an enhanced SU(2) symmetry and central charge $c = 3/2$. While the fixed point is Lorentz invariant, the effective velocities vanish at low energies due to marginally irrelevant operators leading to, e.g., a diverging critical specific heat coefficient. This behavior should occur quite generally in systems where marginally irrelevant terms in the Hamiltonian break Lorentz invariance.

[1] M. Sitte, A. Rosch, J. S. Meyer, K. A. Matveev, and M. Garst, (arXiv:cond-mat/0811.4579).

TT 6.65 Mon 13:00 P1A

Thermal Expansion and Heat Transport of low-dimensional Magnetic Systems close to Quantum Criticality — •Jens Rohrkamp[1], Thomas Lorenz[1], Alexandr Sologubenko[1], Oliver Heyer[1], Markus Garst[2], Fabrizio Anfuso[2], Achim Rosch[2], Karl

Krämer[3], and Mark Turnbull[4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Department of Chemistry and Biochemistry, University of Bern — [4]Carlson School of Chemistry and Department of Physics, Clark University

Compounds with magnetic subsystems representing simple model spin systems with weak magnetic coupling constants are ideal candidates to test theoretical predictions for the generic behavior close to quantum phase transitions. We present measurements of the thermal expansion, magnetostriction and thermal conductivity of the spin-$\frac{1}{2}$-ladder system piperidinium copper bromide $(C_5H_{12}N)_2CuBr_4$ and the spin-$\frac{1}{2}$-chain compound copper pyrazine dinitrate $Cu(C_4H_4N_2)(NO_3)_2$. Both compounds show quantum phase transitions as a function of magnetic field with pressure dependent critical fields. The low-temperature thermal expansion approaches $1/\sqrt{T}$ divergences at the critical fields and shows a complex behavior with various sign changes inbetween.

TT 6.66 Mon 13:00 P1A

Quantum evolution from spin-gap to antiferromagnetic state in the frustrated J_1-J_2 system $(CuCl_{1-x}Br_x)La(Nb_{1-y}Ta_y)_2O_7$ — •Vladimir Gnezdilov[1,2], Peter Lemmens[2], Kwang-Yong Choi[3], and Hiroshi Kageyama[4] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU Braunschweig, Germany — [3]Chung-Ang Univ., Seoul, Korea — [4]IC Kyoto, Japan

The $(CuCl_{1-x}Br_x)La(Nb_{1-y}Ta_y)_2O_7$ frustrated system shows a quantum evolution from a spin-gap to an antiferromagnetic state [1] depending on composition x and y. Pronounced effects are observed in Raman spectra in dependence of x and y. Taking into account all previous experimental observations and models, our Raman data are used to identify a realistic coordinate environment of Cu^{2+} ions in the CuCl layers. Work supported by DFG and ESF-HFM.

[1]. Y. J. Uemyra et al., arXiv:0806.2021v1.

TT 6.67 Mon 13:00 P1A

Low frequency spin dynamics in the S=1/2 Heisenberg chain compound $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) measured by ^{13}C- and ^{14}N-NMR spectroscopy — •M. Günther[1], H. Kühne[1,2], H.-H. Klauss[1], M. Falkner[2], J. Litterst[2], S. Grossjohann[3], W. Brenig[3], A.P. Reyes[4], P.L. Kuhns[4], C.P. Landee[5], and M.M. Turnbull[5] — [1]IFP, TU Dresden — [2]IPKM, TU Braunschweig — [3]ITHP, TU Braunschweig — [4]NHMFL, FSU, USA — [5]DPC, Clark University, USA

The local magnetization and low frequency magnetic dynamics of the antiferromagnetic S=1/2 Heisenberg chain compound CuPzN have been explored both theoretically and experimentally by means of ^{13}C-NMR spectroscopy for the full B vs. T phase diagram with a critical field of B=14.9T [1]. With an in general very satisfying agreement between experiment and theory, we found a divergence of the low frequency spin dynamics in the critical field regime and a spin gap opening linear with field in the saturated phase. On our poster, we also present NMR studies of the ^{14}N-site in the nitrate groups. Since the ^{14}N-nucleus has a finite quadrupole moment, fluctuations of the electrical field gradient(EFG) tensor become visible in the experiment. By analysis of the angular dependence of the NMR properties it is possible to distinguish between the magnetic and EFG fluctuations for the data presented at temperatures between 2K and 55K and fields B<7T.

[1] H. Kuehne et al., arXiv:0804.2170.

TT 6.68 Mon 13:00 P1A

Quantum criticality in the quasi one-dimensional Ising spin-1/2 chain system $BaCo_2V_2O_8$ — •Sandra Niesen, Martin Valldor, Oliver Heyer, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

$BaCo_2V_2O_8$ contains screw chains of CoO_6 octahedra which are running along the c axis of the tetragonal crystal structure and are separated by nonmagnetic Ba^{2+} und V^{5+} ions in the aa plane. Due to a compression of the octahedra along c the threefold degeneracy of the t_{2g} orbitals is lifted and the magnetic ground state can be described by an effective Ising spin-1/2 antiferromagnetic chain. In zero magnetic field $BaCo_2V_2O_8$ shows long-range antiferromagnetic order below $T_N \simeq 5.5$ K with the spins oriented along c. The magnetic field influence is highly anisotropic. For magnetic fields applied in the aa plane T_N is only weakly suppressed, e.g. $T_N \simeq 4.5$ K for $H = 8$ T. In case of H parallel c, however, the Néel order is completely suppressed already for fields above about 4 T. Thus, $BaCo_2V_2O_8$ is ideally suited to study this field-induced quantum phase transition. We have prepared single crystals of $BaCo_2V_2O_8$ by a spontaneous nucleation method and have performed measurements of the magnetization, the specific heat, the thermal expansion, and the magnetostriction. These results will be compared to existing theory.
This work is supported by the DFG through SFB 608.

TT 6.69 Mon 13:00 P1A

Anisotropic length changes in $Sr_3Ru_2O_7$ — •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 $\mu_0 H_c \approx 8$ 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 a symmetry-broken electronic nematic fluid organized into domains.[2]

Because of the strong magnetoelastic coupling, this reduction of symmetry could also be expected to lead to a distortion of the tetragonal lattice planes. The new phase could therefore be characterized by investigating thermal expansion and magnetostriction in the ab-plane perpendicular to the field.

For these measurements, we are testing a new miniaturized capacitive dilatometer, which can be rotated in the field and allows measuring length changes in various orientations relative to field and crystal axes.

This work is in collaboration with F. Weickert, R. Küchler, R.S. Perry and Y. Maeno.

[1] P. Gegenwart et al., PRL **96**, 136402 (2006)
[2] R.A. Borzi et al., Science **315**, 214-217 (2007)

TT 6.70 Mon 13:00 P1A

Quantum Criticality in CeMIn$_5$-Systems Studied by Low-Temperature Thermal Expansion — •Jan Guido Donath[1], Philipp Gegenwart[1,3], Eric D. Bauer[2], John L. Sarrao[2], and Frank Steglich[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico, 87545 USA — [3]I. Physikalisches Institut, Universitaet Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

CeMIn$_5$-115-systems are of tremendous current interest since they are ideal to study the interplay of unconventional superconductivity (SC), long-range magnetic order and non-Fermi liquid behavior (nFL).

In this work, we will present low temperature thermal expansion measurements of $CeIrIn_5$, a heavy fermion superconductor at ambient pressure. By applying high magnetic fields $B > 12$ T, SC is suppressed and nFL behavior develops, which is believed to be connected to a metamagnetic quantum critical point (QCP) at $B \approx 25$ T [1].

Thermal expansion is a powerful tool to analyse quantum critical behavior and make robust statements about the nature of the QCP. We performed measurements in magnetic fields up to B=17.5 T and temperatures 50 mK $\leq T \leq$ 4 K. We will analyse the temperature dependences of our results and compare them with theoretical predictions [2] and other representatives of the 115-family (M=Co, Rh).

[1] Capan *et al.*, PRB **70** 180502 (2004).
[2] Zhu *et al.*, PRL **91** 066404 (2003).

TT 6.71 Mon 13:00 P1A

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

Exotic non-Fermi liquid behavior of the Sommerfeld coefficient C/T was reported for the heavy-fermion compound $YbRh_2Si_2$ [1]. It exhibits antiferromagnetic ordering at $T_N = 72$ mK and a quantum critical point (QCP) can be induced by a magnetic field of $\mu_0 H_c = 60$ mT. The application of hydrostatic pressure yields a shift of T_N to higher temperatures and the appearence of a second phase transition at T_L [2].

Instead of using hydrostatic pressure, similar behavior can be achieved by slightly substituting isoelectronic Co on the Rh site without introducing much disorder. At 7% Co substitution T_N is shifted to 400 mK and T_L to 70 mK.

We investigated the specific heat of a $Yb(Rh_{0.93}Co_{0.07})_2Si_2$ high-

quality single crystal in magnetic fields and in the temperature range between 0.05 and 4 K. The $T-H$ phase diagram has been explored by means of thermodynamics. The nature of the lower transition and the behaviour of C/T close to the QCP at $\mu_0 H_c \approx 200$ mT has been studied in detail.

[1] J. Custers et al. Nature **424**, 524 (2003).
[2] S. Mederle et al., J. Phys. Condens. Matter **14**, 10731 (2002).

TT 6.72 Mon 13:00 P1A

Pressure tuning of magnetism and superconductivity in $CeCu_2Si_2$ — •Koji Kaneko[1,2], Oliver Stockert[1], Julia Arndt[1], Astrid Schneidewind[3,4], Hirale S. Jeevan[1], Christoph Geibel[1], and Franck Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]ASRC, Japan Atomic Energy Agency, Ibaraki, Japan — [3]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [4]Neutronenforschungsquelle Heinz-Maier-Leibnitz (FRM-II), TU München, Garching, Germany

In order to get insights on the relationship between magnetism and superconductivity in $CeCu_2Si_2$, neutron scattering experiments under pressure on A-$CeCu_2Si_2$ were carried out. An application of a small pressure of ∼5 kbar for A-$CeCu_2Si_2$ can change the ground state from antiferromagnetic to superconducting through the coexistence phase, which gives the opposite effect to Ge doping. We started from the development of a new pressure cell made of a special aluminum alloy, in order to overcome difficulties of pressure experiments, such as higher background from the cell. This new pressure cell was succeeded to hold the required pressure of more than 3 kbar, which is sufficient to kill antiferromagnetism and enter into the superconducting state. Neutron scattering experiments on PANDA at FRM-II confirm the disappearance of the long-range antiferromagnetic order under pressure, whereas weak magnetic signal still remains at the ordering wave vector. The identical behavior was observed for the S-$CeCu_2Si_2$ with decreasing temperature[1]. Inelastic neutron scattering experiments are currently in progress.

[1] O. Stockert *et al.*, Physica B **403**, 973 (2008).

TT 7: Postersession Matter at Low Temperature: Materials

Time: Monday 13:00–16:45 Location: P1B

TT 7.1 Mon 13:00 P1B

The effect of temperature and magnetic field on the diffusion of positrons in slightly deformed copper — •Vera Koos, Matz Haaks, Torsten E.M. Staab, and Peter Herzog — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn

The density of lattice defects like dislocations and vacancies can be measured by positron annihilation spectroscopy (PAS) with outstanding sensitivity. This is due to the fact that positrons diffuse through the lattice and can be trapped by open volumes. Diffusion and trapping are temperature dependent. Additionally the diffusion is influenced by magnetic fields forcing the positrons on curved trajectories perpendicular to the fields direction. In slightly deformed metals changes in the diffusion are reflected by changes of the positron annihilation parameters (S-parameter).

In this study we present PAS results on slightly deformed copper over a temperature range from room temperature (300 K) down to 20 mK, using a ^{3}He/^{4}He dilution refrigerator. By comparison with the predictions of an adapted trapping model it could be shown that dislocations change their behavior from a shallow to a deep positron trap at about 100 K. Below trapping in prismatic dislocation loops plays a significant role.

At several temperatures the effect of a magnetic field (0 to 2 Tesla) was studied. Increase of the field causes a decrease in the S-parameter. Within the scope of the trapping model this can be explained by a decrease of the volume scanned by the positron during its diffusive motion.

TT 7.2 Mon 13:00 P1B

Interacting nuclear dipoles of particles involved in atomic tunnelling processes influence the amplitude of polarisation echoes in glassy glycerol — •Gudrun Fickenscher, Masoomeh Bazrafshan, Kathrin Reinhold, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany

In recent years, an unexpected magnetic field effect of the dielectric properties of non-magnetic glasses was discovered, that cannot be described by the otherwise widely accepted standard tunnelling model. It has since been proven, that it is caused by nuclear electric quadrupole moments of the tunnelling entities interacting with local electric field gradients which change their direction as the particle tunnels from one well to the other. Due to its anisotropic nature the interaction of nuclear magnetic dipole moments leads to an analogous effect on a smaller energy scale. We have studied this effect by measuring the dielectric 2-pulse polarisation echo amplitude of various partially deuterated glycerol samples as a function of the delay time and the magnetic field. Numerical calculations were performed assuming particular tunnelling motions as well as different numbers of dipole moments on the tunnelling entity and in its surrounding. With reasonable parameters these calculations fit the data satisfactorily both qualitatively and quantitatively, giving deeper insight into the motion of tunnelling systems in glassy glycerol.

TT 7.3 Mon 13:00 P1B

Low-temperature investigation of the thermal conductivity of bulk metallic glasses — •Daniel Rotfhuss, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg, Germany

The thermal conductivity of glasses at temperatures below 1 Kelvin is generally described by the diffusion of thermal phonons. The mean free path of the phonons is limited by scattering processes between the heat-carrying phonons and the tunneling systems in the glasses. We investigate metallic glasses where the thermal transport is due to both phonons an electrons. In superconducting metallic glasses far below T_c the phonons are dominating the conduction of heat. For the first time measurements of thermal conductivity were performed on a bulk metallic glass down to 6 mK. For this purpose we used a SQUID-based contact-free technique because of its extremly small parasitic heating. Results of amorphous $Zr_{52.2}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$ in the superconduting state are presented which show that the thermal conductivity of the sample scales nearly quadratically in temperature. This suggests that well below T_c the heat transport of superconduting metallic glasses can be described by resonant scattering of phonons by tunneling systems just as in dielectric glasses.

TT 7.4 Mon 13:00 P1B

New Methode to Determine the Specific Heat of Glasses at Ultra-low Temperatures — •Angela Halfar, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, D-69120 Heidelberg

The low temperature properties of glasses are governed by atomic tunneling systems. Due to the structural disorder of glasses the parameters of these atomic tunneling systems are widely distributed. This is the origin of the linear specific heat of glasses at low temperatures, which is a characteristic property of amorphous materials independent of their chemical composition. Measurements of the specific heat of dielectric glasses at ultra-low temperatures are very difficult since even small parasitic heat inputs lead to large systematic errors. To minimize such parasitic heat inputs and to minimize the addenda we have developed a contact-free methode to investigate the specific heat of insulating glasses. It is based on an optical heating system and uses the temperature dependence of the amplitude of polarisation echos as an intrisic thermometer. We shall discuss this new technique and will show first experimental results.

TT 7.5 Mon 13:00 P1B

Antiferromagnetic resonance in multiferroic $YMnO_3$ and $LuMnO_3$ — •D. Kamensky, M. Ozerov, E. Čižmár, J. Wosnitza, and S. Zvyagin — Dresden High Magnetic Field Laboratory (HLD), Forschungszentrum Dresden - Rossendorf, 01314 Dresden, Germany

Multiferroic rare-earth manganites have attracted much attention because of the coexistence of ferroelectric and magnetic order. Combining conventional far-infrared Fourier-transform and THz-range free electron laser electron spin resonance (ESR) techniques, magnetic ex-

citations in the hexagonal multiferroic materials $YMnO_3$ and $LuMnO_3$ have been studied. In the antiferromagnetically (AFM) ordered phase the gap in the excitation spectrum (~ 42 and ~ 48 cm^{-1} for $YMnO_3$ and $LuMnO_3$, respectively) was observed directly. Similar slope of the frequency-field dependences of the AFM resonance modes, ~ 0.5 cm^{-1}/T, was found for both compounds. A fine structure of the AFM resonance absorption has been revealed by means of high-resolution ESR techniques, which can be explained taking into account a finite interaction between the neighboring Mn^{3+} layers.

The work was done in collaboration with A.K. Kolezhuk, D. Smirnov, H.D. Zhou, and C.R. Wiebe.

TT 8: Postersession Transport: Graphene and Carbon Nanotubes

Time: Monday 13:00–16:45 Location: P1B

TT 8.1 Mon 13:00 P1B

Dirac fermion quantization on graphene edges: Isospin-orbit coupling, zero modes and spontaneous valley polarization — •Grigory Tkachov — Max Planck Institute for the Physics of Complex Systems, Dresden

The talk addresses boundary electronic properties of graphene with a complex edge structure of the armchair/zigzag/armchair type. It is shown that the finite zigzag region supports edge bound states with discrete equidistant spectrum obtained from the Green's function of the continuum Dirac equation [1]. The energy levels exhibit the coupling between the valley degree of freedom and the orbital quantum number, analogous to a spin-orbit interaction. The characteristic feature of the spectrum is the presence of a zero mode, the bound state of vanishing energy. It resides only in one of the graphene valleys, breaking spontaneously Kramers' symmetry of the edge states. This implies the spontaneous valley polarization characterized by the valley isospin $\pm 1/2$. The polarization is manifested by a zero-magnetic field anomaly in the local tunneling density of states, and is directly related to the local electric Hall conductivity.

[1] G. Tkachov, arXiv: 0811.2698.

TT 8.2 Mon 13:00 P1B

Time dependent charge and spin transport in graphene nanoribbons — •Claudia Gomes da Rocha, Lakshmi Sankaran, Jens Kunstmann, Luis E.F. Foa Torres, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

Interesting quantum phenomena can be revealed when low dimensional materials are subject to external fields. In our work we theoretically investigate how external fields influence the transport properties of graphene nanoribbons. We demonstrate that armchair-edge nanoribbons subject to a time-periodic gate potential show the so called quantum wagon-wheel effect, in which Fabry-Perot oscillations can be periodically suppressed or recovered as a function of the AC parameters[1]. For zigzag-edge nanoribbons, more intriguing phenomena take place due to the existence of edge states. Essentially, Fabry-Perot oscillations manifest in a limited range of bias and gate voltages and they cannot be totally recovered by tuning the AC gate. Furthermore, zigzag nanoribbons having a Klein edge are expected to yield spin-polarized bands when described by mean-field Hubbard Hamiltonian. Here we also show that the presence of a DC external gate in zigzag-edge systems suppresses the characteristic edge states. This leads to a transition from a completely spin-polarized semiconducting system to one which is non-magnetic and metallic.

[1] L. E. F. Foa Torres, and G. Cuniberti, cond-mat arXiv. 0807.4953

TT 8.3 Mon 13:00 P1B

Ab-Initio Studies of Electronic and Transport Properties of Graphene Nanoribbons — Uwe Treske[1,2], Frank Ortmann[1,2], •Björn Oetzel[1,2], Karsten Hannewald[1,2], and Friedhelm Bechstedt[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 ab-initio DFT calculations for Graphene Nanoribbons (GNRs). We focus our attention on the band structures and gap behavior versus ribbon widths for armchair and zigzag GNRs. Furthermore we study the influence of spin polarization and spin ordering on the band structure and the magnetic behavior of zigzag GNRs. The transmission functions are calculated in the Landauer-Büttiker formalism using the number-of-states approach similarities and differences of quantum transport are discussed for several groups of armchair and zigzag GNRs.

TT 8.4 Mon 13:00 P1B

Microwave graphene nano-transistors — Andreas Betz, •Emiliano Pallecchi, Julien Chaste, Takis Kontos, Gwendal Fève, Jean-Marc Berroir, and Bernard Plaçais — Laboratoire Pierre Aigrain, Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris, France.

We report on microwave characterization of graphene nano-transistors. The samples consist of top-gated graphene flakes connected to source and drain electrodes. We performed room temperature transmission measurements using an RF probe station from which we can access both the transconductance and the gate capacitance. We observed mobility as large as 7800 cm^2/Vs, while the maximum transconductance was 2.5 mS/μm at DC and 0.5 mS/μm at gigahertz frequency. The gate capacitance at the gate voltage corresponding to the maximum transconductance is about 0.9 fF (100 nm gate length). Our measurements show that graphene nano-transistors are characterized by a large transit frequency $f_T = g_m/2\pi C_g$ on the order of 1 THz for a gate length of 100 nm (best device measured). We finally discuss their possible sensitivity as fast charge detectors.

TT 8.5 Mon 13:00 P1B

Trans-conductance of back-gated and top-gated multi-walled carbon nanotube field-effect transistors — •asaf avnon[1] and jaako leppäniemi[2] — [1]Freie universität Berlin,Berlin,Germany — [2]University of Jyväskylä, Jyväskylä, Finland

In this study we have mapped the gate response of thin multi-walled carbon nanotubes (MWNT)-based field-effect transistors (FET). We observe advancing hysteresis in gate-response of back-gated MWCNT FETs and retarding hysteresis in top- gated MWCNT FETs. The hysteresis could be a result of mobile charge carriers trapped in the insulator as it diminishes at low temperatures both in devices with a top-gate and a back-gate. The hysteresis in the gate response could be utilized in future memory applications.

TT 8.6 Mon 13:00 P1B

Scattering dynamics in intra-nanotube quantum dots — •Dario Bercioux[1], Gilles Buchs[2,3], Pascal Ruffieux[3], Pierangelo Gröning[3], Hermann Grabert[1], and Oliver Gröning[3] — [1]Physikalisches Institut and Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands — [3]EMPA Swiss Federal Laboratories for Materials, Testing and Research, nanotech@surfaces, Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland

Room temperature active intratube quantum dots in metallic single-walled carbon nanotubes are realized by means of low dose medium energy Ar^+ irradiation. With this low invasive method defect-induced confinement regions of the order of, or shorter than, 10 nm are produced which are demonstrated to lead to particle-in-a-box-like states with energy separations up to 200 meV, hardly achievable with nowadays' lithography processes. Fourier-transform scanning tunneling spectroscopy compared to results of a Fabry-Pérot electron resonator model yields clear signatures for inter- and intra-valley scattering of electrons confined between consecutive defects. [1] G. Buchs *et al.* arXiv:0812.3883v1 [cond-mat.mes-hall]

TT 8.7 Mon 13:00 P1B

Disorder effects in graphene: A local distribution approach — •Jens Schleede, Gerald Schubert, and Holger Fehske — Institute for Physics, Ernst-Moritz-Arndt Universität Greifswald, Germany

We present a study of different models of local disorder in mono- and bilayer graphene and graphene nanoribbons. In particular, we investigate the Anderson model on a two-dimensional honeycomb lattice and determine the probability distribution of the local density of states using a highly efficient kernel polynomial method. Supplemented by a careful finite-size scaling analysis, this quantity allows for distinguishing extended from localised states. Our findings are corroborated by the evaluation of the time evolution of an initially localised wave packet, which is based on Chebyshev expansion technique. While our results for the 2D infinite systems indicate complete localisation for arbitrary weak Anderson disorder, the finite system sizes of graphene strips (nanoribbons) induce another length scale to the problem. So despite the localisation on large length scales, finite 2D devices may show metallic behaviour for weak disorder. Moreover we show that the ground state properties of graphene are largely affected by the geometric pattern and disorder at their edges.

TT 8.8 Mon 13:00 P1B

Towards entanglement in carbon nanotube based double quantum dots — •Lorenz Herrmann[1,2], Fabien Portier[3], Patrice Roche[3], Christian Glattli[2,3], Takis Kontos[2], and Christoph Strunk[1] — [1]Inst. for Exp. and Appl. Physics, Univ. Regensburg, Germany — [2]Lab. Pierre Aigrain, ENS Paris, France — [3]SPEC, CEA Saclay, France

We investigate carbon nanotube-based double quantum dots with two normal (Ti/Au) and one central superconducting (Al) contact. The characterization of the devices via the normal contacts reveals that the superconducting electrode splits the carbon nanotube into two coupled quantum dots. As an additional feature compared to ordinary double dot systems, we can use our middle electrode (Al) not only to split the nanotube into two dots, but also to inject Cooper pairs into our double dot system. By sending a current from the superconducting to the normal contacts it is possible to divide the current into the two output branches. Since Coulomb charging energy prevents double occupation of one dot, the splitting of a pair into the two different normal contacts is favoured if the gate configuration is such that Coulomb interaction between the dots is strong. That is the case at the so called triple points of the initial stability diagram of the double dot. The splitting of the Cooper pairs thus occurs via a co-tunneling process. We find an enhanced subgap conductance at the triple points, which possibly reflects correlated Andreev processes.

TT 9: Correlated Electrons: Metal-Insulator Transition 1

Time: Monday 14:00–16:45 Location: HSZ 03

TT 9.1 Mon 14:00 HSZ 03

Pressure and doping driven metal-to-insulator transition in V_2O_3 — •Philipp Hansmann[1,2], Alessandro Toschi[2], Giorgio Sangiovanni[2], Maurits Haverkort[1], Tanusri Saha-Dasgupta[3], and Karsten Held[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria — [3]S.N. Bose National Centre for Basic Sciences, Kolkata, India

In the V_2O_3 system chemical doping and application of pressure are usually assumed to have equivalent effects for the physics of the Mott Hubbard metal-to-insulator transition (MIT). Recent experimental evidence, however, shows that application of pressure on the Cr-doped V_2O_3 cannot repristinate the situation of the undoped compound. In order to understand the underlying physical mechanisms in the differently driven MITs we investigate optical and X-ray absorption spectra by means of the local density approximation and its merger with dynamical mean field theory (LDA+DMFT) as well as full multiplet cluster calculations.

TT 9.2 Mon 14:15 HSZ 03

Correlation effects in half-metallic Heusler alloys — •Eberhard Jakobi, Nils Blümer, and Peter van Dongen — KOMET337, Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

Spintronic applications such as giant magnetoresistive or spin valve devices require materials with high spin polarization, ideally half metals at room temperature. Heusler alloys are an important class of candidates for such spintronic materials [1].

For these moderately correlated materials, density functional theory (DFT) appears as a reasonable starting point [2]. However, this description lacks lifetime effects and cannot exhibit Mott transitions.

We present results within dynamical mean-field theory (DMFT), obtained using a second-order weak-coupling impurity solver, which is optimized for treating systems with a large number of valence bands. Correlation effects lead to significant changes in the band-selective densities of states and to corrections in the local moments.

[1] Wurmehl et al, Appl. Phys. Lett. 88 (2006) 032503
[2] Kandpal et al, J. Phys. D: Appl. Phys. 40 (2007) 1507

TT 9.3 Mon 14:30 HSZ 03

LDA+DMFT study of metal-insulator transition in the bulk and at the surface of $Ca_xSr_{2-x}RuO_4$ — •Michael Karolak, Tim Wehling, Frank Lechermann, and Alexander Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg

$Ca_xSr_{2-x}RuO_4$ is an interesting model system to study the interplay of structural distortions and the electronic metal to insulator transition. We present an ab-initio study within the LDA+DMFT framework of this system. In this way we account for changes in the one particle Hamiltonian due to the structural distortions in a first principles manner. We obtain the electronic density of states and the self energy. The mechanism of the metal to insulator transition in the bulk and at the surface of this system is discussed. A strong enhancement of electron correlation effects is found for the low temperature structures.

TT 9.4 Mon 14:45 HSZ 03

LDA+DMFT study of Ca_2RuO_4 and Sr_2RuO_4 using the full on-site Coulomb interaction — •Evgeny Gorelov[1], Eva Pavarini[1], and Alexander I. Lichtenstein[2] — [1]Forschungszentrum Jülich, IFF, 52425 Jülich, Germany — [2]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

The $Ca_{2-x}Sr_xRuO_4$ layered ruthenates display a complex phase diagram. Whereas Sr_2RuO_4 is a correlated metal, the progressive substitution Sr with Ca leads to a number of structural phase changes. Finally, Ca_2RuO_4 exhibits Mott transition at T≈350 K [1].

In this work we calculate the photoemission spectra of Sr_2RuO_4 [2] and study the temperature-induced Mott transition in Ca_2RuO_4 [3].

As a method we use the LDA+DMFT technique. First we construct a material-specific NMTO Wannier basis for the partially filled 4d t_{2g} bands and the corresponding three-band t_{2g} Hubbard Hamiltonian. Then we solve this model within the DMFT approximation retaining the full self-energy matrix and using the Continuous Time QMC impurity solver [4]. This solver allow us to analyze the role played by the spin-flip terms of the on-site Coulomb vertex.

[1] O. Friedt, M. Braden, G. Andre, P. Adelmann, S. Nakatsuji, Y. Maeno, Phys. Rev. B **63**, 174432 (2001).
[2] E. Gorelov, A. N. Rubtsov, A.V. Lukoyanov, V.I. Anisimov and A. I. Lichtenstein, to be published.
[3] E. Gorelov and E. Pavarini, to be published.
[4] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B **72**, 035122 (2005).

TT 9.5 Mon 15:00 HSZ 03

Drastic Spectral Weight Transfer across the Metal-Insulator Transition in $Ca_{2-x}Sr_xRuO_4$ Revealed by Soft-X-ray Photoemission — •H. Fujiwara[1], Z. Hu[1], T. C. Koethe[1], A. Hendricks[1], M. Zell[1], N. B. Brookes[2], S. Nakatsuji[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan

The layered $Ca_{2-x}Sr_xRuO_4$ system shows a very rich phase diagram as a function of the x-composition, temperature and magnetic field. Particularly fascinating is the electronic structure in the range of $0 < x < 0.2$ where the metal-insulator transition (MIT) takes place at a continuously decreasing temperature with x getting closer to 0.2. This transition is accompanied by a drop in the resistivity of several orders of magnitude, comparable to that in V_2O_3 and VO_2. In order

to reveal the mechanism of the MIT in $Ca_{2-x}Sr_xRuO_4$, we have carried out a photoemission study with $h\nu = 700$ eV to obtain reasonable sensitivity to the Ru 4*d* spectral weight. We have found that there is a dramatic transfer of the spectral weight across the MIT. Since x-ray absorption spectroscopy has shown that the orbital occupation of the three t_{2g} bands changes significantly across the MIT, as is the case also in the MITs of V_2O_3 [1] and VO_2 [2], our results suggest the crucial role of the orbital switching for the MIT of $Ca_{2-x}Sr_xRuO_4$.

[1] J.-H. Park, et al., Phys. Rev. B 61, 11506 (2000).
[2] M. W. Haverkort, et al., Phys. Rev. Lett. 95, 196404 (2005).

15 min. break

TT 9.6 Mon 15:30 HSZ 03

Electronic and optical properties of NiS_2 — •Cosima Schuster — Universität Augsburg, D-86135 Augsburg

Crystal field splitting, correlation, and the 3d band width are almost equal in the pyrites MX_2 (M=Fe,Co,Ni; X=S,Se) which gives rise to a large variety of electrical, magnetic and optical properties in these compounds. Of special interest is the metal-insulator-transition in NiS_2 with Se-doping or by applied pressure. It is not accompanied by a change in the lattice symmetry and commonly believed to be driven by electron-electron interactions. In addition, a low-temperature antiferromagnetic phase is observed both in the insulating and metallic regime. To reinvestigate the properties of NiS_2 we perform ab initio calculations using density functional theory. Thereby we focus on the relation between doping and applied pressure and the role of the magnetism in the metal-insulator-transition. The magnetic phase diagram with pressure and doping can be reproduced within the GGA, albeit the magnetic phase is slightly overestimated. The insulating behaviour of NiS_2, however, cannot be described within this approximation. The description in terms of a gap and of the metal-insulator-transition and the optical properties near the transition need more advanced methods. The response functions obtained in the random phase approximation cannot sufficiently describe the optical properties.

TT 9.7 Mon 15:45 HSZ 03

Is NiS_2 a charge-transfer insulator? — •Jan Kuneš[1], Dmitry A Korotin[2], and Vladimir I Anisimov[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Institute of Metal Physics, Russian Academy of Sciences, Yekaterinburg, Russia

The physics NiS_2 and $NiSe_2$ is often described in terms of small respectively negative gap charge-transfer insulator. Using combination of first principles bandstructure and dynamical mean-field approximation, so called LDA+DMFT approach, we investigate the electronic structures of the two materials at ambient conditions and under pressure. While both compounds are similar to charge-transfer insulators in that the ligand p-band is located between the Ni-d lower and upper Hubbard bands, the quasiparticle gap is not of the charge-transfer type. The gap is between a strongly hybridized $p-d$ valence band and a conduction band formed by anti-bonding states of S-S dimer with strong admixture of Ni-d character. The key difference between NiS_2 and $NiSe_2$ determining their groundstates is the stronger dimer splitting in the former.

TT 9.8 Mon 16:00 HSZ 03

Crystal-field level inversion in lightly Mn-doped $Sr_3Ru_2O_7$ — Muhammed A. Hossain[1], Zhiwei Hu[2], Maurits W. Haverkort[2], •Tobias Burnus[2], Chun Fu Chang[2], Stefan Klein[2], Jonathan D. Denlinger[3], Hong-Ji Lin[4], Chien Te Chen[4], Roland Mathieu[5], Y. Kaneko[5], Yoshinori Tokura[5], S. Satow[5], Y. Yoshida[6], Hidenori Takagi[5], Arata Tanaka[7], Ilya S. Elfimov[1], George A. Sawatzky[1], L. Hao Tjeng[2], and Andrea Damascelli[1] — [1]University of British Columbia, Vancouver, Canada — [2]II. Physikalisches Institut, Universität zu Köln — [3]Advanced Light Souce, Berkeley, California — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]University of Tokyo, Japan — [6]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — [7]Hiroshima University, Japan

$Sr_3(Ru_{1-x}Mn_x)_2O_7$, in which 4*d*-Ru is substituted by the more localized 3*d*-Mn, is studied by x-ray dichroism and spin-resolved density functional theory. We find that Mn impurities do not exhibit the same 4+ valence of Ru, but act as 3+ acceptors; the extra e_g electron occupies the in-plane $3d_{x^2-y^2}$ orbital instead of the expected out-of-plane $3d_{3z^2-r^2}$. We propose that the 3*d*–4*d* interplay, via the ligand oxygen orbitals, is responsible for this crystal-field level inversion and the material's transition to an antiferromagnetic, possibly orbitally ordered, low-temperature state.

TT 9.9 Mon 16:15 HSZ 03

On the mechanism for orbital-ordering in $KCuF_3$ — •Eva Pavarini[1], Erik Koch[1], and Alexander I. Lichtenstein[2] — [1]Institut für Festkörperforschung and Institute for Advanced Simulations, Forschungzentrum Juelich — [2]Institute of Theoretical Physics, University of Hamburg

The Mott insulating perovskite $KCuF_3$ is considered the archetype of an orbitally-ordered system. By using the LDA+dynamical mean-field theory (DMFT) method, we investigate the mechanism for orbital-ordering (OO) in this material. We show that the purely electronic Kugel-Khomskii super-exchange mechanism (KK) alone leads to a remarkably large transition temperature of $T_{KK} \sim 350$ K. However, orbital-order is experimentally believed to persist to at least 800 K. Thus Jahn-Teller distortions are essential for stabilizing orbital-order at such high temperatures.

TT 9.10 Mon 16:30 HSZ 03

Predicting pressure-induced phase transitions in the Mott insulator TiOCl — Yuzhong Zhang, •Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The layered Mott insulator TiOCl has been the focus of a lot of recent experimental and theoretical research as it is one of the few inorganic spin-Peierls materials. Still, several important issues remain unsettled, namely the underlying Hamiltonian, the mechanism that is responsible for the incommensurate phase and the nature of the high-pressure phases. We performed thorough density functional theory calculations in order to shed light on these issues. First, we determine the parameters of a very general spin-phonon Hamiltonian[1]. The resulting model for TiOCl has strong antiferromagnetic exchange couplings along one direction with weak but significant frustrating ferromagnetic couplings along the other two directions, and it has strong spin-lattice coupling constants. Using constant pressure Car Parrinello molecular dynamics calculations, we determine the high pressure structures of TiOCl from first principles[2]. We predict two consecutive phase transitions, first from a Mott insulating high symmetry structure to a metallic dimerized structure and then back to a metallic high symmetry structure. The first of the two transitions has since been confirmed by experiment.

[1] Y. Z. Zhang, H. O. Jeschke, and R. Valentí, Phys. Rev. B **78**, 205104 (2008).
[2] Y. Z. Zhang, H. O. Jeschke, and R. Valentí, Phys. Rev. Lett. **101**, 136406 (2008).

TT 10: Superconductivity: Tunneling, Josephson Junctions, SQUIDs

Time: Monday 14:00–16:30 Location: HSZ 105

TT 10.1 Mon 14:00 HSZ 105

Terahertz emission from intrinsic Josephson junctions of high-T_c superconductor Bi2212 — •Lütfi Özyüzer[1,2], Hasan Köseoglu[1], Fulya Türkoglu[1], Cihan Kurter[3], Ulrich Welp[3], Ken E. Gray[3], Alex E. Koshelev[3], Takashi Yamamoto[4], Kazuo Kadowaki[4], Yilmaz Simsek[2], Yuri Koval[2], Paul Müller[2], and Huabing Wang[5] — [1]Department of Physics, Izmir Institute of Technology, Izmir, Turkey — [2]Phys. Inst. III, University of Erlangen-Nurnberg, Germany — [3]Materials Science Division, Argonne National Laboratory, Illinois, USA — [4]University of Tsukuba, Japan — [5]National Institute for Materials Science, Japan

Recent realization of coherent and continuous emission of THz waves from intrinsic Josephson junctions of layered high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+d}$ (Bi2212) is promising to fill electromag-

netic spectrum's Terahertz gap [1]. Large area mesas ranging from 300x100 to 300x40 μm^2 with height greater than 1 μm were formed on Bi2212. Current-voltage and THz emission characteristics were obtained at various temperatures. THz emissions of mesas were studied by Si-composite bolometer and the emission frequencies were obtained.

[1] L. Ozyuzer, A. E. Koshelev, C. Kurter, N. Gopalsami, Q. Li, M. Tachiki, T. Yamamoto, H. Minami, H. Yamaguchi, T. Tachiki, K. E. Gray, W. K. Kwok and U. Welp, Science **318**, 1291 (2007).

*This research is partially supported by TUBITAK (Sci. and Tech. Research Council of Turkey) project number 108T238. L.O. acknowledges support from Alexander von Humboldt Foundation.

TT 10.2 Mon 14:15 HSZ 105

Fabrication of large $Bi_2Sr_2CaCu_2O_{8+\delta}$ mesas for THz emission — •Yilmaz Simsek[1], Lütfi Özyüzer[1,2], Yuri Koval[1], Paul Müller[1], and Huabing Wang[3] — [1]Department of Physics, Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse. 1, D-91058, Erlangen, Germany — [2]Department of Physics, Izmir Institute of Technology, Izmir, Turkey — [3]National Institute of Material Science, Japan

Recently, the observation of THz radiation from $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) single crystals stimulated the research on intrinsic Josephson junctions (IJJ)[1]. We have fabricated large area mesas including many IJJ stacks on Bi-2212 single crystals by electron beam lithography and Ar ion beam etching techniques. As the observed THz emission is probably due to cavity resonances, the fabrication technique was optimized to obtain clear rectangular shapes. We have fabricated large and tall mesas by selective Ar ion beam etching of a Ti layer on Bi-2212. The samples were characterized by dc I-V measurements. We discuss possible resonant features of the I-V characteristics.

[1] L. Ozyuzer, A. E. Koshelev, C. Kurter, N. Gopalsami, Q. Li, M. Tachiki, K. Kadowaki, T. Yamamoto, H. Minami, H. Yamaguchi, T. Tachiki, K. E. Gray, W.-K. Kwok, U. Welp, Science **318**, 1291 (2007).

*L.O. acknowledges support from Alexander von Humboldt Foundation.

TT 10.3 Mon 14:30 HSZ 105

Laser imaging of hot spots and waves in $Bi_2Sr_2CaCu_2O_8$ intrinsic Josephson junctions — •S. Guénon[1], M. Grünzweig[1], H. B. Wang[2], J. Yuan[2], A. Iishi[2], S. Arisawa[2], T. Hatano[2], T. Yamashita[2], D. Koelle[1], and R. Kleiner[1] — [1]Physikalisches Institut & Center for CollectiveQuantum Phenomena, Universität Tübingen, Germany — [2]National Institute for Materials Science, Tsukuba3050047, Japan

Motivated by the discovery of coherent Terahertz emission in large sized stacks of $Bi_2Sr_2CaCu_2O_8$ intrinsic Josephson junctions [1] we used low-temperature scanning laser microscopy (LTSLM) to image local electric field distributions of mesa structures patterned on top of $Bi_2Sr_2CaCu_2O_8$ single crystals [2]. In LTSLM a laser beam at position (x, y) on the sample surface locally warms up an area of about a few μm^2. This locally well defined heat distribution changes the electrical properties of the system, which in turn leads to a voltage change $\Delta V(x, y)$ measured globally across the sample. The mesas (330μm long and 30–70μm wide) were 1 μm thick and consisted of about 670 junctions. In the low-bias regime we find clear signatures of standing electromagnetic waves that essentially are in agreement with the THz emission data in [1]. At high bias voltages we observe the formation of a hot spot, which at some currents is accompanied by standing wave patterns interacting with the hot spot.

[1] L. Ozyuzer *et al.*, Science **318**, 1291 (2007)
[2] H. B. Wang, S. Guénon *et al.*, submitted to Phys. Rev. Lett.; arXiv:0807.2749v1 [cond-mat.supr-con]

TT 10.4 Mon 14:45 HSZ 105

Josephson junctions with ferromagnetic $Fe_{0.75}Co_{0.25}$ and Cu_2MnAl interlayers — •Dirk Sprungmann[1], Kurt Westerholt[1], Hartmut Zabel[1], and Martin Weides[2] — [1]Institut für Experimentalphysik IV / Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]IFF Forschungszentrum Jülich, D-52425 Jülich, Germany

We present our studies on SINFS Josephson junctions using $Fe_{0.75}Co_{0.25}$ and Cu_2MnAl-Heusler alloys for the F-layer. The junctions with $Fe_{0.75}Co_{0.25}$ represent the case of large magnetic exchange energies in the region of 500 meV. We show that these junctions exhibit an extremely short coherence length $\xi_{F1} = 0.16$ nm and $\xi_{F2} = 0.54$ nm and that the stray fields which emanate from the ferromagnetic layer cause increasing flux trapping effects for thicknesses $d_F \geq 1.1$ nm.

The opposite case with very small exchange energies in the region of several meV is realized in junctions with the Heusler alloy Cu_2MnAl. This alloy sputtered at room temperature features a distinct structural disorder which can be reduced by annealing. Because of the correlation between structural order and exchange energy the ferromagnetism can be fine tuned by thermal annealing. We study systematically the influence of the annealing process on the transport properties and correspondingly on the $I_c(d_F)$-characteristic of our junctions.

D. S., K. W. and H. Z. acknowledge financial support by SFB-491, and M. W. by project WE 4359/1-1.

15 min. break

TT 10.5 Mon 15:15 HSZ 105

High frequency properties of Josephson π-junctions — •Georg Wild[1,2], Christian Probst[1], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Str. 8, 85748 Garching — [2]Physik Department, Technische Universität München, Garching

Josephson junctions with ferromagnetic interlayer have attracted much interest due to their potential application as π-phase shift elements. We have developed a self-aligned multilayer process for the fabrication of superconductor/insulator/ferromagnet/superconductor Josephson junctions (S=Nb, I=AlO_x, F=NiPd). Our junctions have RCSJ-like current-voltage characteristics and a Fraunhofer diffraction pattern for the magnetic field dependence of the critical current. The dependence of the I_cR_n-product on the ferromagnet thickness shows a clear crossover from the zero- to the π-state. We have determined the plasma frequency of π-coupled junctions from Fiske resonances. This data is used to explain the different excitations found in microwave spectroscopy experiments at milli-Kelvin temperature.

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

TT 10.6 Mon 15:30 HSZ 105

Visualizing supercurrents in 0-π ferromagnetic Josephson tunnel junctions — •Edward Goldobin[1], Christian Gürlich[1], Tobias Gaber[1], Dieter Koelle[1], Reinhold Kleiner[1], Martin Weides[2], and Hermann Kohlstedt[2] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]Institute of Solid State Physics, Reserch Center Jülich, Germany

So-called 0 and π Josephson junctions can be treated as having positive and negative critical currents. This implies that the same phase shift applied to a Josephson junction causes counterflow of supercurrents in 0 and in π junctions connected in parallel provided they are short in comparison with Josephson penetration depth λ_J.

We have fabricated several 0, π, 0-π, 0-π-0 and 20×(0-π-) planar superconductor-insulator-ferromagnet-superconductor Josephson junctions and studied the spatial supercurrent density distribution $j_s(x, y)$ across the junction area using low temperature scanning electron microscopy. At zero magnetic field we clearly see counterflow of the supercurrents in 0 and π regions. The picture also changes consistently in the applied magnetic field.

TT 10.7 Mon 15:45 HSZ 105

A universal 0-π transition in magnetic triplet superconductor Josephson junctions — •Philip Brydon[1] and Dirk Manske[2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, 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. Using a tunneling Hamiltonian approach, we obtain the currents in an arbitrary triplet superconductor – ferromagnet – triplet superconductor junction, imposing only the condition that the orbital pairing states in the two superconductors are not orthogonal. From this, we predict a sign change of the charge current (a 0-π transition) as the orientation of the barrier magnetic moment is varied. We also show that the spin current flows in opposite directions on either side of the junction, and has a phase-independent contribution arising from spin-flip reflection processes. We confirm our results for three different choices of orbital pairing states using Bogoliubov-de Gennes theory.

TT 10.8 Mon 16:00 HSZ 105

Quantum Dynamics of LC shunted Nb/Al-AlO$_x$/Nb Josephson Junctions — •Christoph Kaiser[1], Thilo Bauch[2], Floriana Lombardi[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH), D-76187 Karlsruhe — [2]Quantum Device Physics Laboratory, Department of Microtechnology and Nanoscience, MC2, Chalmers University of Technology, S-41296 Göteborg, Sweden

Superconducting systems including Josephson junctions (JJs) are good candidates for studying a macroscopic quantum variable if the system is suitably decoupled from its environment.

We investigate the behavior of this macroscopic quantum variable φ in circuits containing a JJ, a capacitor and an inductance. It was shown that φ should be confined by a 2-dimensional potential, leading to two energy scales for the quantum levels in the potential wells.

We designed and fabricated such LC-JJ systems with different inductance values, investigated their quantum dynamics and compared the results to the theoretical expectations. The samples were fabricated in Karlsruhe by a thoroughly optimized Nb/AlO$_x$/Nb process employing electron beam lithography. Afterwards, we explored the quantum mechanical energy levels and the tunnelling rates of our samples in a carefully shielded dilution refrigerator in Göteborg.

Our results are in very good agreement with the theoretical predictions. We achieve the quantum regime for our samples and can clearly identify the predicted energy level splittings in our experimental spectroscopy data.

TT 10.9 Mon 16:15 HSZ 105

Conductance of an array of Josephson junctions in the insulating state — •Sergey Syzranov[1], Konstantin Efetov[1], and Boris Altshuler[2] — [1]Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Physics Department, Columbia University, New York, N.Y. 10027, USA

We study transport in weakly disordered two-dimensional arrays of Josephson junctions in the Coulomb blockade regime. We calculate the conductance of the system at low temperatures and show that it has an activation behaviour with the activation gap close to the charging energy of a single Cooper pair on a superconducting island between the junctions. While a disordered array has a finite conductivity, the conductance of an ideally regular array is independent of its size. The possibility of a new "superinsulating" state is discussed.

TT 11: Transport: Nanoelectronics I - Quantum Dots and Wires, Point Contacts 2

Time: Monday 14:00–16:45 Location: HSZ 301

TT 11.1 Mon 14:00 HSZ 301

Pair tunneling resonance in the single-electron transport regime — •Martin Leijnse[1,3], Maarten Wegewijs[1,2,3], and Herbert Schoeller[1,3] — [1]Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany — [2]Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA-Fundementals of Future Information Technology

We predict a new resonance in non-linear transport through strongly interacting quantum dots, originating from the coherent tunneling of electron pairs (PT). The PT resonance shows up as a peak in the derivative of the differential conductance, d^2I/dV^2, in the *single-electron* transport (SET) regime. The position is determined by the electrochemical potential of one electrode matching the average of two subsequent charge addition energies. Using 4th order perturbation theory in the tunneling coupling[1] for a single level quantum dot (Anderson model), we present an analytic expression for the peak shape, which reveals the bosonic nature of the charge transfer. Awareness of the PT resonance can be crucial for interpretation of experimental low-temperature transport spectroscopy data of semi-conducting, carbon nanotube, or single molecule quantum dots, since it can easily be mistaken for a weak SET resonance judging only by the voltage dependence of its position. We show that the PT resonance can be distinguished from SET by its anomalous temperature- and magnetic field dependence, peak shape and shot-noise signature.

[1] M. Leijnse, M. R. Wegewijs, PRB (in print), arXiv:0807.4027.

TT 11.2 Mon 14:15 HSZ 301

Electron tunneling into a quantum wire in the Fabry-Pérot regime — •Dario Bercioux[1], Stefano Pugnetti[2], Fabrizio Dolcini[2], and Hermann Grabert[1] — [1]Physikalisches Institut and Freiburg Institute for Advanced Studies, Universität Freiburg, D-79104 Freiburg, Germany — [2]Scuola Normale Superiore and NEST CNR-INFM, I-56126, Pisa Italy

We study a gated quantum wire contacted to source and drain electrodes in the Fabry-Pérot regime. The wire is also coupled to a third terminal (tip) at an arbitrary position along its length. We allow for an asymmetry of the tunneling amplitudes between right/left moving electrons and the tip. Electron-electron interaction in the wire is taken into account by means of the inhomogeneous Luttinger liquid model. The current-voltage characteristics of this three-terminal set-up is shown to exhibit very rich physical effects. We analyze configurations where the tip acts as an electron injector or as a voltage probe. When the tip is in the electron-injection configuration we find that electron-electron coupling does not affect the ratio of the currents flowing to the source and drain electrodes [1]. Contrary to the result by Steinberg *et al.*[2], this ratio depends only on the asymmetry in tunneling.

[1] S. Pugnetti, F. Dolcini, D. Bercioux, and H. Grabert, arXiv:0810.2962v1 [cond-mat.str-el].

[2] H. Steinberg, G. Barak, A. Yacoby, L. N. Pfeiffer, K. W. West, B. I Halperin, and K. Le Hur, Nature Phys. **4**, 116 (2008).

TT 11.3 Mon 14:30 HSZ 301

Charge and spin pumping through quantum dots beyond the adiabatic regime — •Fabio Cavaliere[1], Michele Governale[2], and Jürgen König[2] — [1]Dipartimento di Fisica, Università di Genova, LAMIA CNR-INFM, Via Dodecaneso 33, 16146 Genova, Italy — [2]Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

We study charge and spin pumping in an interacting quantum dot connected to normal or ferromagnetic leads, beyond the adiabatic regime. We employ a systematic expansion of the pumped currents in both frequency and tunneling strength. Going beyond the adiabatic regime has important consequences on the pumping characteristics. In the case of normal leads, the pumped current exhibits a sub-linear increase for increasing pumping frequency and its dependence on the phase-difference between the pumping field deviates from that of the adiabatic regime. In the ferromagnetic case, spin and charge currents behave differently as a function of the phase difference, allowing to obtain pure spin pumping without net charge transfer, in sharp contrast to the adiabatic regime [1].

[1] J. Splettstoesser, M. Governale, and J. König, Phys. Rev. B **77**, 195320 (2008).

TT 11.4 Mon 14:45 HSZ 301

Resonant spin pumping with spin-orbit coupling — Markus Jerger[1], •Valentina Brosco[1], Pablo San José[2,1], Gergely Zarand[3], Alexander Shnirman[4], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik , Universität Karlsruhe, Karlsruhe, Germany — [2]Department of Physics, Lancaster University, Lancaster, United Kingdom — [3]Theoretical Physics Department, Budapest University of Technology and Economy, Budapest, Hungary — [4]Institut der Theorie der Kondersierten Materie, Universität Karlsruhe, Karlsruhe, Germany

Adiabatic particle transport in a periodic potential cyclically modulated in time was first proposed by Thouless [1]. Since then, due to to its fundamental interest in relation with the theory of geometric phases and to possible applications in metrology, charge pumping has been studied in a variety of mesoscopic devices. More recently, various authors considered pumping of spin in semiconductor nanostructures.

In the present work we discuss spin pumping in a quantum dot with spin-orbit coupling using a scattering matrix approach [2]. First, we present a general analysis of spin and charge pumping based on the symmetries of the scattering matrix. Then, we focus on spin pumping in the resonant transport regime, we calculate explicitly the pumped spin and charge for some specific pumping cycles and we analyze the conditions to have pure spin currents.

[1] D. J. Thouless, Phys. Rev. B **27**, 6083 (1983).

[2] M. Büttiker, H. Thomas and A. Prêtre Z. Phys. B **94**, 133 (1994);

P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).

TT 11.5 Mon 15:00 HSZ 301

A time dependent approach to obtain transmission coefficients of multi-terminal devices — •Christoph Kreisbeck[1], Viktor Krückl[1], and Tobias Kramer[1,2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

We are interested in the transport behavior of semiconductor nanostructures, where we particularly focus on multi-terminal devices. The conductivity through these devices can be described theoretically within the Landauer-Büttiker formalism, which connects conductance-voltage characteristics with scattering matrices. To obtain the latter we introduce a time dependent approach, which proves to be a very efficient way to calculate transmission coefficients numerically. Moreover this method can go beyond Landauer-Büttiker. This means that we do not have to restrict ourself to asymptotic channels anymore, but we can study localised electron sources as well.

15 min. break

TT 11.6 Mon 15:30 HSZ 301

Dephasing due to phonons in a double dot Aharonov-Bohm interferometer — •Björn Kubala[1], David Roosen[2], Florian Marquardt[1], and Walter Hofstetter[2] — [1]Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, 80333 Munich, Germany — [2]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main, Germany

We investigate an Aharonov-Bohm interferometer consisting of two quantum dots coupled in parallel to two lead electrodes and to a common Einstein phonon mode. Without coupling to phonons transport of noninteracting electrons is fully coherent and the interferometer can be tuned to complete destructive interference even for finite applied bias. If phonons couple differently to the electrons on the two dots, which-path infomation is transferred to the phononic bath and the electronic coherence is diminished. It is only this dephasing due to phonons which enables transport, making the device ideal for studying decoherence issues. In this talk, we focus on results from Keldysh diagrammatic perturbation theory, which are complemented by studies using the numerical renormalization group.

TT 11.7 Mon 15:45 HSZ 301

1D to 0D crossover of decoherence time in small mesoscopic rings — •Maximilian Treiber[1], Oleg Yevtushenko[1], Florian Marquardt[1], Igor V. Lerner[2], and Jan von Delft[1] — [1]Physics Department, ASC, and CeNS, LMU, Theresienstrasse 37, 80333 Munich, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, United Kingdom

We study the decoherence time $\tau_\phi(T)$ in a disordered quasi 1D ring weakly coupled to leads, in the low temperature regime where decoherence is governed by electron interactions. We employ a path integral approach which is free of IR singularities and reproduces the known power-law dependence $\tau_\phi \sim T^{-a}$, where $a = 2/3$ or 1 for the diffusive ($\tau_\phi E_c \lesssim 1$, where E_c is the Thouless energy) [1] or ergodic ($\tau_\phi E_c \geq 1$) [2] regimes, respectively. By incorporating the Pauli principle into the Nyquist noise correlation function, thus excluding large energy transfers ($\omega \gtrsim T$), we are able to also describe the dimensional crossover of τ_ϕ from 1D to 0D as T is lowered below E_c, causing the exponent to change to $a = 2$. The $\sim T^{-2}$ dependence has been predicted before [3], but has so far eluded direct observation. We point out that in the ring geometry it is possible to measure it not only via the smooth part of the magnetoresistance but also via the amplitude of the Altshuler-Aronov-Spivak oscillations.

[1] B. L. Altshuler et al., J. Phys. C, **15**, 7367 (1982).
[2] C. Texier and G. Montambaux, Phys. Rev. B **72**, 115327 (2005); T. Ludwig and A. D. Mirlin, Phys. Rev. B **69**, 193306 (2005).
[3] U. Sivan et al., Europhys. Lett. **28**, 115 (1994).

TT 11.8 Mon 16:00 HSZ 301

Electron-Spin-Resonance (ESR) in Triple Quantum Dots — •Maria Busl[1], Rafael Sánchez[1,2], and Gloria Platero[1] — [1]ICMM, CSIC, Cantoblanco, E-28049 Madrid — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4

In the last years a big effort has been devoted to measure ESR in single and double quantum dots [1]. There, crossed DC and AC magnetic fields with a frequency resonant to the Zeeman splitting in the dots drive electrons to perform spin coherent rotations.

We analyze coherent spin rotations induced by an AC magnetic field in a DC biased triple quantum dot (TQD), both in linear and triangular configuration, filled with one and two extra electrons. We analyze the case where the DC magnetic field is homogeneous and the case where an inhomogeneous DC magnetic field yields to different Zeeman splittings within each dot.

We will discuss how coherent population trapping, which occurs in a TQD filled with one electron[2], is affected by the AC field. There, the electron can be forced to perform single spin rotations induced by the field. Those are stable against decoherence coming from the leads, once the electron drops in the so-called dark state. In the case of two extra electrons, we analyze spin blockade in the presence of the AC magnetic field.

[1] F. H. L. Koppens et al., Nature 442, 766 (2006)
[2] C. Emary, PRB 76, 245319 (2007)

TT 11.9 Mon 16:15 HSZ 301

Understanding energy-resolved spectroscopy of nonequilibrium Luttinger liquids — •So Takei, Mirco Milletari, and Bernd Rosenow — Max-Planck-Institute for Solid State Research

We theoretically analyze a system in which a measurement of an energy-resolved nonequilibrium electronic distribution can be used to gain an understanding on the relaxational properties of a Luttinger liquid (LL). The setup consists of a LL tunnel-coupled to two resonant levels, denoted source and probe, at two points separated by a distance L. The source, whose resonant level is tuned above the chemical potential of the LL, injects high energy electrons into the system. An energy-resolved measurement of the LL distribution is then achieved downstream with the probe by tuning its resonant level. An experimental realization of the setup can be achieved in the context of an edge state in the fractional quantum Hall regime for both the Laughlin sequence of filling fractions $\nu = 1/m$ and the hierarchical edge states with multiple edge excitations.

TT 11.10 Mon 16:30 HSZ 301

Magnetic field dependence of 0.7 Anomaly in Quantum Point Contacts: A Study Using the Functional Renormalization Group — •Florian Bauer and Jan von Delft — Arnold Sommerfeld Center for Theoretical Physics, Munich

We study the magnetic field dependence of the 0.7 anomaly of the conductance through a quantum point contact at zero temperature, using the functional renormalization group (fRG). We model a 1-D quantum wire using a tight-binding chain with short-ranged Coulomb interactions and a prescribed onsite potential to mimick the potential barrier caused by the 2-D constriction. Our fRG results qualitatively reproduce the experimentally observed magnetic field dependence of the conductance anomaly (splitting of the first conductance step into two substeps) and the shot noise. The resulting effective g-factor is strongly enhanced by interactions, in agreement with the experimental observation of anomalously large g factors.

TT 12: Correlated Electrons: Spin Systems and Itinerant Magnets 2

Time: Monday 14:00–16:00 Location: HSZ 304

TT 12.1 Mon 14:00 HSZ 304

Systematic derivation of generalized t-J models from Hubbard models away from half-filling — •Simone Hamerla[1] and Götz S. Uhrig[1,2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

Starting from a fermionic Hubbard model a generalized t-J model is constructed by eliminating charge fluctuations which change the number of double occupancies. The charge fluctuations are eliminated by a

systematic change of basis performed by self-similar continuous unitary transformations [1]. The proliferating terms are truncated according to their spatial extension. The derivation of a generalized t-J model is possible as long as the system is dominated by the local repulsion. In the present work, we focus on the Hubbard model on the linear chain and on the square lattice. There are two main goals: one is to test different choices of the infinitesimal generator, the other is to elucidate the influence of doping.

[1] A. Reischl, E. Müller-Hartmann, G. S. Uhrig, Phys. Rev. B 70, 245124

TT 12.2 Mon 14:15 HSZ 304

Dynamic Spin Excitations and Magnetism in the Hubbard Model — •Sebastian Schmitt — Lehrstuhl für Theoretische Physik II, TU Dortmund

The static and dynamic magnetic susceptibility of the Hubbard model is calculated within the dynamical mean field theory (DMFT) using the enhanced non-crossing approximation (ENCA) as impurity solver. The magnetic properties are discussed for various dopings, temperatures and lattices with and without frustration. Special emphasis is laid on the interpretation in terms of the two fundamental pictures of magnetism, i.e. Stoner-type magnetism of itinerant electronic excitations and Heisenberg spin-magnetism of localized magnetic moments. The transition between these two opposing pictures is discussed. An interesting reentrant behavior is observed for the antiferromagnetic Néel temperature in the intermediate coupling region. Additionally, a dispersionless collective mode is observed in the dynamic magnetic susceptibility for large values of the Coulomb repulsion at very low temperatures, indicating a localized singlet-triplet excitation connected with the breakup of local Kondo-singlets.

TT 12.3 Mon 14:30 HSZ 304

The frustrated ferromagnetic $S = 1/2$ Heisenberg chain in a magnetic field – How multipolar spin correlations emerge from magnetically ordered states — Julien Sudan[1], Andreas Lüscher[1], and •Andreas M. Läuchli[2] — [1]IRRMA, EPF Lausanne, Switzerland — [2]MPI für Physik komplexer Systeme, Dresden, Germany

We present the phase diagram of the frustrated ferromagnetic $S = 1/2$ Heisenberg J_1-J_2 chain in a magnetic field, obtained by large scale exact diagonalizations and density-matrix-renormalization-group simulations. A vector chirally ordered state, metamagnetic behavior and a sequence of spin multipolar Luttinger liquid phases up to hexadecupolar order are found. Starting from classical considerations, we point out that various multipolar correlations are imprinted in a magnetic state and that they can survive the onset of frustration and quantum fluctuations which destroy the convention al magnetic order. Our results also shed new light on previously discovered spin multipolar phases in two-dimensional $S = 1/2$ quantum magnets in a magnetic field. We conclude by presenting numerical results on the dynamical spin structure factor in the various phases which are valuable in identifying multipolar phases in experiments.

TT 12.4 Mon 14:45 HSZ 304

Ferromagnetic mixed-spin chain model for $MnNi(NO_2)_4(en)_2$ (en = ethylenediamine) — •Andreas Honecker[1], Wolfram Brenig[2], Stefan Süllow[3], Matthias Bleckmann[3], and Ralf Feyerherm[4] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, TU Braunschweig — [3]Institut für Physik der Kondensierten Materie, TU Braunschweig — [4]Helmholtz-Zentrum Berlin für Materialien und Energie

$MnNi(NO_2)_4(en)_2$, en = ethylenediamine contains ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. Two energy scales are observed in the field-dependent specific heat of this compound. This behavior is attributed to the existence of an acoustic and an optical mode in the spin wave dispersion. Parameters for a realistic model have been derived from the high-temperature behavior of the magnetic susceptibility.

Here we present numerical results for the specific heat obtained by exact diagonalization and Quantum-Monte-Carlo simulations for the alternating spin chain model. $MnNi(NO_2)_4(en)_2$ orders antiferromagnetically at low temperatures in zero magnetic field, demonstrating relevant antiferromagnetic interchain coupling. This interchain coupling is included in the numerical treatment at the mean-field level.

15 min. break

TT 12.5 Mon 15:15 HSZ 304

Quasiparticle Renormalization of Bulk Conduction Band States in a Ferromagnet at High Binding Energies — •A. Hofmann[1], X. Y. Cui[2], J. Schäfer[1], S. Meyer[1], P. Höpfner[1], L. Patthey[2], E. Rotenberg[3], J. Bünemann[4], F. Gebhard[4], T. Ohm[5], W. Weber[5], and R. Claessen[1] — [1]Physikal. Institut, Universität Würzburg — [2]Paul-Scherrer-Institut, Villigen — [3]Lawrence Berkeley Nat. Laboratory — [4]Universität Marburg — [5]TU Dortmund

Many-body effects in metals can often be captured within the quasiparticle picture, where bare electrons become dressed with bosonic excitations. Angle-resolved photoemission (ARPES) is the probe of choice to detect such energy renormalization. Beyond electron-phonon coupling one expects interaction with spin excitations, which was identified in *surface* states of Fe(110) [1]. For *bulk* states, symmetry planes of k-space yield the desired hole spectral function.

By high-resolution ARPES we have studied the quasiparticle spectra of the ferromagnet Ni for binding energies up to 500 meV. Using a Gutzwiller calculation as reference, we find significant renormalization in the 250-300 meV range, as identified for magnetic bulk bands for the first time. The self-energy is well described within an electron-magnon coupling model, consistent with neutron scattering. The results also relate to a recent theoretical model [2], which describes kinks in correlated systems as transition between different renormalization regimes.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **92**, 097205 (2004).

[2] K. Byczuk *et al.*, Nature Phys. **3**, 168 (2007).

TT 12.6 Mon 15:30 HSZ 304

Collective spin-excitations in Cu L and O K edge Resonant Inelastic X-ray Scattering from $Sr_{14}Cu_{24}O_{41}$ — •Thorsten Schmitt[1], Justina Schlappa[1], F. Vernay[1], V. Strocov[1], V. Ilakovac[2], B. Thielemann[1], H. Ronnow[1], J. Mesot[1], B. Delley[1], and L. Patthey[1] — [1]Paul Scherrer Institut, Villigen PSI, Switzerland — [2]UPMC, Paris, France

The spin-ladder / spin-chain compound $Sr_{14}Cu_{24}O_{41}$ is a low-dimensional spin system, which is known for its complex interplay between charge and spin degrees of freedom. One of the subsystems is formed by 2-leg ladders Cu_2O_3, which have the properties of a spin liquid with a finite spin gap [1]. Resonant inelastic X-ray scattering (RIXS) is a powerful probe of the electronic ground state and the low-energy excitation spectrum of transition-metal oxides, being directly sensitive to the valence electron configuration [2]. Using RIXS at the Cu L_3 and O K edge of $Sr_{14}Cu_{24}O_{41}$ [1,2] we observe collective spin-excitations from the ladders, which we assign to two-triplon modes [3]. At the Cu L_3 resonance the dispersion of the modes was mapped out depending on the momentum transfer with excellent sensitivity over almost the entire first Brillouin-zone, in contrast to inelastic neutron scattering [4]. Site-sensitive RIXS at the O K edge of the chain- and ladder-subsystems give insight into the character of the holes.

[1] T. Vuletic et al., Physics Reports 428, 169-258 (2006).

[2] A. Kotani and S. Shin, Rev. Mod. Phys. 73, 203 (2001).

[3] K. P. Schmidt and G. S Uhrig. Mod. Phys. Rev. Lett. 90, 227204 (2003).

[4] S. Notbohm et al., Phys. Rev. Lett. 98, 027403 (2007).

TT 12.7 Mon 15:45 HSZ 304

Orbitons and bi-orbitons in YVO_3 — •Luis Mäder[1], Eva Benckiser[1,2], Giacomo Ghiringhelli[3], Marco Moretti[3], Graeme R. Blake[4], Nandang Mufti[4], A. Agung Nugroho[4,5], Thomas T. M. Palstra[4], Maurits Haverkort[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung

The aim of the project is the unambiguous observation of a novel kind of elementary excitations in a solid, namely orbitons, propagating orbital excitations. In an orbitally ordered state, one expects that exchange interactions between orbitals on neighbouring sites give rise to a significant dispersion of the orbital excitations. These orbitons are analogous to spin waves in a magnetically ordered state.

Orbital exchange interactions are expected to be strong in the Mott insulator YVO_3.

Here, we report on the observation of orbital excitations in YVO_3 by means of high-resolution resonant inelastic x-ray scattering (RIXS) across the V $L_{3,2}$ (V $2p \rightarrow$ V $3d$) and O K (O $1s \rightarrow$ O $2p$) edges with the new SAXES beamline at the PSI, Villigen. Due to the excellent resolution of 60-70 meV, we are able to resolve the intra-t_{2g} excitations, spin-flip excitations within the t_{2g} shell, and excitations into the e_g levels, in excellent agreement with our recent optical data [1].

Moreover, we find evidence for a bi-orbiton excitation. Finally, our data show that SAXES in principle should allow to study the orbital excitations as a function of the wave vector k.

[1] E. Benckiser *et al.*, New J. Phys. **10**, 053027 (2008).

TT 13: Focussed Session: Superconducting Quantum Circuits

Time: Tuesday 9:30–12:30 Location: HSZ 03

Invited Talk TT 13.1 Tue 9:30 HSZ 03

Photons, Qubits and Computers - A Quantum Mechanics Lab on a Chip — •Andreas Wallraff — Department of Physics, ETH Zurich, CH-8093 Zurich, Switzerland

In our lab we experimentally investigate the interaction of matter and light on the level of single quanta. Our approach, known as circuit quantum electrodynamics [1], combines ideas of atomic physics, quantum optics and solid state physics to perform state of the art quantum mechanics experiments on a single chip. This is achieved by coupling single photons stored in high quality microwave frequency resonators to fully controllable superconducting two-level systems (qubits) realized in macroscopic electronic circuits. In particular, we have recently observed the formation of qubit/light molecules involving one, two or three photons [2], where we probe the quantum nonlinearity of the qubit/field interaction. This experiment unambiguously demonstrates that the radiation field in the on-chip cavity is quantized. We have also performed quantum optics experiments with no photons at all. In this situation, i.e. in pure vacuum, we have been able to resolve the non-resonant interaction of a qubit with the cavity vacuum fluctuations [3]. This interaction leads to a renormalization in the qubit transition frequency, known as the Lamb shift. The high degree of control achievable over a collection of two-level systems and their interactions also renders the circuit QED architecture attractive for quantum information processing.

[1] A. Wallraff et al., Nature (London) 431, 162 (2004).
[2] J. Fink et al., Nature (London) 454, 315 (2008).
[3] A. Fragner et al., Science 322, 1357 (2008).

Topical Talk TT 13.2 Tue 10:00 HSZ 03

Two-photon probe of the Jaynes-Cummings model and controlled symmetry breaking in circuit QED — Frank Deppe[1], Matteo Mariantoni[1], Edwin P. Menzel[1], •Achim Marx[1], Rudolf Gross[1], S. Saito[2], K. Kakuyanagi[2], H. Tanaka[2], K. Semba[2], T Meno[3], H. Takayanagi[4], and E. Solano[5] — [1]Walther-Meissner-Institut and TU München, Germany — [2]NTT Basic Research Laboratories, NTT Corp., Japan — [3]NTT Advanced Technology, NTT Corp., Japan — [4]Tokyo University of Science and International Center for Materials Nanoarchitectronics, Japan — [5]Universidad del País Vasco - Euskal Herriko Unibertsitatea, Spain

Superconducting qubits behave as artificial two-level atoms. Coupling them to on-chip microwave resonators has given rise to the field of circuit quantum electrodynamics. In this work, we report on the observation of key signatures of a two-photon driven Jaynes-Cummings model, which unveils the upconversion dynamics of a superconducting flux qubit coupled to an on-chip resonator. Our experiment and theoretical analysis show clear evidence for the coexistence of one- and two-photon driven level anticrossings of the qubit-resonator system. This results from the controlled symmetry breaking of the system Hamiltonian, causing parity to become a not well-defined property. Our study provides deep insight into the interplay of multiphoton processes and symmetries in a qubit-resonator system. We ackowledge support from SFB 631, NIM, CREST-JST, JSPS-KAKENHI(18201018) and MEXT-KAKENHI(18001002), EuroSQIP, and the Ikerbasque Foundation.

Topical Talk TT 13.3 Tue 10:30 HSZ 03

Landau-Zener Transitions in Qubit-Oscillator Settings — •Sigmund Kohler — Institut für Physik, Universität Augsburg, 86135 Augsburg

The coupling between a qubit and a mode of a transmission line induces Landau-Zener transitions of the qubit upon switching the gate voltage or the magnetic flux that penetrates the superconducting loop. The adiabatic energies of this system are characterized by multiple exact and avoided level crossings for which the usual two-level Landau-Zener formula is no longer applicable. We derive selection rules for the multi-level transitions and present an exact expression for the corresponding transition probabilities [1,2]. Applications include quantum state preparation like single-photon generation and the controllable creation of qubit-oscillator entanglement. If the circuit is driven by a rf signal, the phase of the reflected signal depends on the state of the qubit. We discuss the possibility of monitoring Landau-Zener transitions in that way. A natural generalization addresses the coupling of the qubit to a bath of harmonic oscillator. This defines the dissipative Landau-Zener problem which recently gained interest in the context of adiabatic quantum computation. We derived an exact solution of this problem in the zero-temperature limit [3].

[1] K. Saito *et al.*. Europhys. Lett. **76**, 22 (2006).
[2] D. Zueco, P. Hänggi, and S. Kohler, New. J. Phys. **10**, 115012 (2008).
[3] M. Wubs *et al.*, Phys. Rev. Lett. **97**, 200404 (2006).

15 min. break

Topical Talk TT 13.4 Tue 11:15 HSZ 03

Experiments on the quantum of heat conductance — •Jukka Pekola[1], Matthias Meschke[1], Andrey Timofeev[1], Wiebke Guichard[2], Meri Helle[1], and Mikko Möttönen[1,3] — [1]Low Temperature Laboratory, Helsinki University of Technology, Finland — [2]Institut Neel, C.N.R.S., Grenoble, France — [3]Department of Applied Physics, Helsinki University of Technology, Finland

The fundamental limit to transmit heat via a single channel is governed by the quantum of thermal conductance. This has been demonstrated in experiments on both phonons [1,2] and electrons [3]: here we present two experiments [4,5] on this phenomenon based on electromagnetic coupling (photons). In the first experiment tunable electric impedance is used to modulate the radiated heat between two resistors at different temperatures in a superconducting micro-circuit. In the second experiment we demonstrate electronic refrigeration at the quantum limit using superconductor-normal metal tunnel junctions. We discuss the limits of classical and quantum heat exchange in an electrical circuit.

[1] K. Schwab, E. A. Henriksen, J. M. Worlock, M. L. Roukes, Nature 404, 974 (2000).
[2] C. S. Yung, D. R. Schmidt, A. N. Cleland, Appl. Phys. Lett. 81, 31 (2002).
[3] O. Chiatti, J. T. Nicholls, Y. Y. Proskuryakov, N. Lumpkin, I. Farrer, D. A. Ritchie, Phys. Rev. Lett. 97, 056601 (2006).
[4] M. Meschke, W. Guichard, J. P. Pekola, Nature 444, 187 (2006).
[5] A.V. Timofeev, M. Helle, M. Meschke, M. Möttönen, J.P. Pekola, submitted (2008).

Topical Talk TT 13.5 Tue 11:45 HSZ 03

Preparation of arbitrary quantum states in a microwave resonator — •Max Hofheinz, Haohua Wang, Markus Ansmann, Radoslaw Bialczak, Erik Lucero, Matthew Neeley, Aaron O'Connell, Daniel Sank, James Wenner, John Martinis, and Andrew Cleland — University of California, Santa Barbara, USA

Two-level systems, or qubits, can be prepared in arbitrary quantum states with exquisite control, just using classical electrical signals. Achieving the same degree of control over harmonic resonators has remained elusive, due to their infinite number of equally spaced energy levels. Here we exploit the good control over a superconducting phase qubit by using it to pump photons into a high-Q coplanar wave guide resonator and, subsequently, to read out the resonator state. This scheme has previously allowed us to prepare and detect photon number states (Fock states) in the resonator [1]. Using a generalization of this scheme [2] we can now create arbitrary quantum states of the photon field with up to approximately 10 photons. We analyze the prepared states by mapping out the corresponding Wigner function, which is the phase-space equivalent to the density matrix and provides a complete description of the quantum state.

[1] MH *et al.* Nature **454**, 310 (2008)
[2] Law, Eberly. Phys. Rev. Lett **76**, 1055 (1996)

TT 13.6 Tue 12:15 HSZ 03

Phase diffusion in single-qubit lasers — •Stephan André[1,2],

Valentina Brosco[1,2], Alexander Shnirman[2,3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

Recent experiments explored the dynamics of superconducting qubits, playing the role of artificial atoms, coupled to quantum electrical resonators. Single-qubit lasers were realized by creating a population inversion in the qubit [1]. In contrast to conventional lasers, single-qubit lasers are characterized by a strong qubit-oscillator coupling and a richer noise spectrum for the qubit.

We theoretically investigate the spectral properties of single-qubit lasers, focussing on the effects of the strong coupling and of 1/f-noise [2]. Specifically, we show that low-frequency charge fluctuations can explain the inhomogeneous broadening of the spectrum observed in the experiment.

[1] O. Astafiev *et al.*, Nature **449**, 588 (2007)
[2] S. André *et al.*, arXiv:0807.4607 (2008)

TT 14: Superconductivity: Non-Cuprate Non-Ferropnictide Superconductors

Time: Tuesday 9:30–12:15 Location: HSZ 105

TT 14.1 Tue 9:30 HSZ 105

First principles study of Al and C-doped MgB_2: evolution of two gaps and critical temperature — •Omar de la Peña-Seaman[1,2], Romeo de Coss[2], Klaus-Peter Bohnen[1], and Rolf Heid[1] — [1]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, Germany — [2]Department of Applied Physics, Cinvestav-Merida, Mexico

We have studied the electron-phonon and superconducting properties of the $Mg_{1-x}Al_xB_2$ and $MgB_{2(1-x)}C_{2x}$ alloys within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloys. For both systems, the Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated in the two band model (σ,π) for several concentrations until x(Al) = 0.55 and x(C) = 0.175. Using the calculated $\alpha^2_{ij}F(\omega)$ and a diagonal expression for the Coulomb pseudopotential matrix, μ^*, we solved numerically the Eliashberg gap equations in the two band model without interband scattering. We reproduce the experimental decreasing behavior of $\Delta_\sigma(x)$, $\Delta_\pi(x)$, and $T_c(x)$ for both alloy systems. The role of the interband scattering in the observed behavior of the superconducting gaps and T_c in the Al- and C-MgB_2 alloys is discussed.

TT 14.2 Tue 9:45 HSZ 105

Electronic Raman scattering in non–centrosymmetric superconductors — •Ludwig Klam[1], Dietrich Einzel[2], and Dirk Manske[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Since their recent discovery, non–centrosymmetric superconductors (NCS) form a rapidly growing field of research and represent a completely new class of superconductors which was believed for a long time not to exist at all. We formulate a theory for the polarization–dependence of the electronic (pair–breaking) Raman response for NCS in the clean limit at zero temperature. Possible applications include the systems $CePt_3Si$ and $Li_2Pd_xPt_{3-x}B$ which reflect the two important classes of the involved spin–orbit coupling.

We provide analytical expressions for the Raman vertices for these two classes and calculate the polarization–dependence of the electronic spectra. We predict a two–peak structure and different power laws with respect to the unknown relative magnitude of the singlet and triplet contributions to the superconducting order parameter, revealing a large variety of characteristic fingerprints of the underlying condensate.

TT 14.3 Tue 10:00 HSZ 105

Electronic structure of $SrPt_4Ge_12$: a study by soft x-ray photoelectron spectroscopy and band structure calculations — •Jan Gegner[1], David Regesch[1], Helge Rosner[2], Walter Schnelle[2], Roman Gumeniuk[2], Andreas Leithe-Jasper[2], Hidenori Fujiwara[1], Tim Haupricht[1], H. -H. Hsieh[3], H. -J. Lin[4], C. T. Chen[4], Alim Ormeci[2], Juri Grin[2], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Chung Cheng Institute of Technology, National Defense University,Taoyuan, Taiwan — [4]National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan

We present a comparative study of the electronic structure of the superconducting skutterudite $SrPt_4Ge_{12}$ by means of soft x-ray photoelectron spectroscopy and full potential band structure calculations. Excellent agreement between the measured and the calculated valence spectra is observed, confirming the picture of rather localized, low lying Pt 5*d* states compared to Pt metal. This implicates that the states at the Fermi level stem predominantly from Ge 4*p* electrons. An analysis of the chemical bonding in $SrPt_4Ge_{12}$ based on the electron localizability indicator is given.

Invited Talk TT 14.4 Tue 10:15 HSZ 105

Evidence for a novel superconducting state in high magnetic fields — •Joachim Wosnitza — Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, Germany

In the so-called FFLO state, named after Fulde, Ferrell, Larkin, and Ovchinnikov, the superconducting state can survive even at high magnetic fields above the Pauli paramagnetic limit. The quasi-two-dimensional (2D) organic superconductors have been suggested as good candidates for exhibiting the FFLO state. When applying the magnetic field exactly parallel to the conducting layers the orbital pair breaking is greatly suppressed and the Pauli limit is reached. We performed high-resolution specific-heat and torque-magnetization experiments in magnetic fields up to 32 T for such 2D organic superconductors. In a very narrow region close to parallel orientation we observe additional anomalies below the upper critical field signalling the existence of an additional superconducting phase. The specific-heat data for κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ with T_c = 9.1 K show that the superconducting transition becomes first order for fields above 21 T indicating that the Pauli limit is reached. Below about 3 K, the upper critical field increases sharply and a second first-order transition appears within the superconducting phase. Our results give strong evidence for the realization of the FFLO state in organic superconductors.

Work done in cooperation with R. Lortz, B. Bergk, Y. Wang, A. Demuer, I. Sheikin, G. Zwicknagl, and Y. Nakazawa.

15 min. break

TT 14.5 Tue 11:00 HSZ 105

Doping effect on Pauli limited superconductor $CeCoIn_5$ — •Yoshi Tokiwa — I. Physik. Institut, Georg-August Universitat Gottingen, Friedrich-Hund Platz 1, 37077 Göttingen

We present a study on the proposed FFLO state in the strongly Pauli limited superconductor $CeCoIn_5$ by measuring specific heat of slightly Hg- and Sn-doped compounds, $CeCo(In_{1-x}Hg_x)_5$ and $CeCo(In_{1-x}Sn_x)_5$ with x from 0.01 to 0.08%. The high-field low-temperature (HFLT) superconducting (SC) phase exhibits an extreme sensitiveness to the doping, i. e., HFLT phase being suppressed by ∼0.05% of Hg-doping or ∼0.08% of Sn-doping. Our results suggest a possible relation between the characteristic length scale of HFLT phase and SC coherence length. Interestingly, the HFLT transition temperature T_{HFLT} increases with increasing Hg-doping concentration, while it decreases as Sn is doped. A plot of T_{HFLT} vs T_c at high fields with doping concentration as an implicit parameter shows a scaling of the two, $T_{HFLT} \propto T_c$. We conclude that these results imply SC origin of the HFLT state rather than antiferromagnetism.

This work has been done by the collaboration with R. Movshovich, F. Ronning, E. D. Bauer, J. D. Thompson, P. Papin, A. D. Bianchi, J. F. Rauscher, S. F. Kauzlarich and Z. Fisk.

TT 14.6 Tue 11:15 HSZ 105

Superconducting properties of hydrogen under pressure — Pierluigi Cudazzo[1], Gianni Profeta[1], •Antonio Sanna[2], Andrea Floris[2], Alessandra Continenza[1], Sandro Massidda[3], and E.K.U. Gross[2] — [1]CNISM Dipartimento di Fisica, Universita' degli studi dell'Aquila, L'Aquila Italy — [2]Institut fuer Theoretishe Physik Freie Universitaet, Berlin — [3]SLACS-INFM Dipartimento di Fisica Universita' degli Studi di Cagliari, Cagliari Italy

We present first-principles calculations of the superconducting properties of molecular metallic hydrogen under pressure[1], obtained within the density functional theory of superconductivity [2]. Our study is able to single out the features which drive the system towards superconductivity: mainly, a rich and complex Fermi surface and strongly coupled phonon modes driving the intra- or intermolecular charge transfer. We predict three-gap superconductivity and a critical temperature that rises with increasing pressure up to 242 K at 450 GPa. Our study clearly demonstrates that a very high superconducting critical temperature can be reached purely from electron-phonon and Coulombic electron-electron interactions, thus confirming Ashcroft's early speculations[3].

[1] P. Cudazzo *et al.*, Phys. Rev. Lett **100**, 257001 (2008).
M. Lüders *et al.*, Phys. Rev. B **72**, 024545 (2005).
M. A. L. Marques *et al.*, Phys. Rev. B **72**, 024546 (2005).
[2] L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett **60**, 2430 (1988).
[3] N. Ashcroft, Phys. Rev. Lett. **21** 1748 (1968).

TT 14.7 Tue 11:30 HSZ 105

Superconductivity in quasi-2D systems within the BCS approach: Predictions of high-T_c superconductivity in hydrogen-graphite system — •Nicolas Garcia and Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig

Using the BCS approach, the local density and phonon spectra we calculate the superconducting gap at $T = 0$ K for metalizing hydrogen in a 2D graphene system. The aim is to estimate the critical temperature in quasi 2D graphite-hydrogen system. The calculation is done as a function of the density of conduction electrons n induced by the hydrogen and their effective mass. The results indicate that for $n \sim 5{\times}10^{14}$ cm^{-2} and an effective mass equal to the free electron mass, the superconducting gap has a maximum of 40K with a Maxwell-like distribution as a function of n. The results provide a possible explanation for the recently reported granular superconducting-like behavior in graphite and multigraphene samples.

TT 14.8 Tue 11:45 HSZ 105

Functional renormalization for antiferromagnetism and superconductivity in the Hubbard model — •Simon Friederich — Institut fuer Theoretische Physik, Universitaet Heidelberg

Results of a renormalization group study for the 2-dimensional Hubbard model close to half-filling at finite temperature are presented. Bosonic degrees of freedom corresponding to antiferromagnetic and d-wave superconducting order are introduced, and flow equations for the corresponding coupling constants are deduced from an exact flow equation for the effective average action.

The influence of bosonic fluctuations on the onset of local antiferromagnetic oder is discussed. At low enough temperatures and close to half-filling the discrete symmetry of the lattice is broken and incommensurate antiferromagnetic fluctuations dominate. The phase diagram is shown for the parameter regime close to half-filling in the presence of vanishing as well as non-vanishing next-to-nearest-neighbor hopping t'.

Finally, the potential emergence of d-wave superconducting order at larger distances from half-filling is discussed.

TT 14.9 Tue 12:00 HSZ 105

Discontinuity of capacitance at the onset of surface superconductivity — •Klaus Morawetz[1,2], Pavel Lipavsky[3,4], and Jiri Mares[4] — [1]Forschungszentrum Dresden-Rossendorf, PF 51 01 19, 01314 Dresden, Germany — [2]International Center for Condensed Matter Physics, 70904-910, Brasília-DF, Brazil — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic

The effect of the magnetic field on a capacitor with a superconducting electrode is studied within the Ginzburg-Landau approach. It is shown that the capacitance has a discontinuity at the onset of the surface superconductivity which is expressed as a discontinuity in the penetration depth of the electric field into metals. This new effect establishes a macroscopic signal of the onset of superconducting correlations. This discontinuity is observable with recent bridges for both conventional and high-T_c superconductors.

Phys. Rev. B 78 (2008) 054525-1-13

TT 15: Correlated Electrons: Metal-Insulator Transition 2

Time: Tuesday 9:30–13:00 Location: HSZ 301

TT 15.1 Tue 9:30 HSZ 301

Indications for a line of continuous phase transitions at finite temperatures connected with the apparent metal-insulator transition in two-dimensional disordered systems — •Arnulf Möbius — Leibniz Institute for Solid State and Materials Research IFW Dresden, PO Box 270116, D–01171 Dresden, Germany

In a recent experiment, Lai and coworkers studied the apparent metal-insulator transition of a Si quantum well structure tuning the charge carrier concentration n, see [1]. They observed linear temperature dependences of the conductivity $\sigma(T, n)$ around the Fermi temperature and found that the corresponding $T \to 0$ extrapolation $\sigma_0(n)$ exhibits a sharp bend just at the MIT.
Here, reconsidering data from [1], it is shown that this sharp bend is related to a peculiarity of $\sigma(T = \text{const}, n)$ clearly detectable in the whole T range up to 4 K, the highest measuring temperature in [1]. Since this peculiarity seems not to be smoothed out with increasing temperature, it may indicate a sharp continuous phase transition between the regions of apparent metallic and activated conduction to be present at finite temperature. Hints from other investigations of such a behavior are discussed. Finally, a scaling analysis illuminates similarities to previous experiments and provides understanding of the shape of the peculiarity and of sharp peaks found in $\mathrm{d}\log_{10}\sigma/\mathrm{d}n$ as function of n. Details of this study are given in [2].

[1] K. Lai, W. Pan, D.C. Tsui, S. Lyon, M. Mühlberger, and F. Schäffler, Phys. Rev. B **75**, 033314 (2007).
[2] A. Möbius, Phys. Rev. B **77**, 205317 (2008).

TT 15.2 Tue 9:45 HSZ 301

Scanning tunneling spectroscopy across the insulator-to-metal transition in $La_{0.67}Ca_{0.33}MnO_3$ thin films — •Silvia Seiro[1,2], Yanina Fasano[2,3], Ivan Maggio-Aprile[2], Edmond Koller[2], Rolf Lortz[2,4], and Øystein Fischer[2] — [1]MPI-CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]DPMC-University of Geneva, Quai Ernest-Ansermet 24, 1211 Geneva, Switzerland — [3]Centro Atómico Bariloche, Av. E. Bustillo 9500, 8400 S. C. de Bariloche, Argentina — [4]Department of Physics, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong

We present the temperature evolution of scanning tunneling spectra of $La_{0.67}Ca_{0.33}MnO_3$ thin films across the insulator-to-metal transition. A depletion in normalized conductance is observed over an energy range of a few hundred meV around the Fermi level. This depletion globally narrows upon cooling but is still present in the metallic phase. The link to macroscopic transport behavior is provided by the tunnel conductance at zero bias, which decreases upon cooling in the insulating phase, reaches a minimum close to the insulator-to-metal transition temperature and increases on cooling in the metallic phase. These results are interpreted in terms of dynamical short-range antiferromagnetic/charge order correlations.

TT 15.3 Tue 10:00 HSZ 301

Realistic model Hamiltonians for correlated organics — •Erik Koch — Institut für Festkörperforschung und Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

For a description of strongly correlated materials we have to resort to model Hamiltonians. These generalized Hubbard models have to be simple enough that they can be treated by non-perturbative many-

body approaches, yet complex enough to capture the specifics of real materials. We discuss how to derive such realistic model Hamiltonians for molecular crystals starting ab-initio. We focus in particular on the calculation of screened Coulomb matrix elements for which we use a two-step approach: treating intra-molecular screening with density-functional theory, while describing inter-molecular screening via a lattice of distributed polarizabilities. We discuss the surprising screening effects that appear in highly polarizable lattices and present model Hamiltonians for quasi one- and two-dimensional organics.

TT 15.4 Tue 10:15 HSZ 301

How frustrated is the charge transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ at ambient and elevated pressures? A first principles investigation. — •Harald O. Jeschke, Hem C. Kandpal, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The charge transfer salt κ-(BEDT-TTF)$_2$Cu(CN)$_3$ has been intensely discussed as it possibly represents a realization of a 2D quantum spin liquid. We employ first principles calculations to shed light on the underlying Hamiltonian. We carefully prepare equilibrium structures at ambient and elevated pressure using constant pressure Car Parrinello ab initio molecular dynamics calculations on the basis of the projector augmented wave method. We determine the hopping parameters of the underlying Hubbard Hamiltonian using tight binding fits to the calculated band structures. We find that increasing pressure reduces the frustration of the model.

15 min. break

TT 15.5 Tue 10:45 HSZ 301

LDA+DMFT study of the Sn/Si(111)($\sqrt{3} \times \sqrt{3}$)R30° surface states — •Sergej Schuwalow, Lewin Boehnke, and Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

Experimental studies [1] and LDA+U calculations [2] for the Sn/Si(111)($\sqrt{3} \times \sqrt{3}$)R30° surface suggest a Mott-insulating surface state originating dominantly from strongly correlated Sn (5p) orbitals below about 70K. Interestingly, the Sn atoms form a 1/3 monolayer on an effective triangular lattice. Hence the issue of spin liquid physics may arise due to possible frustration effects.

In the scope of this work, we have first obtained an effective Hamiltonian for the surface states of this system in terms of maximally localized Wannier functions from LDA calculations. From there, we performed DMFT calculations for both a 1-band and a 3-band effective Hamiltonian to map out the temperature-dependent behavior of the spectral function close to the suggested metal-insulator transition and to investigate the importance of the different surface bands. In the case of the 3-band Hamiltonian, the full U matrix was used for the calculations. Finally, we compared the results of our dynamical approach to those obtained within the static LDA+U formalism.

[1] S. Modesti *et al.*, PRL **98**, 126401 (2007)
[2] G. Profeta and E. Tosatti, PRL **98**, 086401 (2007)

TT 15.6 Tue 11:00 HSZ 301

Metal-insulator transition in polymer surfaces modified by low-energy ion irradiation — •Yuri Koval, Irina Lazareva, and Paul Müller — Department for Physik, Universität Erlangen-Nürnberg, Germany

The surface of several polymers like polyimide, PMMA, or PET was graphitized by low-energy (0.15-1.5 keV) ion irradiation at different temperatures (150-700 K). Due to the small penetration depth of ions the thickness of conducting layers is substantially less than 10 nm. Depending on the energy of ions and the temperature of irradiation the sheet conductance can be changed from 10^{-11} S to 10^{-4} S. We show that with increase of the sample conductance the electric transport changes from variable range hopping to semi-metallic type.

Semi-metallic behavior was observed for samples with sheet conductances higher than the quantum conductance g. For samples with lower sheet conductance an exponential law $\sigma=\sigma_0\exp(-(T_0/T)^x)$ typical for variable range hopping transport was found. For samples with a power x=0.5 we have found a correlation between σ_0 and T_0 in the form $\sigma_0=\sigma_{00}\exp(T_0/T^*)^{0.5}$ with σ_{00} equal to the quantum conductance g. Analyzing the low temperature current-voltage characteristics, a similar correlation between the pre-exponential factor and the numerator in the exponent $j=j_0\exp(-(E_0/E)^{0.5})$ was observed, where j is the current density and E is the electric field.

TT 15.7 Tue 11:15 HSZ 301

Mott transitions at variable spin/orbital degeneracy — •Nils Blümer and Elena Gorelik — Institut für Physik, Universität Mainz, Mainz, Germany

The Mott transition between a metal and a paramagnetic insulator is central to the field of strongly correlated electron systems. Much insight into this phenomenon has been gained in numerical studies of the 1-band Hubbard model within dynamical mean-field theory (DMFT). In particular, the phase diagram and the behavior of characteristic observables (such as the effective mass) have been established with high precision - despite the lack of analytic solutions. The physics of multiorbital models is richer (including the possibility of orbital-selective Mott transitions), but also much more challenging.

However, exact analytical results have been derived for the SU(2M) symmetric Hubbard model (where all spins/orbitals are equivalent) in the limit of large band multiplicity $M \to \infty$ [1]. So far, these predictions have only been checked/complemented by self-energy functional calculations with one bath site per orbital [2]; this method has quite substantial errors in the 1- band case [3].

We present numerically exact multigrid Hirsch-Fye quantum Monte Carlo estimates of the phase boundaries at half filling and for up to $M = 8$ bands. We also derive scaling laws which predict the phase boundaries for arbitrary orbital degeneracy M with high accuracy.

[1] S. Florens et al., Phys. Rev. B **66**, 205102 (2002).
[2] K. Inaba et al., Phys. Rev. B **72**, 085112 (2005).
[3] K. Požgajčić, arXiv:cond-mat/0407172v1 (2004).

TT 15.8 Tue 11:30 HSZ 301

Mott transitions in the repulsive SU(3) invariant Hubbard model — •Elena Gorelik and Nils Blümer — Institut für Physik, Universität Mainz, Mainz, Germany

Ultracold fermions on optical lattices are nowadays one of the most exciting fields of both experimental and theoretical studies. They are often considered as model systems for simulating complex condensed matter phenomena. On the other hand, fermionic atoms have large hyperfine multiplets, out of which *several* states can be trapped simultaneously, leading to new degrees of freedom that are unavailable in solid state physics. This feature has attracted a lot of attention as an origin of possible exotic superfluid states in the case of an attractive on-site interaction [1,2].

Here we focus on another important phenomenon that has not yet been addressed within the multiflavor context - the Mott transition in the repulsive case, both as a function of the local interaction U and of the chemical potential. We present the results of a DMFT study, using the multigrid Hirsch-Fye quantum Monte-Carlo impurity solver [3], for the repulsive three flavor fermionic system. The peculiarities and experimentally accessible signatures of Mott transitions in such a multiflavor system are discussed in comparison with the two flavor/spin case.

[1] Á. Rapp et al., Phys. Rev. Lett. **98**, 160405 (2007).
[2] R. W. Cherng et al., Phys. Rev. Lett. **99**, 130406 (2007).
[3] N. Blümer, arXiv:0801.1222 (2008).

15 min. break.

TT 15.9 Tue 12:00 HSZ 301

Phase diagram of the SU(N) Hubbard-Heisenberg model on the honeycomb lattice — •Thomas C. Lang[1], Zi Yang Meng[2], Stefan Wessel[2], Fakher F. Assaad[1], and Alejandro Muramatsu[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Physik III, Universität Stuttgart, Germany

We investigate the phase diagram of the half-filled $SU(N)$ Hubbard-Heisenberg model on the honeycomb lattice in the self-adjoint totally antisymmetric representation. By means of the projective ($T = 0$) quantum Monte Carlo method we simulate the model on lattices ranging up to $L = 15$. For $U = 0$ and in the quantum limit, $N = 2$, decreasing t/J triggers a quantum phase transition from semi-metal to an antiferromagnetic-insulator with no apparent intermediate phase. With increasing symmetry N the Hubbard-Heisenberg model exhibits purely paramagnetic phases. Our aim is to study in detail the phase diagram as a function of N from the quantum limit to the saddle point $N \to \infty$.

TT 15.10 Tue 12:15 HSZ 301

Quantum Monte Carlo study of the half-filled Hubbard model on the honeycomb lattice — •Zi Yang Meng[1], Thomas C. Lang[2], Stefan Wessel[1], Fakher F. Assaad[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

Using projective ($T = 0$) quantum Monte Carlo we investigate the ground-state properties of the half-filled Hubbard model on a honeycomb lattice. Our results confirm previous numerical findings[1] that antiferromagnetic long-range order sets in above a value of $U/t \approx 4.5$. However, examining the quasiparticle gap and the spin gap, we obtain preliminary indications, that the Mott-transition from the semimetal to an insulator occurs at a value of $U/t \approx 3.5$. A separation of two phase transitions allows for the possibility of an intermediate phase between the semi-metal and the antiferromagnetic insulator – a scenario, that has been discussed in recent theoretical studies[2,3]. Further numerical work, aiming at testing such propoals is in progress.

[1] S. Sorella and E. Tosatti, Europhys. Lett. **19**, 699 (1992).

[2] M. Hermele, Phys. Rev. B **76**, 035125 (2007).

[3] B. Uchoa and A. H. C. Neto, Phys. Rev. Lett. **98**, 146801 (2007).

TT 15.11 Tue 12:30 HSZ 301

Magnetic field induced semimetal-to-canted-antiferromagnet transition on the honeycomb lattice — •Martin Bercx and Fakher Assaad — TP1, Universität Würzburg

It is shown that the semi-metallic state with point like Fermi surface of the two-dimensional honeycomb lattice is unstable towards a canted anti-ferromagnetic insulator upon application of an in-plane magnetic field. This instability is already present at the mean-field level; the magnetic field shifts in opposite directions the up and down spin cones thereby generating a finite density of states at the Fermi surface and perfect nesting between the up and down Fermi sheets. This prefect nesting triggers a canted anti-ferromagnetic insulating state. Those conclusions, based on mean-field arguments, are confirmed with projective Quantum Monte Carlo methods on lattices up to 12×12 unit cells.

TT 15.12 Tue 12:45 HSZ 301

First order Mott transition at zero temperature in two dimensions: Variational plaquette study — •Matthias Balzer[1], Michael Potthoff[1], Bumsoo Kyung[2], David Senechal[2], and A.-M.S. Tremblay[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]Département de physique and RQMP, Université de Sherbrooke, Québec, Canada

The nature of the metal-insulator Mott transition at zero temperature has been discussed for a number of years. Whether it occurs through a quantum critical point or through a first order transition is expected to profoundly influence the nature of the finite temperature phase diagram. We study the zero temperature Mott transition in the two-dimensional Hubbard model on the square lattice. Here we use the variational cluster approximation to embed a plaquette of four correlated sites and four or eight uncorrelated bath sites in the lattice. This takes into account the influence of antiferromagnetic short-range correlations. As the method is thermodynamically consistent and focuses on the optimization of a thermodynamical potential, it is ideally suited to distinguish between different phase diagram topologies. By contrast to single-site dynamical mean-field theory, the transition turns out to be first order even at zero temperature.

TT 16: Correlated Electrons: Low-dimensional Systems - Materials 1

Time: Tuesday 9:30–13:00 Location: HSZ 304

TT 16.1 Tue 9:30 HSZ 304

High field ESR study of the new low dimensional S=1/2 system: $Cu(NO_3)_2{\cdot}H_2O$ — •M. Yehia[1], E. Vavilova[1,2], V. Kataev[1], R. Klingeler[1], O. Volkova[3,4], E. Lapsheva[4], V. Shutov[4], O. Savelieva[4], A.N. Vasiliev[4], and B. Büchner[1] — [1]Institute for Solid State Physics, IFW Dresden, 01171 Dresden, Germany. — [2]Kazan Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia. — [3]Institute of Radiotechnics and Electronics, 125009 Moscow, Russia. — [4]Moscow State University, 119991 Moscow, Russia.

$Cu(NO_3)_2{\cdot}H_2O$ is a new low dimensional spin system based on transition metal nitrates. It contains two-dimensional $Cu^{2+}(S = 1/2)$ layers separated by water molecules. ESR, magnetic susceptibility, specific heat and NMR have been measured on single crystalline samples of $Cu(NO_3)_2{\cdot}H_2O$. Specific heat and magnetic susceptibility data imply a phase transition possibly of antiferromagnetic (AFM) nature at $T_N \sim 3.4$ K. However, no long range order is observed in the temperature dependence of ESR measurables. The temperature dependence of the electron spin dynamics has been investigated by NMR. Various spin gap excitations have been observed using high field ESR. We discuss these features by considering the ground state and magnetic excitations of the orthogonal spin-dimers network which is realized in the Cu-layers of this material.

TT 16.2 Tue 9:45 HSZ 304

Electron Spin Resonance in GdI_2H_x — •Georg Andreas Hilscher[1], Joachim Deisenhofer[1], Hans-Albrecht Krug von Nidda[1], Alois Loidl[1], Mikhail Ryazanov[2], Arndt Simon[2], and Reinhard K. Kremer[2] — [1]Experimentalphysik V, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany — [2]Max-Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

The spin dynamics of hydrogen-doped GdI_2H_x ($0 \leq x \leq 1$) have been investigated by electron spin resonance (ESR) spectroscopy. With rising hydrogen concentration the lattice constants of the hexagonal layered structure change: a decreases and c increases [1]. Furthermore, the ferromagnetic Curie temperature T_C, which for pristine GdI_2 lies at approximately 290 K, decreases and the system exhibits a spin-glass-like state for $x > 0.33$. For higher H concentrations the system remains paramagnetic down to 4 K [1]. From the ESR intensity we can estimate the dominant exchange coupling constant within the Gd layers for $x < 0.33$ using the model for the spin susceptibility proposed by Eremin *et al.* [2].

[1] M. Ryazanov, A. Simon, R. K. Kremer, H. Mattausch, Sol. State Chem. **178**, 2339 (2005).

[2] I. Eremin, P. Thalmeier, P. Fulde, R. K. Kremer, K. Ahn, A. Simon, Phys. Rev. B **64**, 064425 (2001).

TT 16.3 Tue 10:00 HSZ 304

Magnetic field-induced ordering in a metal-organic spin-1/2 dimer system – a candidate for a Kosterlitz-Thouless transition — •U. Tutsch[1], B. Wolf[1], M. Lang[1], T. Kretz[2], H.-W. Lerner[2], M. Wagner[2], S. Wessel[3], T. Saha-Dasgupta[4], H. Jeschke[5], and R. Valenti[5] — [1]Phys. Inst., Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany — [2]Inst. f. Anorg. Chemie, Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany — [3]Inst. f. Theor. Phys. III, Universität Stuttgart, D-70550 Stuttgart, Germany — [4]S.N. Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700098, India — [5]Inst. f. Theor. Phys., Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany

We have investigated the spin-1/2 metal-organic dimer system $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91) by means of high-resolution susceptibility measurements at very low temperatures ($0.04\ \text{K} \leq T \leq 0.5\ \text{K}$) and magnetic fields up to $B = 7.5$ T. The spins, located on the Cu^{2+} ions, are coupled into dimers by a hydroquinone-derived linker, giving rise to an *intra*-dimer exchange interaction of $J_1/k_B \approx 10$ K. As suggested by *ab initio* calculations, the *inter*-dimer couplings J_i have a quasi-two-dimensional (quasi-2d) character with a very weak interlayer coupling. Quantum Monte Carlo simulations for 2d and various strongly anisotropic 3d coupling schemes are used to model our susceptiblity data yielding clear signatures of a B-induced ordering phenomenon. A very good agreement is obtained for the 2d scenario, making TK91 a good candidate for the very rare phenomenon of a magnetic Kosterlitz-Thouless transition.

TT 16.4 Tue 10:15 HSZ 304

Crystal water induced switching of magnetic active orbitals in $CuCl_2$ — •Miriam Schmitt[1], Oleg Janson[1], Marcus

Schmidt[1], Stefan Hoffmann[1], Walter Schnelle[1], Stefan-Ludwig Drechsler[2], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW Dresden, Germany

Low dimensional transition metal compounds show an intimate interplay between the crystal structure and their magnetism. Nevertheless, it is a widespread belief that crystal water has just a moderate, renormalizing influence on the magnetic properties due to a modification of interactomic distances. In contrast, the dehydration of $CuCl_2{\cdot}2H_2O$ to $CuCl_2$ leads to a dramatic change in magnetic behavior and ground state – driving a classical example of a 3D antiferromagnet (T_N=4.3 K) to a quasi 1D system with long range order below T∼23 K. Combining electronic structure calculations based on DFT, model calculations and thermodynamical measurements we reveal the microscopic origin of this surprising behavior. Regarding our calculations $CuCl_2$ can be well described as a frustrated J_1–J_2 Heisenberg chain with ferromagnetic exchange J_1 and $J_2/J_1 \sim$ -1.5 predicting a helical ground state. The hydration of $CuCl_2$ flips the magnetically active orbitals, resulting in a fundamental change of the coupling regime. As $CuCl_2$ consists edge-shared Cu-Cl_4 plaquettes with the magnetically active orbital in the chain plane, $CuCl_2{\cdot}2H_2O$ forms its magnetically active orbitals out of the former chain plane resulting in isolated plaquettes arranged back to back. This new arrangement strongly reduces the former in-chain interactions yielding an almost isotropic 3D coupling.

TT 16.5 Tue 10:30 HSZ 304

Magnetocaloric effect near a B induced quantum critical point in an S = 1/2 antiferromagnetic Heisenberg chain — •Deepshikha Jaiswal-Nagar[1], Georg Hofmann[1], Yeekin Tsui[1], Katarina Remović-Langer[1], Ulrich Tutsch[1], Bernd Wolf[1], Andrey Profofiev[1,2], Wolf Assmus[1], Andreas Honecker[3], and Michael Lang[1] — [1]Phys. Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany — [2]Inst. f. Festkörperphys., TU Wien, 1040-Wien, Austria — [3]2 Inst. f. Theor. Physik, Georg-August-Universität at Göttingen, 37077, Göttimgen, Germany

The magnetocaloric effect (MCE), i.e., heating or cooling of a system under adiabatic conditions in response to an external magnetic field, is an important tool for exploring quantum critical points (QCP's), as it is expected to diverge at the QCP. The competition between different ground states at a QCP leads to an accumulation of entropy at the QCP at finite temperature and hence to a variety of interesting properties in thermodynamic quantities like the MCE. A one-dimensional spin S = 1/2 antiferromagnetic Heisenberg chain (AfHC) is quantum critical in magnetic fields up to the saturation field Bs, above which it undergoes a transition to a ferromagnetically polarized state. In this talk, we present MCE data on a metal-organic polymer system built from Cu2+ (S = 1/2) ions, which is shown to be a very good realization of an AfHC. We obtain field-induced temperature changes which are an order of magnitude larger than those of paramagnetic salts! Our data compare favorably with theoretical results based on exact diagonalization of finite systems.

TT 16.6 Tue 10:45 HSZ 304

Magnetic properties of a novel quasi-2D Cu(II)-trimer system — •Bernd Wolf[1], Katarina Removic-Langer[1], Eiken Haussühl[2], Leonore Wiehl[2], Francesca Sauli[3], Nils Hasselmann[3], Peter Kopietz[3], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, SFB/TR 49, D-60438 Frankfurt — [2]Institut für Geowissenschaften, Universität Frankfurt, D-60438 Frankfurt — [3]Institut für Theoretische Physik, Universität Frankfurt, SFB/TR 49, D-60438 Frankfurt

The rational design of low-dimensional quantum spin systems with novel exchange coupling topologies is of interest since it allows the testing of fundamental concepts in theoretical solid state physics. Up to now, only a few examples for 2D coupled-trimer systems are known. We have managed to synthesize a new magnetic Cu(II)-trimer system $2b{*}3CuCl_2{*}2H_2O$ (b = betaine), where the trimers form a quasi-2D quantum spin system with an unusual intralayer exchange coupling topology, which in principle supports ring-exchange processes. We discuss the structural aspects together with magnetic susceptibility and magnetization data. In addition, a theoretical model, enabling us to describe the magnetic properties over a wide temperature and field range is presented. The low-energy description and effective parameters are obtained from numerical calculations based on four coupled trimers. The model calculations indicate that for certain ranges of the inter-trimer coupling constants, which might be experimentally accessible, the low-energy properties of $2b{*}3CuCl_2{*}2H_2O$ will be dominated by non-trivial four-spin exchange processes.

TT 16.7 Tue 11:00 HSZ 304

Electronic structure and exchange coupling of a frustrated S=1/2 pyrochlore $Hg_2Cu_2F_6S$ — •Deepa Kasinathan[1], Klaus Koepernik[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Spin systems with geometric frustration have a macroscopic number of degenerate low lying states. An interesting question to answer for such kind of systems is: "Which state is chosen as the ground state at low T?" Our talk will focus on the pyrochlore compound $Hg_2Cu_2F_6S$ which exibits a perfectly cubic CuF_6 octahedral environment.[1] This is quite unusual for a Cu^{2+} ion which is normally in the 4+2 coordination. The lack of distortion for the CuF_6 octahedron leads to a 2-fold degenerate e_g band complex at the Fermi level. Since the system is insulating due to the presence of strong Coulomb repulsion, this 2-fold degeneracy is strongly disfavoured because it would lead to metallicity. Orbital or charge ordering can lift this degeneracy. Strong magnetic frustrations will also play a role in determining the ground state of this system due to the presence of 3D linkages of corner sharing Cu_4 tetrahedra. We will present results from density functional theory (DFT) calculations within the LDA and LDA+U methodology. We will discuss the role of total energies, hoppings and possible orbital ordering (visible in the spin density) in this compound.

[1]. S. Kawabata et al., J. Phys. Soc. Japan Vol 76, No.8, 084705 (2007).

15 min. break.

Invited Talk TT 16.8 Tue 11:30 HSZ 304

Two Dimensional Electron Gases at Oxide Interfaces — •Jochen Mannhart — Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Two-dimensional electron gases based on conventional semiconductors such as Si or GaAs have played a pivotal role in fundamental science and technology. The high mobilities achieved enabled the discovery of the integer and fractional quantum Hall effects and are exploited in high electron mobility transistors. Recent work has shown that 2-DEGs can also exist at oxide interfaces. These electron gases typically result from reconstruction of the complex electronic structure of the oxides, so that the electronic behavior of the interfaces may differ from the behavior of the bulk.

In the presentation I will provide an overview of our studies of the properties of these unusual electronic systems and explore whether electron gases at oxide interfaces have the potential to be used in nanoscale electronic devices.

TT 16.9 Tue 12:00 HSZ 304

The Two-Dimensional Electron Gas between $LaAlO_3$ and $SrTiO_3$: A Fascinating System for Electronic Devices — •Christoph Richter, Rainer Jany, Stefan Thiel, Christof Schneider, German Hammerl, and Jochen Mannhart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany

The conducting, two-dimensional electron gas that is formed at the interface between the band insulators $LaAlO_3$ and $SrTiO_3$ is characterized by remarkable fundamental properties and has therefore generated intense scientific interest. In the presentation we will demonstrate that this apparently fragile, ultrathin electronic system can be used to fabricate robust electronic devices.

We will report on field effect transistors that use the two- dimensional electron gas as drain source channel as well as on diodes with unique properties.

TT 16.10 Tue 12:15 HSZ 304

Profiling the interface electron gas of $LaAlO_3/SrTiO_3$ heterostructures by hard X-ray photoelectron spectroscopy — •G. Berner[1], M. Sing[1], K. Goss[1], A. Wetscherek[1], A. Müller[1], A. Ruff[1], S. Thiel[2], J. Mannhart[2], S.A. Pauli[3], C.W. Schneider[3], P.R. Willmott[3], and R. Claessen[1] — [1]Experimentelle Physik IV, Universität Würzburg — [2]Experimentelle Physik VI, Universität Augsburg — [3]Paul Scherrer Institut, CH-5232 Villingen, Switzerland

Oxide heterostructures are of special interest due to unexpected new physics occurring at the interface. One heavily discussed topic is the quasi-two-dimensional electron gas (2DEG), which emerges at the in-

terface of the two band insulators $LaAlO_3/SrTiO_3$, if at least 4 unit cells of $LaAlO_3$ are grown on TiO_2-terminated $SrTiO_3$. Moreover, both a magnetic and a superconducting phase at low temperatures have been reported for the ground state of the 2DEG. We have studied this buried interface by angle dependent hard x-ray photoemission spectroscopy (HAXPES), which is a powerful tool to get insight in both change in chemical state and vertical distribution of the additional charge at the interface. The distinct angle-dependence of the intensity ratio of the Ti^{3+} 2p and Ti^{4+} 2p core lines indicates that the thickness of the 2DEG is much smaller than the HAXPES probing depth of 4 nm. It is observed that the carrier density varies between differently prepared heterostructures and increases with increasing numbers of $LaAlO_3$ overlayers. Our results point to electronic reconstruction in the overlayer as driving mechanism for the 2DEG formation and is supportive for the recently observed 2D superconductivity.

TT 16.11 Tue 12:30 HSZ 304

Resonant soft x-ray scattering studies of buried interfaces — •Jochen Geck[1,2], Hiroki Wadati[2], Enrico Schierle[3], P. Kommissinskiy[4], L. Alff[4], D.G. Hawthorn[5], T. Higuchi[6], Y. Hikita[6], H.Y. Hwang[6], S.-W. Huang[7], D.J. Huang[7], H.-J. Lin[7], L.H. Tjeng[8], H.-H. Wu[7,8], E. Weschke[3], C. Schüssler-Langeheine[8], and G.A. Sawatzky[2] — [1]IFW Dresden, Germany — [2]University of British Columbia, Canada — [3]Helmholtz-Zentrum Berlin, Germany — [4]University of Technology Darmstadt, Germany — [5]University of Waterloo, Canada — [6]University of Tokyo, Japan — [7]National Synchrotron Radiation Research Center, Taiwan — [8]University of Cologne, Germany

Resonant soft x-ray scattering (RSXS) is a unique experimental tool to access the electronic properties of buried interfaces in heterostructures that contain transition metal oxides. In this contribution, studies of $SrTiO_3/LaAlO_3$, $SrTiO_3/(La,Ca)MnO_3$ and $NdGaO_3/(La,Ca)MnO_3$ interfaces are presented. Specifically, RSXS was employed to examine the electronic reconstruction of Ti 3d and O 2p valence states at the interfaces of $SrTiO_3/LaAlO_3$ superlattices. Similarly, we used resonant soft x-ray reflectivity to investigate the electronic structure at the interfaces of $SrTiO_3/(La,Ca)MnO_3$ and $NdGaO_3/(La,Ca)MnO_3$ thin film systems.

TT 16.12 Tue 12:45 HSZ 304

Ab initio Quantum Monte Carlo study of interlayer binding in graphitic nanostructures — •Norbert Nemec and Richard Needs — Dept. of Physics, University of Cambridge, UK

The electronic structure of graphitic systems is studied using ab initio quantum Monte Carlo methods implemented in the CASINO code. The diffusion Monte Carlo method allows the exact handling the long-ranged correlations responsible for the London dispersion forces that dominate the interlayer binding. The finite size errors caused by the limited volume of the simulation cell are reduced by a careful extrapolation to infinite size giving a reliable theoretical prediction of the interlayer binding of graphite and related nanostructures.

TT 17: Correlated Electrons: Quantum-Critical Phenomena 1

Time: Tuesday 14:00–16:15 Location: HSZ 03

TT 17.1 Tue 14:00 HSZ 03

Radiography of weakly ferromagnetic metals with polarized neutrons — •Michael Schulz[1,2], Peter Boeni[2], Elbio Calzada[1,2], Martin Muehlbauer[1,2], Andreas Neubauer[2], Christian Pfleiderer[2], and Burkhard Schillinger[1,2] — [1]FRM II, Garching, Germany — [2]E21, Physik Department TUM, Garching, Germany

The depolarization of a neutron beam passing through a ferromagnet crucially depends on the magnetic properties of the sample. Combining neutron depolarisation measurements with neutron radiography allows obtaining spatially resolved information about these properties. For measuring the depolarization, we have installed a longitudinal polarized beam setup at the ANTARES beamline consisting of ^3He polarizers and flat coil spin flippers. With this setup we have performed radiography with polarized neutrons in the weak itinerant ferromagnets $Pd_{1-x}Ni_x$ in order to determine the spatial distribution of the Curie temperatures T_C in the samples. The results show that the single crystals are rather inhomogeneous showing large variations in T_C. The data allows firstly to cut out small crystals with improved homogeneity for neutron scattering experiments and secondly to provide feedback for improving the growth techniques for the crystals. In the future we hope to use the potential of this method to map out magnetic domains across large volume samples.

TT 17.2 Tue 14:15 HSZ 03

Experimental Investigation of $Pd_{1-x}Ni_x$ at the border of Quantum Criticality — •Christian Franz[1], Christian Pfleiderer[1], Michael Schulz[1,2], Björn Pedersen[2], and Peter Böni[1] — [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

Polycrystals of the transition metal system $Pd_{1-x}Ni_x$ display ferromagnetic quantum criticality at a critical concentration x_c assumed to be well described by the SCR theory. We report comprehensive studies of the magnetic field and temperature dependence of the magnetization, resistivity, Hall effect and specific heat of Czochralsky grown $Pd_{1-x}Ni_x$ for four Ni-concentrations near x_c. Only the lowest Ni-concentration has crystallized as a single crystal, while the higher concentrations remained polycrystalline. For large values of x the typical behavior of a weakly ferromagnetic metal akin stoichiometric compounds like Ni_3Al, YNi_3 or $ZrZn_2$ is observed. In contrast, for low concentrations two regimes may be distinguished. Moreover, an analysis of the mode-mode coupling as inferred from the magnetic field dependence of the magnetization suggests that the it stays positive for all x as expected of quantum criticality. But the concentration dependence of the spontaneous moment indicates that $Pd_{1-x}Ni_x$ stays ferromagnetic on local scales even for very small concentrations. This suggests that quantum criticality in $Pd_{1-x}Ni_x$ is more complex then previously thought.

TT 17.3 Tue 14:30 HSZ 03

Polarized neutron tomography of Ni_3Al and Fe_2TiSn — •Andreas Neubauer[1], Michael Schulz[1], Christian Pfleiderer[1], Peter Böni[1], Anke Köhler[2], Nadja Wizent[2], and Günther Behr[2] — [1]Physik Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, PF270116, 01171 Dresden, Germany

The transition metal compounds Ni_3Al and Fe_2TiSn are weakly ferromagnetic metals, for which the magnetic properties are extremely sensitive to composition. We have attempted the growth of polycrystalline and single-crystal rods of these compounds with an UHV compatible image furnace. The polycrystalline starting material as well as the floating-zoned rods have been characterized by means of conventional bulk properties and EDX. As a new method we have additionally carried out polarized neutron tomography. The depolarization of the neutron beam proves to be extremely sensitive to tiny variations of the ferromagnetic transiton temperature, thus providing key information on the metallurgical phase diagram and the ideal growth conditions. The possible implications of our observations for the nature of quantum criticality in these compounds will be discussed.

TT 17.4 Tue 14:45 HSZ 03

Pressure Dependence of the Magnetization and Magnetotransport in Ferromagnetic Pr_5Si_3 — Christian Franz[1], •Stefan Legl[1], Christian Pfleiderer[1], Philipp Niklowitz[1], Dmitri Souptel[2], and Günther Behr[2] — [1]Physik Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, PF270116, 01171 Dresden, Germany

Pr_5Si_3 is an easy-plane ferromagnet with a comparatively low Curie temperature. We report the pressure dependence of the magnetization under pressures up to 18 kbar at magnetic fields up to 9 T. We have further measured the magnetotransport properties under pressure up to 60 kbar and magnetic field up to 14 T using a Bridgman pressure cell. Anomalous contributions to the Hall signal allow us to track the magnetic state up to the highest pressures studied. Our data suggest that the magnetic state of Pr_5Si_3 fairly abruptly develops an addi-

tional modulation for pressure in excess of $\sim$ 25 kbar, thus avoiding ferromagnetic quantum criticality.

15 min. break.

TT 17.5 Tue 15:15 HSZ 03

Evidence for Unusual Magnetic Order in Cubic FeGe beyond its Quantum Phase Transition — •Heribert Wilhelm[1], Alessandro Barla[2], Martin Forthaus[3], Rudolf Rueffer[4], Marcus Schmidt[5], and Mohsen Abd-Elmeguid[3] — [1]Diamond Light Source Ltd, Chilton, OX11 0DE, UK — [2]Experiments Division, CELLS-ALBA, E-08193 Bellaterra, Barcelona, Spain — [3]II. Physikalisches Institut, Universität zu Köln, 50937 Köln — [4]European Synchrotron Radiation Facility, BP220, F-38043 Grenoble, France — [5]Max Planck Institut für Chemische Physik fester Stoffe, 01187 Dresden

Transport measurements on the cubic modification of FeGe under high pressure have shown that the long-wavelength helical order (T_C = 280K, at $p = 0$) is suppressed at a critical pressure $p_c \approx$ 19GPa [1]. The metallic ground state persisting above p_c can be described by band-structure calculations if zero-point motion is included. However, the electrical resistivity shows that the ground state can not be described by Fermi-liquid theory in a wide pressure range above p_c. This non-Fermi liquid behavior suggests that the phase transition occurs without quantum criticality. New information based on nuclear forward scattering measurements ($p <$ 25GPa, $T >$ 3K) revealed a finite but disordered magnetic moment above p_c and low temperature. The implication of this finding to the metallic ground state and an updated phase diagram will be discussed.

[1] P. Pedrazzini et al., Phys. Rev. Lett. 98, 047204 (2007).

TT 17.6 Tue 15:30 HSZ 03

Pressure Dependence of the Magnetotransport Properties of MnSi — •Robert Ritz, Christian Pfleiderer, Andreas Neubauer, Philipp Niklowitz, and Peter Böni — Physik Department E21, Technische Universität München, D-85748 Garching, Germany

The temperature dependence of the resistivity of the itinerant-electron magnet MnSi suggests the emergence of an extended non-Fermi liquid regime above a critical pressure $p_c = 14.6$ kbar. Various neutron scattering studies suggest that this state may not be related to quantum criticality, where one of the most promising scenarios concerns the spontaneous formation of topologically non-trivial spin textures composed of skyrmions. We report measurements of the low-temperature magnetoresistance and Hall-effect under pressure in excess of 40 kbar and magnetic field up to 14 T. We discuss our findings in the light of the recent discovery of a skyrmion lattice and a related topological Hall effect in MnSi at ambient pressure.

TT 17.7 Tue 15:45 HSZ 03

Novel coupled spin-electron liquid in the layered cobaltate Na_xCoO_2 — •Peter Lemmens[1], Dietrich Wulferding[1], Vladimir Gnezdilov[1,2], Alexander Doering[1], Chengtian Lin[3], Guo-Jun Shu[4], and Fang-Cheng Chou[5] — [1]IPKM, TU Braunschweig, Germany — [2]ILTP, Kharkov, Ukraine — [3]MPI-FKF, Stuttgart, Germany — [4]Center for Condensed Matter Sciences, Taipei, Taiwan — [5]Nat. Synchrotron Radiation Research Center, HsinChu, Taiwan

In the layered cobaltate Na_xCoO_2 certain compositions (x=0.71) show a depression of long range magnetic ordering and a coexistence of itinerant and localized charge carriers with a comparably high conductivity and a Curie-Weiss like magnetic susceptibility. In Raman scattering a divergence of quasi-elastic fluctuations is observed towards low temperatures supporting a scenario of a novel coupled spin-electron liquid state. Work supported by DFG and ESF-HFM.

TT 17.8 Tue 16:00 HSZ 03

Ferromagnetic quantum phase transition in $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider, Vasile Moshnyaga, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen

We report synthesis of $Sr_{1-x}Ca_xRuO_3$ thin films, which have been grown epitaxially on $SrTiO_3$ substrates by metalorganic aerosol deposition technique characterized by x-ray diffraction and room-temperature STM. The physical properties were investigated by electrical resistivity and magnetization measurements. We observe a continuous suppression of itinerant electron magnetism with T_C=160K for $SrRuO_3$ with increasing Ca concentration x in $Sr_{1-x}Ca_xRuO_3$ towards $T_C \to 0$ for $x_c \approx 0.8$. Non-Fermi liquid behaviour in the electrical resistivity is analysed for thin films with x=0.8 and x=1 down to mK temperatures.

TT 18: Superconductivity: Fabrication and Characterization

Time: Tuesday 14:00–16:00 Location: HSZ 105

TT 18.1 Tue 14:00 HSZ 105

Crystal Growth and Characterization of $Ba_{1-x}K_xFe_2As_2$ — •Andreas Erb, Franz Czeschka, Monika Bahurupi, and Rudolf Gross — Walther Meissner Institut für Tieftemperaturforschung, Bayerische Akademie der Wissenschaften, Walther Meissnerstr. 8, 85748 Garching, Germany

We report on the growth and characterization of single crystals of $Ba_{1-x}K_xFe_2As_2$ by electrical transport and magnetization measurements. The crystals were grown from high temperature solutions using tin as a flux. Crystals of several mm size in a-b direction can be grown exhibiting sharp superconducting transitions in both resistive and magnetic measurements. We discuss the problem of intrinsic inhomogeneity of the as-grown crystals as a consequence of the phase diagram for this solid solution system. We also outline scenarios for the application of other crystal growth techniques. This work is supported by DFG within the Research Unit 538.

TT 18.2 Tue 14:15 HSZ 105

Preparation and Analysis of the new Superconductors $RO_{1-x}F_xFeAs$ (R = La, Ce, Nd, Sm, Gd) — •Anke Köhler, Günter Behr, Jochen Werner, Daniel Koksch, Rüdiger Klingeler, Norman Leps, Jorge E. Hamann-Borrero, and Bernd Büchner — IFW Dresden, PF 270116, D-01171 Dresden

Polycrystalline samples of $RO_{1-x}F_xFeAs$ ($0 \le x \le 0.25$) were prepared in a two step method, similar described by Zhu et al. . In the first step FeAs is prepared which is milled afterwards. In the second step the FeAs powder is mixed together with rare-earth-oxides, -flourides and -pure element powders and pressed into pellets under a well defined pressure. Then, the samples were heated in an evacuated silica tube at 940°C and 1150°C. The composition of the samples and particularly the fluorine content was determined by wavelength-dispersive X-ray spectroscopy (WDX) in the electron microscope. The polycrystalline samples consist of the $RO_{1-x}F_xFeAs$ phase mainly, only small amount of RO_yF_z and FeAs are found. We find that the measured fluorine content can deviate from the initial weight. In the lanthanum compound $LaO_{1-x}F_xFeAs$, e.g., we found a good agreement mainly for x>0.05, but the fluorine hardly goes into the sample for x<0.05. For the samarium compound again we measure less fluorine in the sample as weighted for all fluorine contents. These measured values are taken into account when drawing the electronic phase diagrams of $LaO_{1-x}F_xFeAs$ and $SmO_{1-x}F_xFeAs$. Furthermore, we studied which preparation steps are crucial for the fluorine incorporation.

TT 18.3 Tue 14:30 HSZ 105

Growth and anisotropy of La(O,F)FeAs thin films deposited by pulsed laser deposition — •Elke Backen[1], Silvia Haindl[1], Tim Niemeier[1], Ruben Hühne[1], Thomas Freudenberg[1], Jochen Werner[2], Günter Behr[2], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

$LaFeAsO_{1-x}F_x$ thin films were deposited successfully on (001)-oriented $LaAlO_3$ and MgO substrates from stoichiometric $LaFeAsO_{1-x}F_x$ polycrystalline targets with fluorine concentrations up to x = 0.25 by pulsed laser deposition (PLD). Room temperature deposition and post annealing yield films with a pronounced c-axis texture and a strong biaxial in-plane orientation. Transport measurements show metallic resistance and onset of superconductivity at 11 K.

$\mu_0 H_{c2}$(T) was determined by resistive measurements and yield $\mu_0 H_{c2}$ values of 3 T at 3.6 K for the perpendicular field direction and 6 T at 6.4 K for the parallel field direction to the sample surface.

TT 18.4 Tue 14:45 HSZ 105

Texture and anisotropy of PLD-grown superconducting $LuNi_2B_2C$ thin films — •Tim Niemeier[1], Ruben Hühne[1], Günter Fuchs[1], Anke Köhler[2], Günther Behr[2], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]Institute for Metallic Materials, IFW Dresden, P.O. Box 270116, D-01171 Dresden — [2]Institute for Solid State Physics, IFW Dresden, P.O. Box 270116, D-01171 Dresden

Epitaxial thin films of $LuNi_2B_2C$ were deposited on MgO single crystal substrates using Pulsed Laser Deposition from a stoichiometric target. The film thicknesses are around 200 nm. For optimized deposition parameters, a sharp c-axis texture, high in-plane order and a good reproducibility were achieved. The residual resistivity is around 5 $\mu\Omega$cm, which is about 2-3 times higher than the best values reported for single crystals, resulting in RRR values of about 15. The temperature behaviour of the upper critical field was measured using a Quantum Design PPMS between 2K and T_c and reveals a significantly higher H_{c2} than in single crystals whereas the anisotropic behaviour of H_{c2} is qualitatively similar. Potential reasons for the increase of H_{c2} are discussed.

15 min. break.

TT 18.5 Tue 15:15 HSZ 105

Ion-beam assisted deposition of textured transition metal nitride films — •Martin Kidszun, Ruben Hühne, Bernhard Holzapfel und Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Ion-beam assisted deposition (IBAD) offers the opportunity to prepare thin textured films on non-textured substrates. A textured nucleation was observed in materials with a rocksalt structure like MgO or TiN under appropriate deposition conditions. Therefore, the IBAD approach was used to investigate, if other superconducting transition metal nitrides can be textured in a similar way. The films were prepared on amorphous Si3N4 seed layers in a reactive process using pulsed laser deposition of pure metals in combination with a nitrogen containing ion-beam. The texture development was studied in-situ using reflection high-energy electron diffraction. It was found, that NbN reveals a textured nucleation similar to MgO or TiN. The biaxial texture was stabilised to thicker layers using homoepitaxial growth. Highly textured NbN layers were realised on amorphous substrates with an in-plane alignment below 5°. In dependence of the nitrogen pressure applied during the homoepitaxial growth, superconducting transition temperatures up to 14 K were observed. A clear correlation between structural and superconducting properties was found. Additionally, the oxygen incorporated in the NbN layer has a significant influence on the superconducting properties. Finally, a textured nucleation was also found for the reactive preparation of ZrN using ion-beam assisted laser deposition.

TT 18.6 Tue 15:30 HSZ 105

Magnetic measurements under pressure of the non-centrosymmetric superconductor Li_2Pd_3B synthesized by a semi-open method — •P. Badica[1,2], G. Jakob[1], A. Beleanu[1], V. Ksenofontov[1], and C. Felser[1] — [1]Mainz University, Mainz, Germany — [2]National Institute of Materials Physics, Bucharest, Romania

Samples of the non-centrosymmetric superconductor Li_2Pd_3B were synthesized from mixtures of the elements. A simple semiopen method is proposed using endings-pressed stainless steel tubes placed in a vacuum furnace. Heating regime employed a short-time overheating at 900 ° C and a slow cooling step between 720 to 550 ° C with a constant cooling rate of 1 ° C/min. Extra amount of Li was necessary to compensate losses and the optimum starting composition was $Li_{2.4}Pd_3B$. Superconducting properties, such as lower and upper critical fields and critical temperature T_c, were measured by magnetic measurements (MPMS magnetometer) under hydrostatic pressures up to 2 GPa (using a self-made pressure capsule). Superconducting properties are decreasing with pressure. For example, under normal pressure samples show a critical temperature of 8-8.2 K and a sharp superconducting transition, while the results indicate for the decrease rate dT_c/dP a value of 0.12 K/GPa. This value is about 3 times lower than the reported value measured by transport measurements on arc-melted samples.

TT 18.7 Tue 15:45 HSZ 105

Phase evolution of $BaHfO_3$ pinning centers in YBCO thin films fabricated with the TFA-MOD process — •Thomas Thersleff, Sebastian Engel, Jens Hänisch, Robert Kluge, Ruben Hühne, Ludwig Schultz, and Bernhard Holzapfel — IFW-Dresden, P.O. Box 270116, 01171 Dresden, Germany

Exploiting the exceptional electrical and magnetic properties of superconducting $YBa_2Cu_3O_{7-\delta}$ (YBCO) coated conductors for the commercial market requires both an economical deposition process as well as a means of enhancing the pinning of magnetic flux lines to increase performance of these materials in applied magnetic fields. Introducing nanosized $BaHfO_3$ (BHO) particles into a YBCO layer deposited using the well-documented chemical solution deposition route known as TFA-MOD is one way to achieve both of these goals. However, the conversion from a precursor solution to crystalline YBCO is complicated and not fully understood, particularly when nanoparticles are added. This contribution takes a closer look at the phase evolution of these nanoparticles in the TFA-MOD-based process. Films with varying concentrations of BHO particles were quenched at different temperatures during the conversion process. Transport and inductive measurements on the fully reacted samples with BHO particles indicate an increased pinning effect with higher dopant concentrations. X-ray results reveal the formation of BHO particles before YBCO is observed, suggesting they precipitate at the substrate. Finally, FIB cuts and TEM cross-section images provide a robust characterization of these films at various stages of the conversion process.

TT 19: Correlated Electrons: Metal-Insulator Transition 3

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

TT 19.1 Tue 14:00 HSZ 301

On the spin-state and metal-insulator transition in $R\mathbf{BaCo_2O_{5.5}}$ — •T.C. Koethe[1], Z. Hu[1], Hua Wu[1], C. Schüssler-Langeheine[1], J.C. Cezar[2], F. Venturini[2], N.B. Brookes[2], H.H. Hsieh[3], H.-J. Lin[3], C.T. Chen[3], S.N. Barilo[4], S.V. Shiryaev[4], G.L. Bychkov[4], and L.H. Tjeng[1] — [1]II.PhysikalischesInstitut Universität zu Köln — [2]ESRF, Grenoble, France — [3]NSRRC, Hsinchu, Taiwan — [4]Belarus Academy of Sciences,Minsk, Belarus

The novel layered perovskite $R\mathrm{BaCo_2O_{5.5}}$ (R = rare earth) has attracted considerable interest in the last decade. It shows an intriguing mix of properties, including giant magneto-resistance, metal-insulator and antiferro-ferromagnetic transitions, and a sign change of the thermoelectric power across these transitions. Explanation of these properties is subject of on-going debate. The so-called spin-blockade mechanism together with the occurrence of a spin-state transition of the octahedral Co^{3+} ions was proposed [Maignan *et al.*, PRL **93** 026401 (2004)]. Other scenarios invoke, for example, order-disorder effects, involving essentially all possible spin state configurations for the octahedral and pyramidal Co^{3+} ions. Using high quality single crystals and bulk sensitive photoelectron and x-ray absorption spectroscopy, we were able to identify the spin-state of the Co ions, thereby arriving at a very different scenario than proposed so far in the literature. We also find that the transfer of spectral weight near the Fermi level across the metal-insulator transition is very modest, in contrast to existing assumptions but in agreement with our observation on the evolution of the spin-state as a function of temperature.

TT 19.2 Tue 14:15 HSZ 301

Spin blockade, orbital occupation and charge ordering in $\mathbf{La_{1.5}Sr_{0.5}CoO_4}$ — •Chun Fu Chang[1], Zhiwei Hu[1], Hua Wu[1], Tobias Burnus[1], Nils Hollmann[1], Mohammed Benomar[1], Thomas Lorenz[1], Arata Tanaka[2], Hong-Ji Lin[3], Hui-Huang Hsieh[4], Chien-Te Chen[3], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

— [2]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [3]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30077, Taiwan — [4]ChungCheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan

Using Co-$L_{2,3}$ and O-K x-ray absorption spectroscopy, we reveal that the charge ordering in $La_{1.5}Sr_{0.5}CoO_4$ involves high spin (S=3/2) Co^{2+} and low spin (S=0) Co^{3+} ions. This provides evidence for the spin blockade phenomenon as a source for the extremely insulating nature of the $La_{2-x}Sr_xCoO_4$ series. The associated e_g^2 and e_g^0 orbital occupation accounts for the large contrast in the Co-O bond lengths, and in turn, the high charge ordering temperature. Yet, the low magnetic ordering temperature is naturally explained by the presence of the non-magnetic (S=0) Co^{3+} ions. From the identification of the bands we infer that $La_{1.5}Sr_{0.5}CoO_4$ is a narrow band material.

TT 19.3 Tue 14:30 HSZ 301

Application of Sum Rules to Resonant Magnetic Diffraction — •Marcel Buchholz[1], Christian Schüssler-Langeheine[1], Maurits W. Haverkort[1,2], Hsueh-Hung Wu[1,3], Chun-Fu Chang[1], Matthias Cwik[1], Mohammed Benomar[1], Enrico Schierle[4], Arata Tanaka[5], Markus Braden[1], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institut für Festkörperforschung, Stuttgart — [3]NSRRC, Hsinchu, Taiwan — [4]Helmholtz-Zentrum Berlin — [5]ADSM, Hiroshima University, Japan

Sum rules relating the spin and orbital moment to integrals over the x-ray magnetic circular dichroism (XMCD) signal are well established and widely used to determine fundamental quantum numbers for ferromagnetic systems.

Resonant magnetic diffraction is closely related to the XMCD effect and can be used to apply sum rules also to magnetically ordered systems without net magnetic moment like antiferromagnets or magnetically ordered systems with multiple sublattices. We tested this approach using holmium metal as a model system. The determination of the proper phase turns out to be a crucial point in the analysis.

We applied the sum-rule analysis to Sr- and Ca-doped La_2CoO_4 and compare the results to microscopic model calculations.

Supported by the DFG through SFB 608 and by the BMBF through 05 ES3XBA/5.

TT 19.4 Tue 14:45 HSZ 301

Pressure-induced superconductivity in the Mott insulator $GaNb_4S_8$ — Xin Wang[1], •Martin K. Forthaus[2], Karl Syassen[1], Mathias Kraken[3], Jochen Litterst[3], Hubertus Luetkens[4], Dirk Johrendt[5], and Mohsen M. Abd-Elmeguid[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germnay — [2]II. Physikalisches Institut, Iniversität zu Köln, Köln, Germany — [3]Institut für Physik der kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [4]Paul Scherrer Institut, Villigen, Switzerland — [5]Department Chemie und Biochemie, LMU München, München, Germany

$GaNb_4S_8$ (cubic fcc $GaMo_4S_8$ type structure) belongs to a new class of Mott insulators in which the electronic conduction originates from hopping of localized electrons (S = 1/2) among widely separated tetrahedral Nb_4 metal clusters. The magnetic susceptibility ($\chi(T)$) of $GaNb_4S_8$ shows Curie-Weiss behavior ($100 \leq T \leq 300$ K) and reveals a sudden drop around 30 K but no long range magnetic order has been detected down to 1.6 K. Recent strutural investigation shows that the drop of $\chi(T)$ is associated with a tetragonal distortion. We find pressure-induced superconductivity in $GaNb_4S_8$ with $T_C = 2.1$ K at $p = 10$ GPa which increases with pressure up to 4 K at 23 GPa. As our μSR experiments at ambient pressure clearly shows that the tetragonal distortion in $GaNb_4S_8$ is associated with the onset of short range magnetic order, we discuss the possibility of a nonconventional pressure-induced superconducting state.

TT 19.5 Tue 15:00 HSZ 301

The local/non-local duality of 5f electrons in actinide compounds: A mean-field study — •Duc-Anh Le[1], Sebastien Burdin[2], Peter Fulde[1], and Gertrud Zwicknagl[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Theoretical Physics, University of Cologne, Germany — [3]Institute for Mathematical and Theoretcal Physics, TU Braunschweig, Germany

The local/non-local duality of 5f electrons in actinide compounds has been observed in a great variety of experiments including photoemission spectroscopy, inelastic neutron scattering, muon spin relaxation measurements, and x-ray inelastic scattering. A general microscopic mechanism leading to the partial localization of 5f orbitals has been proposed within the so-called 'dual model' (D. V. Efremov, et al., Phys. Rev. B 69, 115114 (2004)). It is a generalized multi-orbital Hubbard model which includes the direct Coulomb interaction as well as the Hund's rule correlations. Using a generalized slave boson method (F. Lechermann, et al., Phys. Rev. B 76, 155102 (2007)), we study this model for an electronic filling corresponding to the prototype compound UPt3. We then analyse the calculated phase diagram and discuss the local/non-local and magnetic/non-magnetic phases in terms of orbitally dependent quasi-particle residues and partial electronic occupations.

TT 20: Correlated Electrons: (General) Theory 1

Time: Tuesday 15:30–16:30 Location: HSZ 301

TT 20.1 Tue 15:30 HSZ 301

Anyons as Landau Quasi-Particles - Kitaev's Toric Code in a magnetic Field — •Kai Phillip Schmidt[1], Sébastien Dusuel[2], Ronny Thomale[3], and Julien Vidal[4] — [1]Lehrstuhl für theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany — [4]LPTMC, Jussieu, 75252 Paris Cedex 05, France

Kitaev's Toric Code is an exactly solvable two-dimensional spin model which is relevant for topological quantum computation. Elementary excitations are abelian anyons which are strictly local due to conservation laws. In the presence of a finite external magnetic field, the anyonic excitations gain a kinetic energy and they start to interact. Using perturbative continuous unitary transformations, we set up a true quasi-particle description of the abelian anyons inside the topological phase. We study one-particle properties like the anyon dispersion but also the formation of bound states including two or more anyon excitations. These collective modes turn out to be fermions or bosons. Finally, we study the full phase diagram of the model which turns out to be very rich including multi-criticality and self-duality on different lines in parameter space. The critical properties of the model therefore strongly depend on the direction of the magnetic field. Apart from perturbative continuous unitary transformations we use exact diagonalization as a complentary tool.

TT 20.2 Tue 15:45 HSZ 301

Entanglement and relative local entropies: Introducing a quantitative measure of correlations in correlated electron systems — •Krzysztof Byczuk[1], Walter Hofstetter[2], and Dieter Vollhardt[3] — [1]Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, PL-00-681 Warszawa, Poland — [2]Institut fur Theoretische Physik, Johann Wolfgang Goethe-Universitaet, D-60438 Frankfurt/Main, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

We employ the concept of entanglement and relative local entropies to provide a quantitative measure of the strength of correlations in interacting electronic systems. As an application we solve the Hubbard model within the dynamical mean-field theory and extract the entanglement local entropy as well as the relative local entropy, using different Hartree-Fock-like ground states as reference states. The strength of the correlations in the paramagnetic and antiferromagnetic phase, expressed by the relative entropies with respect to the Hartree-Fock solutions, is discussed.

TT 20.3 Tue 16:00 HSZ 301

Upper bound of truncation errors in continuous unitary transformations — •Nils A. Drescher[1], Tim Fischer[1], and Götz S. Uhrig[1,2] — [1]Technische Universität Dortmund, Lehrstuhl für The-

oretische Physik I, 44221 Dortmund, Germany — [2]School of Physics, University of New South Wales, Kensington 2052, Sydney NSW, Australia

Self-similar continuous unitary transformations (CUTs) are a method to systematically derive effective models for many-particle-systems of finite or infinite size. They allow us to separate Hilbert spaces of different numbers of quasiparticle. Technically this is done by solving the flow equations for the coefficients of the various terms in the Hamiltonian. In order to keep the number of equations finite truncations are inevitable. The choice of an efficient truncation scheme which preserves the relevant physics is a highly non-trivial task. Here we present the mathematical derivation of a method to quantify the truncation error so that different truncation schemes can be compared without bias. Thereby we can establish rigorous bounds on the accuracy of the ground state energy calculated by CUT. Exemplary results a shown for zero and one dimensional systems[1,2].

[1] S. Dusuel and G.S. Uhrig, Journal of Physics A: Mathematics and General 37, 9275- (2004).

[2] C. Knetter, K.P. Schmidt, and G.S. Uhrig, Journal of Physics A: Mathematics and General 36(29), 7889 (2003).

TT 20.4 Tue 16:15 HSZ 301

Simulating strongly correlated fermions with unitary networks — •Carlos Pineda and Jens Eisert — University of Potsdam, 14476 Potsdam, Germany

One of the central challenges in the numerical study of quantum many-body systems is to efficiently identify ground state properties of strongly correlated two- and higher-dimensional quantum systems. Recently, it has become clear that efficiently contractable tensor networks offer new perspectives for such simulations: In one dimension, the density-matrix renormalization group method and entanglement renormalization can both be grasped as such networks, with natural higher-dimensional analogues [1,2,3,4]. In this work, we introduce a framework of unitary tensor networks for fermions, which is not overburdened by encountering non-local string operators in the spin representation. In fact, there is only a constant overhead in the effort to compute local expectation values. We present a formalism of dynamical relabeling of fermions and dicuss first results on this framework.

[1] G. Vidal, Phys. Rev. Lett. 99, 220405 (2007).

[2] C.M. Dawson, J. Eisert, T.J. Osborne, Phys. Rev. Lett. 100, 130501 (2008).

[3] M.-C. Banuls, D.P.-García, M.M. Wolf, F. Verstraete, J.I. Cirac, Phys. Rev. A 77, 052306 (2008).

[4] U. Schollwoeck, Rev. Mod. Phys. 77, 259 (2005).

TT 21: Transport: Fluctuations and Noise

Time: Tuesday 14:00–16:15 Location: HSZ 304

Invited Talk TT 21.1 Tue 14:00 HSZ 304

Correlated charge detection in quantum dots — •Klaus Ensslin — ETH Zurich, Switzerland

Quantum point contacts placed close to quantum dots can be used as charge detectors with time resolution. This way it is possible to measure the statistics of charge transport through quantum structures or the interference of individual electrons. If the quantum dot or double dot is probed by two charge detectors the detector signals may be correlated or anti-correlated depending on the locations between which a single electron is transported. This allows to fully characterize the tunneling processes of electrons in a double dot systems. For quantum dots tuned off resonance this method allows to also measure co-tunneling rates. These experiments are performed in standard n-type AlGaAs heterostructures, but also in p-type material, InAs nanowire quantum dots as well as in graphene quantum structures.

TT 21.2 Tue 14:30 HSZ 304

Electron counting with a two-particle emitter — •Janine Splettstoesser[1], Sveta Ol'khovskaya[2], Michael Moskalets[1,2], and Markus Büttiker[1] — [1]Département de Physique Théorique, Université de Genève, CH-1211 Genève, Switzerland — [2]Department of Metal and Semiconductor Physics, NTU "Kharkiv Polytechnic Institute", 61002 Kharkiv, Ukraine

Recently an on-demand coherent single-electron source has been realized experimentally giving the possibility of initializing quantum states for, e.g., electronic quantum information. However, a suitable setup for high-speed single-electron detection is still missing. We consider two driven cavities (capacitors) connected in series via an edge state. The cavities are driven such that they emit an electron and a hole in each cycle. Depending on the phase lag the second cavity can effectively absorb the carriers emitted by the first cavity and nullify the total current or the set-up can be made to work as a two-particle emitter. We examine the precision with which the current can be nullified and with which the second cavity effectively counts the particles emitted by the first one.

TT 21.3 Tue 14:45 HSZ 304

Control of the conductance and noise of driven carbon-based Fabry-Perot devices — •Luis E. F. Foa Torres and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany.

Here we report on the suppression and revival of the Fabry-Perot conductance interference pattern through a carbon-based three terminal device [1]. By using Green functions techniques in the Floquet replica space as our general framework, we show that control of the interference pattern can be achieved by tuning the ac field strength and frequency. For frequencies matching integer multiples of the level spacing of the system a manifestation of the wagon-wheel effect in the quantum domain takes place as the conductance remains irresponsive to the external field. When this condition is not satisfied, tuning the intensity of the ac gating induces an alternation of suppression and partial revival of the conductance interference pattern. In contrast, the phase sensitive current noise behaves as in the static case only when the frequency is commensurate with twice the mean level spacing. This scenario is tested for the case of carbon nanotubes, where the scaling properties of noise with tube radius and length are also explored.

[1] L. E. F. Foa Torres and G. Cuniberti, arxiv: 0807.4953.

15 min. break.

TT 21.4 Tue 15:15 HSZ 304

Tunable dynamical channel blockade in double-dot Aharonov-Bohm interferometers — •Daniel Urban and Jürgen König — Unversität Duisburg-Essen and CeNIDE

We study electronic transport through an Aharonov-Bohm interferometer with single-level quantum dots embedded in the two arms. The full counting statistics in the shot-noise regime is calculated to first order in the tunnel-coupling strength. The interplay of interference and charging energy in the dots leads to a dynamical channel blockade, resulting in enhanced cumulants. This effect is tunable by the magnetic flux penetrating the Aharonov-Bohm ring.

The origin of the blockade lies in the decoupling of the double dot's Hilbert space into two subspaces, one containing the singlet and one containing the three triplet states: Consequent filling of an empty dot with two electrons from the source results in the singlet state, i.e. the triplet can only be reached by tunneling out to the drain. Since the subspaces differ in their transport properties, this leads to super-Poissonian noise. When the flux assumes integer multiples of the flux quantum, tunneling out is suppressed, so that the subspaces decouple and the second and higher cumulants diverge.

[1] D. Urban and J. König, arXiv:0811.4723

TT 21.5 Tue 15:30 HSZ 304

Phonon assisted noise in molecular junctions — •Federica Haupt[1], Tomas Novotny[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-121 16 Praha 2, Czech Republic

Effects due to electron-phonon scattering in molecular junctions are relevant not only because they ultimately affect the characteristics and the stability of the device, but also because they can be used to extract information on the junction itself. In particular, inelastic transport spectroscopy is an important investigation tool for atomic- and

molecular devices, and more information is expected to be provided by noise measurements.

In this work we investigate the effects of phonon scattering on the current noise through nanojunctions. Using the extended Keldysh-Green's function formalism we derive an expression for cumulant generating function in the case of weak electron-phonon coupling. We present analytic results for the case of a single broad level and identify, both in the inelastic current and in the noise, physically distinct contributions based on their voltage dependence. We apply our theory to an experimentally relevant set-up [1] and predict the inelastic contribution to current noise in the presence of phonon heating effects.

[1] R. H. M. Smit, Y. Noat, C. Untied, N.D. Lang, M.C. van Hemert, and J.M. van Ruitenbeek, Nature 419, 906 (2002).

TT 21.6 Tue 15:45 HSZ 304

Time-Resolved Counting Statistics for a Quantum Point Contact — •Adam Bednorz[1,2] and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institute of Theoretical Physics, University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

We show that the naive formulation of time-resolved full counting statistics fails for high frequencies and leads to results, which could be interpreted as negative probabilities. We propose to construct a properly time-ordered positive-operator-valued measure, that combines counting statistics with detector backaction parametrized by a characteristic time τ [1]. The standard counting statistics is recovered in long time limit. In high frequency limit, for a weak coupling between the system and detector, the generating functional of counting statistics gains an additional Gaussian white noise component, that saves the positivity of the probability. It agrees with experiments since otherwise at strong coupling the noise measurements would be considerably modified due to the detector backaction. Finally, we also show that with more than one detector these nonclassical correlations can be directly measured.

[1] A. Bednorz and W. Belzig, Phys. Rev. Lett. **101**, 206803 (2008).

TT 21.7 Tue 16:00 HSZ 304

Electron counting statics in transport through double quantum dots — •Clive Emary[1], David Marcos[2], Ramon Aguado[2], and Tobias Brandes[1] — [1]Institut für Theor. Physik, TU Berlin — [2]Departamento de Teoria de la Materia Condensada, CSIC, Madrid

The double quantum dot is an important paradigm of quantum transport, representing a quantum two level system (qubit) connected to leads. We present several new aspects of the transport through a double quantum dot in the Coulomb blockade regime. On the one hand we discuss finite-frequency full counting statistics of the transport electrons and investigate the visibility of coherent effects at finite temperatures and bias; on the other, we study the effects of higher-order electron tunneling process usually neglected in standard treatments.

TT 22: Correlated Electrons: Quantum-Critical Phenomena 2

Time: Wednesday 9:30–13:00 Location: HSZ 03

Invited Talk TT 22.1 Wed 9:30 HSZ 03

Thermal expansion and magnetostriction close to quantum criticality — •Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln

Quantum phase transitions occur in materials at zero temperature upon tuning an external parameter, e.g., magnetic field to an instability of the ground state. A coupling of the quantum critical fluctuations to the lattice degrees of freedom can be exploited to probe quantum criticality at finite temperatures. We discuss the resulting anomalous signatures in thermal expansion, magnetostriction and the Grüneisen parameter, which provide a valuable tool not only to detect but also to classify a quantum phase transition. A smoking gun for the existence of such a transition is, e.g., the divergence of the Grüneisen parameter with an exponent characteristic for its universality class. We also explain that a negative thermal expansion naturally accompanies such transitions, and that its sign changes indicate the entropy distribution in the phase diagram. As examples, we discuss (a) quantum critical metamagnetism, a concept introduced for the bilayer ruthenate $Sr_3Ru_2O_7$, and (b) the critical properties of the spin-ladder compound $(C_5H_{12}N)_2CuBr_4$, that exhibits a diverging thermal expansion.

TT 22.2 Wed 10:00 HSZ 03

Low-temperature thermal expansion of $Nb_{1-y}Fe_{2+y}$ — •Stefan Lausberg[1], Manuel Brando[1], Rafik Ballou[2], F Malte Grosche[3], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Laboratoire Louis Néel, CNRS, B.P. 166, 38042 Grenoble Cedex 9, France — [3]Cavendish Laboratory, Cambridge CB30HE, United Kingdom

The hexagonal C14 Laves phase system $Nb_{1-y}Fe_{2+y}$ exhibits a magnetically ordered ground state, the nature of which strongly depends on the concentration y. Stoichiometric $NbFe_2$ shows low-temperature ($T_N = 10$ K) spin-density-wave (SDW) order, while slight Fe-excess induces low-moment ferromagnetism (FM). A quantum critical point (QCP) is expected on the Nb-rich side at $y \sim -0.015$, where signatures of logarithmic Fermi-liquid breakdown have been reported [1]. The presence of a QCP can be thermodynamically tested by measuring the thermal expansion coefficient $\alpha(T)$: In metals close to a QCP, a divergence of the Grüneisen ratio $\Gamma = \alpha/c_p$ has been proposed, since α is more singular than c_p, while in metals with a Fermi-liquid ground state, α/T and c_p/T are constant. We report measurements of α for different single crystals with y close to the QCP. Surprisingly, we find an extremely large α coefficient, similar to that of heavy-fermion materials [2], and it increases with decreasing temperature. The behavior of the resulting Γ parameter will be discussed.

[1] M. Brando et al., PRL **101**, 026401 (2008).
[2] R. Küchler et al., Physica B **378-380**, 36 (2006).

TT 22.3 Wed 10:15 HSZ 03

Probing the quantum critical behavior of $CeCoIn_5$ via thermal expansion measurements — •Sebastian Zaum[1,2], Kai Grube[1], Roland Schäfer[1], Eric D. Bauer[3], Christoph Meingast[1], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The heavy-fermion compound $CeCoIn_5$ is an unconventional superconductor. Its tetragonal crystal structure leads to anisotropic superconducting properties with an upper critical field of $B_{c2} = 5$ T and 11.8 T along the a- and c-axes, respectively. At its upper critical field $B_{c2} \parallel c$, $CeCoIn_5$ reveals a quantum critical point with pronounced deviations from Fermi-liquid behavior. We have measured the thermal expansion α_i ($i = a$, c) and magnetostriction λ_i longitudinal and transverse to the magnetic field. As expected, α_i/T changes its sign at B_{c2} and diverges with decreasing temperature. The effect of the quantum critical behavior on α_a, however, is qualitatively different from that on α_c. While α_c shows at $T = 0.3$ K a crossover to a weaker divergence, α_a does not change its singular behavior down to the lowest measured temperature of 50 mK.

TT 22.4 Wed 10:30 HSZ 03

Divergence of the Magnetic Grüneisen Ratio at the Field-Induced Quantum Critical Point in $YbRh_2Si_2$ — Yoshi Tokiwa[1,2], Teodora Radu[1], •Philipp Gegenwart[2], Christoph Geibel[1], and Frank Steglich[1] — [1]Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden — [2]I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We study quantum criticality in the heavy-fermion metal $YbRh_2Si_2$ by means of the low-temperature magnetization and specific heat[1]. The magnetic Grueneisen ratio $\Gamma_{\rm mag} = -(dM/dT)/C$ is derived, which is found to diverge in the approach of the field-induced quantum critical point. The data are compared with theoretical predictions for quantum criticality in heavy-fermion metals.

[1] T. Tokiwa et al., arXiv:0809.3705v2.

TT 22.5 Wed 10:45 HSZ 03

Thermoelectric power in the quantum critical regime of $YbRh_2Si_2$ and $CeNi_2Ge_2$ — •Stefanie Hartmann, Niels Oeschler, Cornelius Krellner, Nubia Caroca-Canales, Christoph Geibel, and Frank Steglich — MPI CPfS, Dresden, Germany

The heavy-fermion compounds $YbRh_2Si_2$ and $CeNi_2Ge_2$ are situated very close to a quantum critical point (QCP). $YbRh_2Si_2$ exhibits an antiferromagnetic ground state with $T_N = 70$ mK and a tiny critical field $B_c \approx 60$ mT. In $CeNi_2Ge_2$ a non-magnetic ground state is observed. While in $CeNi_2Ge_2$ a 3-dim. spin-density wave scenario is realized, the QCP in $YbRh_2Si_2$ is shown to be of anomalous nature with a critical break-down of the Kondo scale. We report on low-temperature thermopower $S(T)$ results in the quantum critical regimes of both compounds. S/T logarithmically diverges upon cooling down to 100 mK in the critical region of $YbRh_2Si_2$, reflecting the strongly diverging heavy quasi-particle mass upon approaching the QCP. However, a decrease and a sign change in S/T for $B < B_c$ point toward a "small"Fermi surface on the magnetic side. In the quantum critical regime of $CeNi_2Ge_2$, S/T remains comparably small and does not exhibit a divergence for $T \to 0$. In the field-induced Landau-Fermi-liquid regime, both compounds exhibit a constant S/T below T_{LFL} as expected for a renormalized metal-like state.

15 min. break

TT 22.6 Wed 11:15 HSZ 03

Tuning the magnetic behavior in $Yb(Rh_{1-x}Co_x)_2Si_2$ with Chemical Pressure — •Christoph Klingner, C. Krellner, C. Geibel, and F. Steglich — Max-Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

In recent years $YbRh_2Si_2$ has been intensively investigated due to its proximity to an antiferromagnetic quantum critical point (QCP). As expected for Yb-Kondo lattice compounds the magnetic ordering of $YbRh_2Si_2$ (T_N=70mK) is stabilized by applying pressure. The complementary method of doping with Cobalt results in chemical pressure allowing therefore an investigation of the magnetic phase diagram and the physical behavior of the stabilized antiferromagnetic ordered state. A thorough understanding of the physical properties of this series, particularly for small amounts of Cobalt doping, are of high interest to understand the phenomena at the QCP in $YbRh_2Si_2$. In this contribution we report on the growth of a series of single crystals $Yb(Rh_{1-x}Co_x)_2Si_2$ with concentrations x from 0 to 1. The crystallographic parameters as well as low temperature properties studied by resistivity, specific heat and magnetization measurements will be presented and compared to already existing pressure data on $YbRh_2Si_2$. The qualitative agreement of the magnetic phase diagrams obtained from hydrostatic and chemical pressure experiments can be shown. With increasing x the change of the physical properties of the series $Yb(Rh_{1-x}Co_x)_2Si_2$ can be understood originating from the interplay of the Kondo- and RKKY- dominated exchange interaction.

TT 22.7 Wed 11:30 HSZ 03

Low-temperature magnetic phase diagram of the heavy-fermion compound $YbCo_2Si_2$ — •Luis Pedrero, Christoph Klingner, Manuel Brando, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Str. 40, 01187 Dresden, Germany

We report on the first high-resolution DC magnetization $M(H,T)$ measurements on a single crystal of $YbCo_2Si_2$. M was measured down to 50 mK and fields up to 12 T with the field $H \perp c$ axis. The magnetic phase diagram of $YbCo_2Si_2$ was deduced from the isothermal curves along with susceptibility and heat-capacity measurements.
Two antiferromagnetic phase transitions have been detected at $T_N = 1.65$ K and $T_L = 0.9$ K. The signatures at T_N suggest that the phase transition is 2^{nd} order and it is suppressed by a field $\mu_0 H_N = 1.9$ T. At T_L latent heat has been observed in the heat capacity in zero field and hysteresis effects in the M *vs.* H confirm the 1^{st} order nature of the transition. The entropy below both transitions and the M value at H_N point to a local character of the Yb $4f$ quasi-hole, resulting in a very small Kondo temperature compared to the one in $YbRh_2Si_2$ [1]. However, the data at 50 mK reveals the presence of a kink in M *vs.* H at $\mu_0 H_N = 10.6$ T, very similar to the one observed $YbRh_2Si_2$ at $\mu_0 H_N = 9.9$ T, where a suppression of the Kondo fluctuations or a Lifshitz transition have been proposed [1,2]. The $T-H$ phase diagram as well as the nature of the high-field transition will be discussed.

[1] Y. Tokiwa et al. Phys. Rev. Lett. **94**, 226402 (2005).
[2] P. M. C. Rourke et al., submitted (2008).

TT 22.8 Wed 11:45 HSZ 03

Conduction Electron Spin Resonance (CESR) of the itinerant magnets $ZrZn_2$ and $NbFe_2$ — •Tobias Förster[1], Jörg Sichelschmidt[1], Manuel Brando[1], Noriaki Kimura[2], Rafik Ballou[3], and Frank Steglich[1] — [1]Max Planck Inst. f. Chem. Physik Fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden,Germany — [2]Center f. Low Temp. Scien., Tohoku University, Sendai, Miyagi 980-8578, Japan — [3]Inst. Nèel, CNRS, B.P. 166, 38042 Grenoble Cedex 9, France

The two Laves phase compounds $ZrZn_2$ and $NbFe_2$ belong to the rather small group of low temperature itinerant magnets. $ZrZn_2$ has a cubic structure and shows a ferromagnetic (FM) order with a small ordered moment at T_C=27.5 K. When applying pressure the FM phase transition becomes first order and disappears around 16.5 kbar[1]. The properties of $ZrZn_2$ are well described by the concept of a marginal Fermi liquid[1]. In the light of these recent findings we reinvestigated the CESR on high quality single crystals of this compound.
$NbFe_2$ has a hexagonal structure and possesses a magnetically ordered ground state (T_N=10 K) which is believed to be of spin-density-wave (SDW) type. Signatures of a logarithmic Fermi-liquid breakdown [2] suggest the existence of a quantum critical point on the Nb-rich side of the phase diagram. In our contribution, we will present the first CESR measurements on a slightly Nb-rich single crystal with T_N=3.6 K, which shows an intriguing and unusual behavior.

[1] R. Smith et al., Nature **455**, 1220 (2008).
[2] M. Brando et al., Phys. Rev. Lett. **101**, 026401 (2008).

TT 22.9 Wed 12:00 HSZ 03

Nonequilibrium quantum criticality in open electronic systems — •So Takei[1,2], Aditi Mitra[3], William Witczak-Krempa[1], Yong Baek Kim[1], and Andrew J. Millis[4] — [1]University of Toronto, Toronto, Canada — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [3]New York University, New York, U.S.A. — [4]Columbia University, New York, U.S.A.

A theory is presented of quantum criticality in open (coupled to reservoirs) itinerant electron magnets, with nonequilibrium drive provided by current flow across the system. Both departures from equilibrium at conventional (equilibrium) quantum critical points and the physics of phase transitions induced by the nonequilibrium drive are treated. Nonequilibrium-induced phase transitions are found to have the same leading critical behavior as conventional thermal phase transitions. The theory is also extended to the case of a coupled bilayer system of itinerant electron magnets where coupled critical dynamics between the two order parameters becomes possible.

TT 22.10 Wed 12:15 HSZ 03

Color Superfluidity and Trion Formation in Ultracold Fermionic Systems — •Akos Rapp — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77 D-50937 Cologne Germany

We investigate the low temperature properties of the three component Hubbard model. This system might be realized by trapping 3 different hyperfine states of ultracold Li-6 atoms in optical lattices. Studies concerning the SU(3) symmetric attractive case based on a Gutzwiller variational method in $d = \infty$ suggest (see Phys. Rev. Lett. 98, 160405 (2007) and Phys. Rev. B 77, 144520 (2008)) that there is a continuous phase transition happening between a weak coupling color superfluid and a strong coupling trionic ground state. We construct and investigate the properties of the quantum field theory describing this quantum phase transition.

TT 22.11 Wed 12:30 HSZ 03

Infinite randomness fixed point of the superconductor-metal quantum phase transition — •Bernd Rosenow[1], Adrian Del Maestro[2], Markus Mueller[3], and Subir Sachdev[4] — [1]Max-Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]University of British Columbia , Vancouver, BC V6T1Z1, Canada — [3]University of Geneva, 1211 Geneva, Switzerland — [4]Harvard University, Cambridge, MA 02138, USA

We examine the influence of quenched disorder on the superconductor-metal transition, as described by a theory of overdamped Cooper pairs which repel each other. The self-consistent pairing eigenmodes of a quasi-one dimensional wire are determined numerically. Our results [1] support the recent proposal [2] that the transition is characterized

by the same strong disorder fixed point describing the onset of ferromagnetism in the random quantum Ising chain in a transverse field.

[1] A. Del Maestro, B. Rosenow, M. Müller, and S. Sachdev, Phys. Rev. Lett. **101**, 035701 (2008).

[2] J. A. Hoyos, C. Kotabage, and T. Vojta, Phys. Rev. Lett. **99**, 230601 (2007).

TT 22.12 Wed 12:45 HSZ 03

Quantum phase transitions in systems of coupled spin dimers — •Sandro Wenzel[1], Wolfhard Janke[1], and Stefan Wessel[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04109 Leipzig — [2]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

We study quantum phase transitions in two-dimensional periodic arrangements of coupled spin-1/2 dimers, using a combination of quantum Monte Carlo simulations and effective field theories. Our numerical results on both ground-state properties and the finite-temperature scaling behavior in the quantum critical regime indicate, that depending on the spatial arrangement of the dimers, deviations occur to the scaling behavior of the three-dimensional Heisenberg universality class. We discuss the numerical evidence [1] for such unconventional quantum criticality, and possible relations to low-energy continuum theory beyond the conventional non-linear sigma model action.

[1] S. Wenzel, L. Bogacz, W. Janke, Phys. Rev. Lett. **101**, 127202 (2008).

TT 23: Transport: Nanoelectronics III - Molecular Electronics

Time: Wednesday 9:30–12:30 Location: HSZ 105

TT 23.1 Wed 9:30 HSZ 105

Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives: A density functional study — •Fabian Pauly[1,2], Janne Viljas[1,2], and Juan Carlos Cuevas[3] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

We study theoretically the length dependence of both conductance and thermopower in metal-molecule-metal junctions made up of dithiolated oligophenylenes contacted to gold electrodes [1]. We find that while the conductance decays exponentially with increasing molecular length, the thermopower increases linearly as suggested by recent experiments [2]. We also analyze how these transport properties can be tuned with methyl side groups. Our results can be explained by considering the level shifts due to their electron-donating character as well as the tilt-angle dependence of conductance and thermopower. Qualitative features of the substituent effects in our density functional calculations are explained using a tight-binding model. In addition, we observe symmetry-related even-odd transmission channel degeneracies as a function of molecular length.

[1] F. Pauly, J. K. Viljas, and J. C. Cuevas, Phys. Rev. B 78, 035315 (2008).

[2] P. Reddy, S.-Y. Jang, R. A. Segalman, and A. Majumdar, Science 315, 1568 (2007).

TT 23.2 Wed 9:45 HSZ 105

Opto-electronic properties of gold nanoparticle arrays — •Christoph Weiss, Markus A. Mangold, and Alexander W. Holleitner — Walter Schottky Institute, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

The field of plasmonics has drawn a lot of interest in recent years. It deals with the interaction of metal clusters with light. Special attention was given to the fact that the exciting electric field is strongly enhanced at the surface of metal nanoparticles. Another topic where substantial research efforts are undertaken is the field of molecular electronics. Our research combines the two fields by examining the interaction of light with metal-molecule junctions. To this end, ordered hexagonal arrays of alkanethiol coated gold nanoparticles are produced by self-assembly. In such an array the nanoparticles are separated by nanometer-sized gaps. The nanoparticle arrays are manipulated with a focused ion beam and their opto-electronic properties are probed in the UV and visible spectrum. The strong plasmonic absorption of the nanoparticles can be readily observed in the photoresponse of arrays with alkanethiol coated gold nanoparticles.

We acknowledge the fruitful collaboration with J. Liao, M. Calame, C. Schönenberger, and the NCCR Nanoscience of the Swiss National Science Foundation (SNF) and thank for financial support by the DFG excellence initiative Nanosystems Initiative Munich (NIM).

TT 23.3 Wed 10:00 HSZ 105

Conductance of DNA molecular wires: bridging molecular dynamics and model Hamiltonians — •Benjamin Woiczikowski[2], Rafael Gutierrez[1], Rodrigo Caetano[1], Tomas Kubar[2], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany.

We present a hybrid method based on a combination of quantum/classical molecular dynamics (MD) simulations [1] and a model Hamiltonian approach to describe charge transport through biomolecular wires.[2] Our approach maps the molecular electronic structure (obtained from the MD simulations) onto a tight-binding model. The latter is then coupled to a bosonic bath which describes fluctuation effects from the solvent and from the conformational dynamics. We apply this approach to the case of pG-pC and pA-pT oligomers as typical cases. We show that conformational fluctuations are crucial in determining charge transport. Especially, our results indicate that pA-pT shows a much larger current than pG-pC, in contrast to transport calculations performed on static configurations.

[1] T. Kubar, P. B. Woiczikowski, G. Cuniberti, and M. Elstner, J. Phys. Chem. B 112, 7937 (2008).

[2] R. Gutierrez, R. Caetano, B. Woiczikowski, T. Kubar, M. Elstner, and G. Cuniberti, submitted (2008).

TT 23.4 Wed 10:15 HSZ 105

Screw motion of a DNA duplex during translocation through a nanopore: A coarse-grained model — •Rafael Gutierrez[1], Jewgeni Starikov[2], Dirk Hennig[3], Hiroaki Yamada[4], Gianaurelio Cuniberti[1], and Bengt Norden[5] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Theoretical Solid State Physics, University of Karlsruhe, D-76131 Karlsruhe, Germany — [3]Institute for Physics, Humboldt University of Berlin, D-12489 Berlin, Germany — [4]Yamada Physics Research Laboratory, Niigata 950-2002, Japan — [5]Department of Physical Chemistry, Chalmers University of Technology, SE-412 96, Gothenburg, Sweden

Based upon the structural properties of DNA and their counterion-water surrounding in solution, we have introduced a screw model describing DNA translocation through artificial nanopores in a qualitatively correct way.[1] This model represents DNA as a "screw", whereas the counterion-hydration shell is a "nut". When an electrical potential is applied across a membrane with a nanopore, the "screw" and "nut" begin to move with respect to each other, so that their mutual rotation is coupled with their mutual translation. As a result, there are peaks of electrical current connected with the mutual translocation of DNA and its counterion-hydration shell, if DNA has some non-regular base-pair sequence. The calculated peaks of current strongly resemble those observed in the pertinent experiments.

[1] E. B. Starikov, D. Hennig, H. Yamada, R. Gutierrez, G. Cuniberti, and B. Norden, submitted (2008)

TT 23.5 Wed 10:30 HSZ 105

Charge-memory polaron effect in molecular junctions — •Dmitry A. Ryndyk[1], Pino D'Amico[1], Gianaurelio Cuniberti[2], and Klaus Richter[1] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Institute for Material Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden

The charge-memory effect, bistability and switching between charged and neutral states of a molecular junction, as observed in recent STM

experiments, is considered within a minimal polaron model. We show that in the case of strong electron-vibron interaction the rate of spontaneous quantum switching between charged and neutral states is exponentially suppressed at zero bias voltage but can be tuned through a wide range of finite switching timescales upon changing the bias. We further find that, while junctions with symmetric voltage drop give rise to random switching at finite bias, asymmetric junctions exhibit hysteretic behavior enabling controlled switching. Lifetimes and charge-voltage curves are calculated by the master equation method for weak coupling to the leads and at stronger coupling by the equation-of-motion method for nonequilibrium Green functions.

TT 23.6 Wed 10:45 HSZ 105

Spin-Vibration Coupling and Kondo Effect in Transport through Single-Molecule Magnets — •Falk May[1], Maarten R.Wegewijs[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik,J. W. Goethe-Universität, D-60438 Frankfurt, Germany — [2]Institut für Theoretische Physik, Lehrstuhl A, RWTH Aachen, D-52056 Aachen, Germany

We study transport properties of a single-molecule magnet (SMM) strongly coupled to electronic leads in the low temperature limit using the numerical renormalization group. These molecules can be characterized by a large spin and magnetic anisotropies arising from spin-orbit coupling of magnetic ions and ligand field effects. We address the important question of the coupling of the spin to a localized molecular vibration, which can also be anisotropic. We find a rich interplay with effects of intrinsic quantum spin-tunneling, responsible for the Kondo effect in such systems [1], for example a Kondo resonance induced solely by zero-point quantum vibrations.

[1] C. Romeike et al., Phys. Rev. Lett. **96**, 19 (2006)

15 min. break

TT 23.7 Wed 11:15 HSZ 105

Vibrational Nonequilibrium Effects in Single-Molecule Conductance — •Rainer Härtle and Michael Thoss — Theoretische Chemie, Lichtenbergstrasse 4, D-85747 Garching, Germany

Vibrational nonequilibrium effects in charge transport through single-molecule junctions are theoretically investigated by employing a master equation and a nonequilibrium Green's function approach. For molecules that are asymmetrically bound to the leads, vibrationally coupled charge transport, in particular through a single non-degenerate electronic level, exhibits pronounced rectification and negative differential resistance, which can be solely attributed to vibrational nonequilibrium and electron-hole pair creation processes. Focusing on molecular bridges with multiple electronic states, it is shown that electronic-vibrational coupling triggers a variety of vibronic emission and absorption processes, which influence the conductance properties and mechanical stability of single-molecule junctions profoundly. These processes are analyzed in detail for generic model systems of molecular junctions and for more realistic models that are based on ab-initio quantum chemistry calculations.

TT 23.8 Wed 11:30 HSZ 105

Entangled excitation dynamics in biomolecules due to spatially correlated environmental fluctuations — •Peter Nalbach and Michael Thorwart — Freiburg Institute for Advanced Studies, Albert-Ludwigs Universität Freiburg, Albertstr. 19, 79104 Freiburg

In photosynthetic light harvesting complexes, absorbed photons induce excitations of biomolecular chromophores. The excitation moves until it reaches the reaction center where it transfers its energy to chemical reaction energy. A single excitation in two chromophores can be described by a quantum two level system (TLS) where the chromophore coupling is of Förster-type and is described as tunnelling between the two sites. In order to compare the energy transferred to a reaction center with the loss to the environment (formed by vibrational and rotational states of the molecular complexes or charge fluctuations in the solvent-protein host), a coupling of the TLS to an environment is introduced. The environment is characterized by a rather small reorganization energy, leading to slow bath-induced fluctuations. We investigate two coupled TLSs and show that quantum coherent energy transfer is efficiently supported by a slow (non-Markovian) bath which has spatial correlations extending over distances larger than the biomolecule distance. We discuss the inter-chromophore coupling generated by the slow bath modes which couple to both TLSs, its dependence on spatial distance and its influence on the coherent dynamics of the excitations.

TT 23.9 Wed 11:45 HSZ 105

Phthalocyanine based molecular switches — •Thomas Brumme, Cormac Toher, Florian Pump, and Gianaurelio Cuniberti — Insitute for Materials Science, TU Dresden

Me-Phthalocyanine (MePc) molecules have potential applications as switches in molecular electronics. Recent experiments performed by the group of R. Berndt at the University Kiel indicate that SnPc can be changed between an in-plane and an out-of-plane conformation by means of STM induced tunneling. To control this switching it is crucial to understand the underlying transport mechanism.

We have studied the electronic transport properties of structural conformations of various MePc molecules on a Au(111) surface. In particular, the possibility of switching the larger metal atoms in an STM experiment between an in-plane and an out-of-plane conformation has been investigated. We used an STM-tip/molecule/surface configuration in order to work out which transport regime could induce this shift. The electronic transport properties and the geometry of the system were calculated for different applied bias voltages. We also investigated the variation of the transport characteristics through the MePc molecule with increasing current.

TT 23.10 Wed 12:00 HSZ 105

Interplay of Mechanical and Electrical Degrees of Freedom in Molecular Junctions — •Florian Pump[1], Cormac Toher[1], Ruslan Temirov[2], Olga Neucheva[2], Serguei Soubatch[2], Stefan Tautz[2], Michael Rohlfing[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden — [2]Institut für Bio- und Nanosysteme 3, JARA, Forschungszentrum Jülich, D-52425 Jülich — [3]Department of Physics, University of Osnabrück, D-49069 Osnabrück

The electronic transport properties of molecular junctions are very sensitive to the contact configuration which is usually not very well known. One type of setup which allows more control over the contact geometry uses an STM (scanning tunnelling microscope) tip as one of the electrodes enabling the investigation of both the electronic and geometric structure of the junction. We present, using the non-equilibrium Green function formalism in combination with DFT [2-4], the results of our recent calculations related to a set of experiments studying PTCDA on metallic surfaces [1]. The calculations allow for the systematic investigation of the effect of the contact geometry on the transport properties of molecular junctions, which should in turn improve the agreement between theory and experiment.

[1] R. Temirov, A. Lassise, F. B. Anders, and F. S. Tautz, Nanotechnology **19**, 065401 (2008).
[2] F. Pump *et al.*, Appl. Phys. A **93**, 335 (2008).
[3] A. R. Rocha *et al.*, Phys. Rev. B **73**, 085414 (2006).
[4] A. Pecchia and A. Di Carlo, Rep. Prog. Phys. **67**, 1497 (2004).

TT 23.11 Wed 12:15 HSZ 105

Control of the Conductance in Molecular Switch Junctions — •Daijiro Nozaki, Cormac Toher, Florian Pump, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden, Germany

We explore the usability of molecules with bistable characteristics as reversibly tunable molecular switches driven by external stimulation such as light [1] or current-pulse [2]. We have modeled three molecular switch-junctions formed with silicon contacts and azobenzene derivatives which have bistable cis- and trans-conformations. Using the nonequilibrium Green's function approach implemented with the density-functional-based tight-binding theory [3], we analyzed electron transmission, on/off ratios, potential energy surfaces along reaction coordinate from cis- to trans-conformation, and the stability of the molecular switches in ambient conditions along MD pathways.

The numerical results have shown that transmission spectra in *cis*-conformations are more conductive than *trans*-ones inside of the bias window in three models. I-V characteristics also lead to the same trends. Additionally, the transmission along MD pathways have shown that the *cis*-conformations are always more conductive than *trans*-ones at room temperature. Therefore, the azobenzene derivative-based molecular switches can be expected to work as robust switching components.

[1] M. del Valle *et al.*, Nature Nanotech. **2**, 176 (2007).
[2] H. Riel *et al.*, Small, **2**, 973 (2006).
[3] A. Pecchia *et al.*, Rep. Prog. Phys. **67**, 1497 (2004).

TT 24: Correlated Electrons: (General) Theory 2

Time: Wednesday 9:30–13:00 Location: HSZ 301

TT 24.1 Wed 9:30 HSZ 301

Finite-Temperature Variational Cluster Approach (VCA) — •Gang Li, Maximilian Kiesel, and Werner Hanke — Institute for Theoretical Physics and Astrophysics, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The Variational Cluster Approach (VCA) proliferates the many-body physics, contained in an exact solution of a "reference system", i.e. a cluster, in a controlled manner to the infinite-system size limit of strongly correlated lattice models. This approach has been found for the 2D single-band Hubbard model to reproduce salient features of the ($T = 0$) ground-state phase diagram [1], single-particle excitations [2] and, most recently, two-particle, i.e. magnetic excitations [3]. Here, we describe an implementation of the continuous-time QMC technique as a "cluster solver". This new method allows to consider finite temperature properties as well as a significantly large number of electronic (orbital) degrees of freedom in the underlying many-body model.

[1]. M. Aichhorn, E. Arrigoni, M. Potthoff, W. Hanke, Phys. Rev. B. **74**, 024508 (2006).

[2] M. Aichhorn, E. Arrigoni, Z. B. Huang, W. Hanke, Phys. Rev. Lett. **99**, 257002 (2007).

[3] S. Brehm, E. Arrigoni, M. Aichhorn, W. Hanke, arXiv: 0811.05213 (21.11.08).

TT 24.2 Wed 9:45 HSZ 301

The Dynamical Vertex Approximation: spatial correlations beyond Dynamical Mean Field Theory — •Alessandro Toschi[1], Andrey Katanin[2,3], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Austria — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institute of Metal Physics, Ekaterinburg, Russia

Progress in going beyond the purely local description of the Dynamical Mean Field Theory (DMFT) has been recently obtained through cluster extensions of the method, which include spatial correlations within the cluster size. Long-range spatial correlations may be, however, of vital importance: They are responsible for a rich variety of phenomena, ranging from magnons and screening of the Coulomb interaction to quantum criticality. Our new diagrammatic approach, coined "Dynamical Vertex Approximation" (DΓA)[1,2], provides for a systematic treatment of the effects of long-range spatial correlations beyond DMFT. Specifically, we use the DΓA with a Moriyaesque λ correction for studying the impact of antiferromagnetic fluctuations on the spectral function in the whole phase diagram of the Hubbard model in three[1] and intwo dimensions[2,3] . The diagrammatic nature of DΓA, moreover, makes the algorithm well suited for a generalization to the more realistic case of multi-band Hamiltonians.

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

[2] K.Held, A. Katanin, and A. Toschi, Prog. Theo. Phys. Suppl, **176**, in print (arXiv: 0807.1860).

[3] A. Katanin, A. Toschi, and K. Held, arXiv:0808.0689 submitted to Phys. Rev. B

TT 24.3 Wed 10:00 HSZ 301

Long-range correlations beyond DMFT: the ladder dual fermion approach — •Hartmut Hafermann[1,3], Alexei N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute for Molecules and Materials, Radboud University of Nijmegen, 6525 ED Nijmegen, The Netherlands

The dual fermion approach is a systematic perturbative extension of dynamical mean-field theory to describe the physics of strongly correlated lattice fermions. We generalize the approach to include long-range correlations via a ladder approximation to the self-energy. The method is applied to the two-dimensional Hubbard model. While the mean-field solution fails to describe the physics in the vicinity of the antiferromagnetic instability, the ladder approximation recovers good agreement to quantum Monte-Carlo results. Inclusion of the long-range correlations leads to the formation of a pseudogap in the local density of states.

TT 24.4 Wed 10:15 HSZ 301

Analytic Continuation of Quantum Monte Carlo Data by Stochastic Analytic Inference — •Sebastian Fuchs[1,2], Mark Jarrell[2], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803, USA

The maximum entropy method is the standard tool for the analytic continuation of imaginary-time quantum Monte Carlo data. It uses arguments of Bayesian logic to obtain the most probable energy spectrum given the imaginary-time input data.

In the past efforts where made to provide an alternative to this standard approach [2]. It was proposed to perform an average over a wide range of spectra using Monte Carlo techniques instead of selecting a single spectrum. So far, the method lacked a rigorous rule to eliminate a free regularization parameter inherent in the algorithm.

We propose an algorithm that is based on Bayesian inference. It utilizes Monte Carlo simulations to both calculate a weighted average of possible spectra and to provide a strict criterion for the elimination of the regularization parameter.

Our implementation is based on the libraries of the ALPS project [3]. ALPS is an open source effort providing libraries and simulation codes for strongly correlated quantum mechanical systems.

[1] M. Jarrell, G. E. Gubernatis, Phys. Rep. **269**, 133 (1996).

[2] A. Sandvik, PRB **57**, 10287 (1998); K. Beach, cond-mat/0403055

[3] `http://alps.comp-phys.org`

Invited Talk TT 24.5 Wed 10:30 HSZ 301

Theory of time-resolved optical and photoemission spectroscopy for correlated electron systems — •Marcus Kollar — Theoretische Physik III, Universität Augsburg, 86135 Augsburg

In pump-probe experiments the real-time dynamics of interacting electrons is measured by first driving the sample out of equilibrium with a pump pulse, and then probing its state with a second pulse after a controlled time delay. In time-resolved (TR) optical spectroscopy the reflected electrical field is measured, whereas in TR photoemission spectroscopy the spectrum of the emitted electrons is analyzed. These experimental signals can be related to the two-time optical conductivity and to the real-time electronic Green function, respectively. Both quantities can be calculated using nonequilibrium dynamical mean-field theory (DMFT), which maps an interacting lattice system onto an effective time-dependent single-site problem. TR optical spectroscopy has the advantage of full time resolution [1], whereas TR photoemission spectroscopy provides momentum resolution of the electronic Green functions but suffers from some energy-time uncertainty restrictions [2]. We present explicit results for the Falicov-Kimball model [1,2], for which we model the pump excitation by a sudden parameter change in the Hamiltonian [3]. We identify characteristic signatures in the experimental signals, e.g., for as-yet-unobserved electronic collapse-and-revival oscillations, the type of which are well-known from cold atom experiments.

[1] M. Eckstein and M. Kollar, Phys. Rev. B **78**, 205119 (2008).

[2] arXiv:0809.4282; [3] Phys. Rev. Lett. **100**, 120404 (2008).

15 min. break

TT 24.6 Wed 11:15 HSZ 301

Adiabatic parameter change across the metal-insulator transition in the Falicov-Kimball model — •Martin Eckstein and Marcus Kollar — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86153 Augsburg

We obtain the exact time evolution of the fermionic Falicov-Kimball model during a slow variation of the interaction parameter, using dynamical mean-field theory (DMFT) for nonequilibrium. For this purpose we adapt the DMFT equations which were derived for a sudden interaction quench [1] and solve them numerically. We analyze the dependence of the excitation energy on the ramp speed in the adiabatic limit, and find different power laws when the system is driven within the insulating phase, within the metallic phase, or between the two phases. Possible reasons for this behavior are discussed.

[1] M. Eckstein and M. Kollar, Phys. Rev. Lett. **100**, 120404 (2008).

TT 24.7 Wed 11:30 HSZ 301

Time evolution of correlations in strongly interacting fermions after a quantum quench — •Salvatore R. Manmana[1], Stefan Wessel[2], Reinhard M. Noack[3], and Alejandro Muramatsu[2] — [1]Institute of Theoretical Physics (CTMC), EPF Lausanne, CH-1015 Lausanne, Schweiz — [2]Institut für Theoretische Physik III, Universität Stuttgart — [3]Fachbereich Physik, Philipps-Universität Marburg

Using the adaptive time-dependent density matrix renormalization group, we study the time evolution of density correlations of interacting spinless fermions on a one-dimensional lattice after a sudden change in the interaction strength. Over a broad range of model parameters, the correlation function exhibits a characteristic light-cone-like time evolution representative of a ballistic transport of information. Such behavior is observed both when quenching an insulator into the metallic region and also when quenching within the insulating region. However, when a metallic state beyond the quantum critical point is quenched deep into the insulating regime, no indication for ballistic transport is observed. Instead, stable domain walls in the density correlations emerge during the time evolution, consistent with the predictions of the Kibble-Zurek mechanism.

TT 24.8 Wed 11:45 HSZ 301

Influence of orbital degeneracy on the two particle spectral function — •Berlinson Dominikus Napitu[1,2] and Jamal Berakdar[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Institut für Physik- Heinrich-Damerow-Strasse 4 Halle (Saale)

We studied the evolution of two particle spectral function of the orbitally degenerate Hubbard model with the same and different bandwidth. The calculation of single particle spectra is based on dynamical mean field theory (DMFT) together with quantum monte carlo (QMC) while for two particle spectra the ladder approximation is implemented. The influence of temperature is also considered.

TT 24.9 Wed 12:00 HSZ 301

Band formation vs. local correlations: NiO — •T. Haupricht[1], R. Gierth[1], J. Weinen[1], S. G. Altendorf[1], A. Hendricks[1], Y.-Y. Chin[1,2], Z. Hu[1], J. Gegner[1], H. Fujiwara[1], D. Regesch[1], H. H. Hsieh[3], H.-J. Lin[2], C. T. Chen[2], and L. H. Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

Modeling the electronic structure of NiO is a true theoretical challenge. Even though the general agreement between the experimental valence-band photoemission (PES) spectrum of NiO and the results of a single-site cluster configuration interaction calculation is very good, some structures in the spectrum remain unexplained. These shortcomings have been recognized already when looking at the Ni $2p$ core level spectra, and were attributed to so-called non local screening effects involving neighboring Ni clusters [v. Veenendaal et al., PRL 70 (1993)]. We therefore set out to measure the valence band PES of NiO impurities in MgO thin films. Comparing the NiO impurity valence band spectrum to that of bulk NiO we find that there are indeed remarkable differences. On the other hand we find that the correspondence of the experimental NiO impurity valence band and the result of the cluster calculation is very good. We also compare our experimental data to the results of recent LDA+DMFT calculations [Kuneš at al., PRL 99 (2007); Kuneš at al., PRB 75 (2007); Taguchi et al., PRL 100 (2008)] with reasonable results but also showing characteristic discrepancies.

TT 24.10 Wed 12:15 HSZ 301

Pseudogap phase in hole-doped high-temperature superconductors — •Steffen Sykora and Klaus W. Becker — Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden

One of the most important unsolved problems in the understanding of copper-oxide superconductors is the pseudogap phase which is a most unusual state of matter. ARPES experiments have revealed a gap-like behavior on parts of the Fermi surface, leaving a non gapped segment known as Fermi arc around the diagonal of the Brillouin zone. Two main interpretations of the origin of the pseudogap have been proposed: either the pseudogap is a precursor to superconductivity, or it arises from another order competing with superconductivity. In this paper, the pseudogap phase is investigated in the framework of a novel renormalization scheme. We present results for the one-particle spectral function $A_{\mathbf{k}}(\omega)$ near the Fermi level for different values of wave vector $\mathbf{k}$, doping and temperature. The results show an excellent agreement with recently puplished ARPES measurements. The origin of the pseudogap will be discussed.

TT 24.11 Wed 12:30 HSZ 301

Renormalization approach to the two-dimensional Periodic Anderson Model — •Alexander Mai and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden

Despite the success of numerical methods in the treatment of strongly correlated electron systems, analytical approaches are still needed to obtain a deeper understanding of the underlying physics. We apply the Projector-based Renormalization Method (PRM) to the Periodic Anderson Model (PAM) in two dimensions to study the valence transition in heavy fermion systems and its dependence on the different model parameters. In order to investigate superconductivity we extend the model by adding a conduction electron phonon coupling. We discuss the superconducting solution with respect to the different parameters of the model and the valence transition in the PAM.

TT 24.12 Wed 12:45 HSZ 301

Ab initio correlated electronic structure of Cu oxide and Fe-As compounds: a quantum chemical perspective — •Liviu Hozoi, Mukul Laad, and Peter Fulde — Max-Planck-Institut fuer Physik komplexer Systeme, Dresden

Wavefunction-based methods from modern quantum chemistry are applied to the study of the electronic structure of correlated transition-metal compounds. Whereas the correlation treatment is performed in direct-space, a k-space representation can be obtained later on after accounting for the (strong) short-range correlations. In some cases, a balanced treatment of the short-range interactions, onsite and intersite, is essential for achieving even a qualitatively correct picture.

In cuprates, we find that the Fermi surface (FS) of the hole doped material evolves from small hole pockets in the deeply underdoped region to one with both hole- and electron-like sheets at slightly higher doping and to a large FS consistent with Luttinger's theorem at still higher hole concentrations. Our results offer a route toward a resolution of the controversy generated by the apparent inconsistency between Shubnikov-deHaas measurements and the Luttinger sum rule for underdoped cuprates, as well as with recent Hall-effect data suggesting an electron-like Hall constant for hole doped cuprates at low T.

The multiorbital correlated electronic structure of the recently discovered Fe-As superconducting compounds is also discussed. We compute the ground-state for the undoped case and provide new insight into the nature of doped holes and electrons.

TT 25: Superconductivity: Cuprate High-Temperature Superconductors 1

Time: Wednesday 9:30–13:00 Location: HSZ 304

TT 25.1 Wed 9:30 HSZ 304

Stripe-like charge order in $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ studied by resonant soft X-ray diffraction — •Jörg Fink[1,2], Enrico Schierle[1], Viktor Soltwisch[1], Eugen Weschke[1], Hermann Dürr[1], Jochen Geck[2,3], Patrick Ribeiro[2], Bernd Büchner[2], David Hawthorn[3], and George Sawatzky[3] — [1]Helmholtz Zentrum Berlin — [2]IFW Dresden — [3]University of British Coulombia, Vancouver, Canada

In the doped cuprates there exists a complex interplay between lattice, charge and spin degrees of freedom leading to the appearance of stripe phases. In the stripe phases antiferromagnetic antiphase magnetic domains are separated by periodically spaced domain walls to which the holes segregate. We used resonant soft X-ray scattering with photon energies near the O K and the Cu L3 edges to study the charge order-

ing in the system $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$. This method is the only one in which static charge ordering can be directly detected. A complete phase diagram could be derived for the charge ordering which will be compared with structural and spin ordering. In addition,information on the amplitude and on the doping dependence of the wave lenght of the charge ordering is provided. The results support strong coupling scenarios for the mechanism of stripe formation.

TT 25.2 Wed 9:45 HSZ 304

Evidence for Fermi surface reconstruction in the static stripe phase of $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$, $x = 1/8$ — •V. B. Zabolotnyy[1], A. A. Kordyuk[1,2], D. S. Inosov[1,3], D. V. Evtushinsky[1], R. Schuster[1], B. Büchner[1], N. Wizent[1], G. Behr[1], S. Pyon[4], T. Takayama[4], H. Takagi[4], R. Follath[5], and S. V. Borisenko[1] — [1]Institute for Solid State Research, IFW-Dresden, P.O.Box 270116, D-01171 Dresden, Germany — [2]2Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [4]Department of advanced materials, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa 277-8561, Japan — [5]BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

We present a photoemission study of $La_{0.8-x}Eu_{0.2}Sr_xCuO_4$ with doping level x=1/8, where the charge carriers are expected to order forming static stripes. Though the local probes in direct space seem to be consistent with this idea, there has been little evidence found for such ordering in quasiparticle dispersions. We show that the Fermi surface topology of the 1/8 compound develops notable deviations from that observed for $La_{2-x}Sr_xCuO_4$ in a way consistent with the FS reconstruction expected for the scattering on the antiphase stripe order.

TT 25.3 Wed 10:00 HSZ 304

Renormalization of the longitudinal bond-stretching phonon branch in $La_{1.95}Sr_{0.05}CuO_4$ probed by inelastic neutron scattering technique — •A. Hamann[1], D. Lamago[1,2], L. Pintschovius[1], K. Yamada[3], M. Fujita[3], and D. Reznik[1,2] — [1]Institut für Festkörperphysik, KIT, 76021 Karlsruhe, Germany — [2]LLB, CEA Saclay, 99191 Gif sur Yvette, France — [3]Institute for Materials Research, Tohoku Univ., Katahira, Sendai 980-8577, Japan

$La_{2-x}Sr_xCuO_4$ becomes superconducting (sc) for $0.06 \leq x < 0.3$, where optimal doping of $x = 0.15$ results in T_c up to 38 K. The mechanism leading to SC remains to be understood. Neutron scattering experiments revealed anomalous phonon behavior that hints at an enhanced electron-phonon coupling possibly connected to dynamic stripe order [1].

We report our latest measurements on non-sc $La_{1.95}Sr_{0.05}CuO_4$. Shell model predictions including resolution effects were used to fit the data. We found that in comparison to the sc-samples the anomalous phonon behavior becomes much less pronounced.

[1] D. Reznik et al., Nature **440**, 1170 (2006)

TT 25.4 Wed 10:15 HSZ 304

Charge stripes and electron phonon coupling in cuprates — •A. C. Komarek[1], A. Hiess[2], H. Hiraka[3], K. Ikeuchi[3], M. v. Zimmermann[4], M. Fujita[3], K. Yamada[3], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpcher Str. 77, 50937 Köln, Germany — [2]Institut Laue-Langevin, BP 156, 6 rue Jules Horowitz, 38042 Grenoble Cedex 9, France — [3]Institute for Material Research, Tohoku University, Katahira, Sendai 980-8577, Japan — [4]Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron, 22603 Hamburg, Germany

The role of electron-phonon coupling and its relevance to the pairing meachanism in high-temperature superconductivity is still a matter of controversy. The $(La,Sr)_2CuO_4$ (LSCO) system appears well suited for a study of the electron phonon coupling as the lattice dynamics is less complex than that of other cuprates. The strongest signatures of electron-phonon coupling are found in the longitudinal bond-stretching branches. In general these modes couple to charge fluctuations on the metal sites. In particular, the polarization patterns of modes propagating along the [100]-direction correspond to the distortions expected for the stripe ordering, which occurs in Nd-codoped LSCO and in $La_{1.88}Ba_{0.12}CuO_4$. We have searched for charge stripe order and studied the electron phonon coupling in the spin glass phase of LSCO ($x = 0.05$). Furthermore, the response of the electron phonon anomaly in LSCO ($x \approx 0.12$) on Zn- and Ni-doping was analysed.

TT 25.5 Wed 10:30 HSZ 304

Static and fluctuating stripe order in 1/8-doped LNSCO and LSCO — •Hsueh-Hung Wu[1,2], Marcel Buchholz[1], Christoph Trabant[1], Franziskus Heigl[3], Enrico Schierle[4], Matthias Cwik[1], Markus Braden[1], Liu-Hao Tjeng[1], and Christian Schüssler-Langeheine[1] — [1]II. Physikalisches Institut, Universitaet zu Koeln, Germany — [2]NSRRC, Hsinchu, Taiwan — [3]ALBA, Barcelona, Spain — [4]Helmholtz-Zentrum Berlin

We have studied the stripe order in $La_{1.475}Nd_{0.4}Sr_{0.125}CuO_4$ (LNSCO) and $La_{1.88}Sr_{0.12}CuO_4$ (LSCO) using resonant soft x-ray diffraction (RSXD). In both systems, a pronounced charge order (CO) peak was found at the oxygen K and copper $L_{2,3}$ edges. While for LNSCO, Nd stabilizes the static CO, no static CO has been found in LSCO [1]. In fact, earlier experiments from the isostructural nickelate system indicates that RSXD is suited to observe not only static, but also fluctuating order. This is particularly interesting for fluctuating CO, which is very difficult to probe with inelastic neutron diffraction. For LNSCO, the CO signal vanishes near the tetragonal to orthorhombic structural transition; in LSCO, the signal vanishes slightly above the critical temperature similar to what has been found for the spin order [2]. The resonance of the CO signal in both samples looks very similar at the O K edge, while some differences at the Cu $L_{2,3}$ edges are found. The spectroscopic interpretation of these findings will be discussed.

[1] M. Fujita *et al.*, Phys. Rev. Lett. **88**, 167008 (2002).
[2] H. Kirmura *et al.*, Phys. Rev. B **59**, 6517 (1999).

TT 25.6 Wed 10:45 HSZ 304

Interplay of charge stripe order with structural distortions: a high pressure x-ray study — •M. v. Zimmermann[1], M. Huecker[2], J.M. Tranquada[2], M. Debessai[3], J.S. Schilling[3], and G.D Gu[2] — [1]Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron, 22603 Hamburg, Germany — [2]Brookhaven National Laboratory, Upton, New York 11973, USA — [3]Dept. of Physics, Washington University, St. Louis, Missouri 63130, USA

The stability of charge stripe order in $La_{2-x}Ba_xCuO_4$ (LBCO) is still poorly understood. At x=1/8 LBCO exhibits a pronounced suppression of superconductivity and a static ordering of of spins and charge into a stripe pattern. At the same doping a structural transition from the usual orthorhombic phase (LTO) into the low temperature tetragonal phase (LTT) is observed. By the application of pressure the stability of the LTT and the LTO phase can be tuned and thus the influence of these structural distortion on the stripe order be studied. Using high energy x-ray diffraction the presence of charge stripes in a lattice without long range distortions could be found, indicating that electronic effects also contribute to the stablity if stripe order.

15 min. break

TT 25.7 Wed 11:15 HSZ 304

Electron-Phonon Interaction in Strongly Correlated Systems — •giorgio sangiovanni[1] and olle gunnarsson[2] — [1]Vienna University of Technology — [2]Max-Planck Institute - Stuttgart

Oxygen isotope effect on the low-energy dispersion kink has been recently reported by Iwasawa et al. using high-resolution laser photoemission [1], suggesting a major role of the half-breathing oxygen phonon in high-temperature superconducting cuprates. The same phonon mode displays a huge anomaly approximately half-way to the zone boundary in the dispersion and in the width detected by inelastic neutron scattering [2]. In order to get a strong coupling to the half-breathing and other phonon modes in theoretical calculations electronic correlations turn out to be an essential ingredient.

[1] H. Iwasawa, *et al.*, Phys. Rev. Lett. **101**, 157005 (2008)
[2] D. Reznik, *et al.*, Nature **455**, E6 (2008)

TT 25.8 Wed 11:30 HSZ 304

Momentum dependence of the electron-phonon coupling, phonon-induced pairing interaction, and self-energy effects in $YBa_2Cu_3O_7$ within the local density approximation — •Dirk Manske[1], Rolf Heid[2], Roland Zeyher[1], and Klaus-Peter Bohnen[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Forschungszentrum Karlsruhe, Germany

Using the local density approximation (LDA) and a realistic phonon spectrum we calculate the momentum and frequency dependence of the electron-phonon coupling in $YBa_2Cu_3O_7$ and determine its consequences for the phonon-induced pairing interaction and for the electronic self-energy in the normal state.

The phonon-induced interaction has a pronounced peak for large momentum transfers and the interband contributions between bonding and antibonding band are of the same magnitude as the intraband ones. The dimensionless coupling constant in the d-wave channel λ^d, relevant for superconductivity, is only 0.022, i.e., even about ten times smaller than the small value of the s-wave channel.

For electronic states at the Fermi energy, the maximum in the real part of the phonon-induced self-energy at low frequencies is about a factor 5 too small compared to the experiment, resulting in a very small and smooth change in the slope of the electronic dispersion [1].

These findings suggest that phonons are not the important low-energy excitations, and cannot produce well-pronounced kinks in $YBa_2Cu_3O_7$, at least, within LDA.

[1] R. Heid, K.-P. Bohnen, R. Zeyher, D. Manske, PRL **100**, 137001 (2008).

TT 25.9 Wed 11:45 HSZ 304

Theory of two-particle excitations and the magnetic susceptibility in high-T_c cuprate superconductors — •Sascha Brehm[1], Enrico Arrigoni[2], Markus Aichhorn[3], Maximilian Kiesel[1], and Werner Hanke[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau Cedex, France

Two-particle (2-p) excitations such as spin and charge excitations play a key role in high-T_c cuprate superconductors (HTSC). On the basis of a parameter-free theory, which extends the Variational Cluster Approach (a recently developed embedded cluster method) to 2-p excitations, the magnetic excitations of HTSC are shown to be reproduced for a Hubbard model within the relevant strong-coupling regime [1]. In particular, the resonance mode in the underdoped regime, its intensity, "hour-glass"dispersion and doping dependence are in good overall agreement with experiments [1]. Combined with the earlier results for the phase diagram and one-particle excitations, such as the electron-hole asymmetry in the doping dependence of AF and SC phases [2] and the presence of a gap dichotomy of the nodal and antinodal SC gaps [3], a consistent picture emerges, which lends substantial support to Hubbard-model descriptions of high-T_c cuprate superconductivity.

[1] S. Brehm et *al.*, arXiv:0811.0552.
[2] M. Aichhorn et *al.*, Phys. Rev. B 75, 235117 (2006).
[3] M. Aichhorn et *al.*, Phys. Rev. Lett. 99, 257002 (2007).

TT 25.10 Wed 12:00 HSZ 304

Raman study of $La_{2-x}Sr_xCuO_4$: Evidence of universal electronic properties — •Bernhard Muschler[1], Wolfgang Prestel[1], Leonardo Tassini[1], Seiki Komiya[2], Yoichi Ando[2], Michael Lambacher[1], Andreas Erb[1], and Rudi Hackl[1] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching — [2]CRIEPI, Komae, Tokyo 201-8511, Japan

We report results of electronic Raman scattering (ERS) experiments in $La_{2-x}Sr_xCuO_4$ single crystals in the doping range $0.02 \leq x \leq 0.30$. Due to the momentum resolution of ERS we are able to independently analyze the nodal and the antinodal carriers. We extract static carrier relaxation rates from the Raman spectra by applying an extended Drude analysis. For the nodal carriers we find doping independent scattering rates which trace the transport data measured on the same crystal. For the antinodal carriers we find an evolution of the relaxation rates with doping. The relaxation rates are isotropic for $x > 0.20$. In the range $0.16 \leq x \leq 0.20$ the carrier lifetimes become momentum dependent. Below optimal doping there is a peak superimposed on the usual response of the carriers which originates from charge ordering fluctuations. This peak is observed in the nodal and the antinodal response for $x \leq 0.05$ and $x \geq 0.05$, respectively. The temperature dependence indicates the existence of a quantum critical point at $x = 0.18$ which is related to a charge ordering instability.

This work is supported by the DFG under Grant No. Ha2071/3-4 in the Research Unit FOR538.

TT 25.11 Wed 12:15 HSZ 304

Comparison of ARPES and Raman spectra — •Wolfgang Prestel[1], Bernhard Muschler[1], Nathalie Munnikes[1], Michael Lambacher[1], Andreas Erb[1], Yoichi Ando[2], Shimpei Ono[3], Toshizo Fujita[2], Andrea Damascelli[4], Hiroshi Eisaki[5], Martin Greven[6], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching — [2]Osaka University, Osaka 567-0047, Japan — [3]CRIEPI, Komae, Tokyo 201-8511, Japan — [4]UBC, Vancouver, BC V6T 1Z4, Canada — [5]AIST, Tsukuba 305-8568, Japan — [6]Stanford University, Stanford, CA 94305, USA

Cuprate superconductors are strongly correlated metals. In the overdoped range the electrons can be described in terms of Landau quasiparticles. They manifest themselves as well defined peaks in the angle-resolved photoemission (ARPES) spectra. Using ARPES results we can quantitatively predict the normal state Raman spectra above a doping of $p \approx 0.21$. For $p < 0.21$ we find discrepancies between simulation and experiment in the B_{1g} channel becoming increasingly strong for decreasing p. At optimal doping we compare ARPES data and Raman measurements also in the superconducting state. Here we use an analytic expression which reproduces the ARPES data quantitatively in the entire Brillouin zone. Similarly as in the normal state, the B_{2g} spectra are well reproduced, while there are discrepancies in B_{1g} symmetry.

The project has been supported by the DFG under grant number Ha2071/3-4 via the Research Unit FOR538.

TT 25.12 Wed 12:30 HSZ 304

Two component dynamics of the superconducting order parameter revealed by time-resolved Raman scattering — •Ilka Mahns[1], R. Pelangi Saichu[1], Arne Goos[1], Stephan Binder[1], Patrick May[1], Stefan G. Singer[1], Benjamin Schulz[1], Andrivo Rusydi[1,2], Julia Unterhinninghofen[3], Dirk Manske[4], Prasenjit Guptasarma[5], Mark S. Williamsen[5], and Michael Ruebhausen[1] — [1]Institut fuer Angewandte Physik, Universitaet Hamburg, Germany. Center for Free Electron Laser Science (CFEL), Hamburg, Germany — [2]Department of Physics, NUS, Singapore — [3]Institut fuer Theoretische Physik, Universitaet Bremen, Germany — [4]Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, Germany — [5]Department of Physics, University of Wisconsin,USA

The nature of the interaction between holes leading to superconductivity is encoded in the properties of the superconducting order parameter. These properties are reflected by the energy and the time scales on which the order parameter reacts to an external perturbation. Here, we present unique results detecting the dynamics of the superconducting order parameter in Bi-2212 by employing a time-resolved pump-probe Raman experiment. We find two different coupling mechanisms that contribute equally to the relaxation of the pair breaking peak. A model that couples holes through phonons is able to reproduce only one part of the condensate dynamics, thus, outlining also the importance of hole-spin interactions.

TT 25.13 Wed 12:45 HSZ 304

Charge-Transfer Excitons In Underdoped $Ca_{2-x}Na_xCuO_2Cl_2$ — •R. Schuster[1], S. Pyon[2], M. Knupfer[1], J. Fink[1,3], M. Azuma[4], M. Takano[4], H. Takagi[2], and B. Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Department of Advanced Materials Science, University of Tokyo, Kashiwa 277 8581, Japan — [3]BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [4]Inst. Chem. Res., Kyoto Univ., Uji, Kyoto-fu 611-0011, Japan

Employing electron energy-loss spectroscopy we show that small values of doping in the system $Ca_{2-x}Na_xCuO_2Cl_2$ strongly influence the formation and dynamics of charge-transfer excitons in the Cu-O plane. We find a remarkable redistribution of spectral weight between the two modes seen in the insulator yielding a single sharp feature for non-zero doping; accompanied by a strong suppression of the dispersion. Our data may provide evidence for a prominent role of the magnetic background on the dynamics of charge-transfer excitations in underdoped cuprates.

TT 26: Transport: Graphene and Carbon Nanotubes

Time: Wednesday 14:00–19:00 Location: HSZ 03

Invited Talk TT 26.1 Wed 14:00 HSZ 03

Nanotube and Graphene ElectroMechanics — •Adrian Bachtold — CIN2 (CSIC-ICN) Barcelona, Campus UAB, Spain

Carbon nanotubes and graphene have attracted a lot of attentions as high-frequency mechanical resonators. For instance, nanotube resonator devices hold promise for ultralow mass detection or quantum electromechanical experiments. However, the detection of the mechanical vibrations remains very challenging. In this talk, I will present a novel detection method of the vibrations of nanotubes and graphene, which is based on atomic force microscopy. This method enables the detection of the resonances up to 3.1 GHz with subnanometer resolution in vibration amplitude. Importantly, it allows the imaging of the mode-shape for the first eigenmodes. I will also report on a new artificial nanofabricated motor in which one short nanotube moves relative to another coaxial nanotube. The motion is shown to be controlled by how the atoms are arranged within the two nanotubes. The motion is actuated by imposing a thermal gradient along the device, allowing for sub-nanometer displacements. This is, to our knowledge, the first experimental demonstration of displacive actuation at the nanoscale by means of a thermal gradient.

TT 26.2 Wed 14:30 HSZ 03

Quantum spin Hall state in gapless graphene? — •Martina Hentschel and Grigory Tkachov — MPI für Physik komplexer Systeme, Dresden

We demonstrate the possibility of a quantum spin Hall state in a two-dimensional gas of massless Dirac fermions as is realized in graphene [1]. To this end we use a generalized zigzag-confinement model that admits a spin-orbit interaction. At a certain critical strength the spin-orbit coupling induces a phase transition of the quantum-spin-Hall type. It is characterized by the existence of a novel type of edge states consisting of a Kramers pair of counter propagating modes with opposite spin orientations (i.e. exhibiting spontaneous quantum Hall effects of opposite signs). These edge states are capable of accumulating an integer spin. They exist without any excitation gap in the bulk, due to which our system stands out among other quantum spin Hall systems studied earlier [2-4]. We show that the local density of states is discontinuous at the transition and its energy dependence reflects the phase diagram of the system.

[1] G. Tkachov and M. Hentschel, arXiv: 0803.0713.
[2] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
[3] B. A. Bernevig and S. C. Zhang,
Phys. Rev. Lett. **96**, 106802 (2006).
[4] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann,
L. W. Molenkamp, X.-L. Qi, and S.-C. Zhang
Science **318**, 766-770 (2007).

TT 26.3 Wed 14:45 HSZ 03

Transport properties of the graphene edge state — •Michael Wimmer, Inanc Adagideli, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

A graphene edge in zigzag configuration supports a localized state, the graphene edge state. Despite being localized at the graphene boundary, recent numerical studies within the nearest-neighbor tight-binding model found that transport in the graphene edge state is influenced little by edge defects [1].

We investigate systematically the transport properties of the graphene edge state for corrections to the nearest-neighbor tight-binding model. In particular we find that the nearest-neighbor tight-binding model—the paradigm model of graphene—is not suitable for describing edge state transport, as exponentially small corrections (such as next-nearest neighbor hopping, see also Ref. [2]) alter the transport properties of the edge state fundamentally.

[1] F. Muñoz Rojas *et al.*, Phys. Rev. B **74**, 195417 (2006), L. Zârbo *et al.*, Europhys. Lett. 80, 47001 (2007).
[2] M. Wimmer *et al.*, Phys. Rev. Lett. **100**, 177207 (2008).

TT 26.4 Wed 15:00 HSZ 03

Exchange phenomena in transport across graphene armchair nanoribbon quantum dots — •Sonja Koller[1], Leonhard Mayrhofer[1,2], and Milena Grifoni[1] — [1]Universität Regensburg — [2]Fraunhofer IWM Freiburg

Taking into account interaction effects, we have investigated spectrum and transport properties of finite size graphene armchair nanoribbons (ACNRs). In wide ribbons, the long-ranged part of the Coulomb interaction dominates, yielding charging and spin-charge separation effects. For narrow ribbons, short-ranged processes become relevant. Those can involve not only two bulk electrons, but also one bulk electron and one electron localized in an edge state, which arises at both zig-zag ends of the stripe. In particular, this edge-bulk interaction strongly influences spectrum and transport properties of the system. In transport, the most prominent feature is the occurrence of a pronounced negative differential conductance for a completely symmetric, unpolarized setup. Further, we discuss the transport characteristics of ACNRs in magnetic field and with collinearly polarized contacts.

TT 26.5 Wed 15:15 HSZ 03

Time dependent transport in graphene nanosystems — •Viktor Krückl[1], Christoph Kreisbeck[1], and Tobias Kramer[1,2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

In recent experiments the Quantum Hall Effect in graphene is measured for high magnetic fields leading to numerous different filling factors. In order to characterise these effects, we investigate the local density of states for the massless Dirac Hamiltonian in crossed electric and magnetic fields. We predict a unique substructure for each Landau level and present analytical expressions to describe their composition. For more complex setups we present an algorithm which solves the time dependent problem. The numerical data corresponds up to a very high accuracy to the aforementioned analytically solvable problem. Within this computational scheme also other phenomena like the Zitterbewegung can be studied.

15 min. break

TT 26.6 Wed 15:45 HSZ 03

Functional RG on graphene nanodisks — •Michael Kinza, Jutta Ortloff, and Carsten Honerkamp — Universität Würzburg, Institut für Theoretische Physik und Astrophysik

Graphene-nanodisks are nanometer-sized graphene structures with a closed edge. They are promising candidates for future nanoelectronic devices. In a tight-binding approximation trigonal zigzag nanodisks with size N (which is proportional to the number of edge atoms) have 2N-fold degenerated zero-energy-states. By using the functional renormalization group an effective Hamiltonian for these zero-energy-states is derived and used to explore spin-resolved transport through the nanodisks coupled to metallic electrodes in the coulomb blockade regime.

TT 26.7 Wed 16:00 HSZ 03

A theory of ballistic transport in disordered graphene — •Alexander Schuessler[1], Pavel Ostrovsky[1], Igor Gornyi[1], and Alexander Mirlin[1,2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

We develop an analytic theory of ballistic electron transport in disordered graphene in a "short-and-wide"geometry [1]. Considering a sample of a large width W, we analyze the evolution of the conductance, the shot noise, and the full statistics of the charge transfer with increasing length L, both at the Dirac point and at a finite gate voltage. The transfer matrix approach combined with the disorder perturbation theory and the renormalization group is used. We also discuss the crossover to the diffusive regime and construct a "phase diagram" of various transport regimes in graphene. Our analytical results are in agreement with experimental observations [2,3].

[1] A. Schuessler et al., arXiv: 0809.3782.
[2] R. Danneau et al., Phys. Rev. Lett. **100**, 196802 (2008).
[3] L. DiCarlo et al., Phys. Rev. Lett. **100**, 156801 (2008).

TT 26.8 Wed 16:15 HSZ 03

Tomonaga-Luttinger liquid parameters of magnetic waveguides in graphene — •W. Häusler[1,2], A. De Martino[1,3], T. K. Ghosh[1,4], and R. Egger[1] — [1]Institut für Theoretis-

che Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany — [3]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Strasse 77, D-50937 Köln, Germany — [4]Department of Physics, Indian Institute of Technology-Kanpur, Kanpur 208016, India

Electronic waveguides in graphene formed by counterpropagating snake states in suitable inhomogeneous magnetic fields are shown to constitute a realization of a Tomonaga-Luttinger liquid. Due to the spatial separation of the right- and left-moving snake states, this non-Fermi liquid state induced by electron-electron interactions is essentially unaffected by disorder. We calculate the interaction parameters accounting for the absence of Galilei invariance in this system, and thereby demonstrate that non-Fermi liquid effects are significant and tunable in realistic geometries.

TT 26.9 Wed 16:30 HSZ 03

Universal conductivity and shot noise in graphene quantum billiards — •Adam Rycerz[1,2] and Michael Wimmer[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040, Germany — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, PL-30059 Kraków, Poland

We study the ballistic electron transport through two types of quantum billiards in undoped graphene: a finite section of the Corbino disc, and a long insulating nanoribbon attached to the leads in a way that the current is flowing *perpendicularly* to the main ribbon axis. We found such a *closed* and an *open* billiard behave similarly when changing geometrical parameters. Namely, both billiards show the *pseudodiffusive regime*, in which the conductance is equal to that of the dissipative medium characterized by the conductivity $\sigma_0 = 4e^2/\pi h$, whereas the Fano factor $\mathcal{F} = 1/3$. In the opposite *tunneling regime*, the conductance shows power-law decay with a distance between leads, and the shot-noise is Poissonian ($\mathcal{F} = 1$). Additionally, in the crossover region between tunneling and pseudodiffusive regimes, the conductance $G \approx (1-\mathcal{F}) \times 4e^2/h$, what shows the transport is dominated by a single evanescent mode with the fourfold (*spin* and *valley*) degeneracy.

TT 26.10 Wed 16:45 HSZ 03

Conductance of graphene ribbons in the presence of chemical adsorbates — Petra Dietl[1], •Georgo Metalidis[1], Pablo San-Jose[1,2], Dmitri Golubev[1], Elsa Prada[1,2], Henning Schomerus[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Department of Physics, Lancaster University, Lancaster, LA1 4YB, United Kingdom

Chemical adsorbates on a graphene sheet have a large influence on its transport properties, making graphene a candidate system for chemical sensors. The influence of adsorbates on the graphene conductivity is twofold. On one hand they can dope the graphene sheet, thus increasing its conductance, while on the other hand the adsorbates form scattering centers that will decrease the conductance. We have investigated the interplay between these competing effects and observed some interesting properties, one of them being an extremely long localization length for certain types of adsorbates.

TT 26.11 Wed 17:00 HSZ 03

Band gap engineering of carbon nanotubes using pulsed high magnetic fields — •Sungho Jhang[1], Yurii Skourski[2], Dominik Preusche[1], Joachim Wosnitza[2], and Christoph Strunk[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Dresden High Magnetic Field Laboratory, Forschungszentrum Dresden-Rossendorf, Germany

Due to the Aharonov-Bohm (AB) phase generated around the nanotube circumference, the band structure of carbon nanotubes is expected to be strongly influenced by the magnetic field. We report magnetotransport experiments on ballistic carbon nanotubes up to 60 Tesla. We present that the band gap of carbon nanotubes is modulated with the application of magnetic field parallel to the tube axis, and show how initially metallic (or semiconducting) tube evolves into semiconducting(or metallic) tube as we increase the magnetic field. In addition, we find fine structures in the magnetoconductance and explain the phenomena due to the beating effect in the AB interference between clockwise and counterclockwise electronic motions around the tube.

15 min. break

TT 26.12 Wed 17:30 HSZ 03

Exchange effects in single wall carbon nanotube quantum dots — •Christoph Schenke, Sonja Koller, Leonhard Mayrhofer, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg

Various transport experiments have been performed on single wall carbon nanotube quantum dots (SWNTs) in recent years. Some of them revealed exchange effects - as predicted in a mean-field approach by [1]. Using the powerful technique of bosonization we were able to derive the full spectrum of interacting finite-size SWNTs. The long- and short-range parts of the Coulomb interaction are responsible for charging and exchange effects, respectively. In particular we find that the ground state of a SWNT with two electrons in the last shell can be a triplet or a singlet, depending on the magnitude of the exchange coupling. The latter is at largest for small diameter SWNTs [2].

An additionally applied parallel magnetic field induces a Zeeman-splitting between the energy levels of the system. We evaluated the current - bias voltage - gate voltage characteristics for zero and finite magnetic fields. We found a quantitative agreement with the experimental results in [3] where, in particular, a singlet-triplet crossing by sweeping the magnetic field was observed.

[1] Y. Oreg, K. Byczuk and B.I. Halperin, Phys. Rev. Lett. 85, 365 (2000).
[2] L. Mayrhofer and M. Grifoni, Eur. Phys. J. B63, 45 (2008).
[3] S. Moriyama et al., Phys. Rev. Lett. 94, 186806 (2005).

TT 26.13 Wed 17:45 HSZ 03

Ultra-sensitive carbon nanotube resonant tunneling transistor — Soren Andresen[1,3], •Lorenz Lechner[2], Fan Wu[2], Romain Danneau[2], and Pertti Hakonen[2] — [1]Niels Bohr Institute, Copenhagen, Denmark — [2]Low Temperature Laboratory, Helsinki University of Technology, Helsinki, Finland — [3]Nanoscience Center, University of Copenhagen, Copenhagen, Denmark

We have studied resonant tunneling field-effect transistors (RTFET) made from single-walled carbon nanotube quantum dots in the Fabry-Pérot regime. We show excellent charge sensitivity of $8.0 \cdot 10^6$ e/Hz$^{1/2}$ with a carrier frequency of 719 MHz at 4.2 K. This resolution is comparable to the best values so far reported for radio frequency single electron transistors (RF-SET). Unlike RF-SETs operating in the Coulomb blockade regime our device can work as an electron interferometer up to temperatures of 23 K.

TT 26.14 Wed 18:00 HSZ 03

Coupling between chirality and pseudospin in a 2D Dirac fermion semi-confinement: New type of polarization and electronic functionalities — •Grigory Tkachov and Martina Hentschel — Max Planck Institute for the Physics of Complex Systems, Dresden

We introduce a novel type of polarization - chiral pseudospin polarization (CPP) - that represents a nonmagnetic analogue of electron spin polarization [1]. It can be realized in two-dimensional carbon or semiconductor systems exhibiting massless Dirac fermions of two opposite chiralities. The CPP occurs as a boundary effect arising from a correlation between the chirality and effective spin degrees of freedom, which is unique to time-reversal invariant Dirac fermion confinement. The CPP can be probed by tunneling, resulting in a zero-bias conductance anomaly and a singular particle-hole asymmetric local density of states. We use our findings to interpret recent scanning tunneling experiments on monoatomic graphite steps and outline possible applications motivated by the search for new functionalities brought by Dirac quasiparticles into nanoelectronics.

[1] G. Tkachov and M. Hentschel, arXiv: 0810.0632.

TT 26.15 Wed 18:15 HSZ 03

Ballistic electrons in graphene antidot lattices - a numerical study — •Jan Bundesmann, Jürgen Wurm, Michael Wimmer, Inanc Adagideli, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Motivated by recent experiments at the University of Regensburg we study quantum transport properties of charged carriers in graphene antidot lattices. To this end we perform numerical quantum transport simulations on a tight-binding honeycomb lattice with antidots cut out of the lattice using recursive Greens function methods.

Our main focus lies on magnetoconductance and weak localization due to scattering from antidots. We find that the magnetic field profile of the weak localization curve is similar to results from semiclassics

and random matrix theory of chaotic cavities.

We further discuss the relevance of intervalley scattering on the magnitude of the weak localization peak.

TT 26.16 Wed 18:30 HSZ 03

Symmetry Classes in Graphene Quantum Dots — •Jürgen Wurm[1,2], Adam Rycerz[1,3], Inanc Adagideli[1], Michael Wimmer[1], Klaus Richter[1], and Harold Baranger[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Department of Physics, Duke University, Durham, NC 27708, USA — [3]Marian Smoluchowski Institute of Physics, Jagiellonian University, 30059 Krakow, Poland

In view of the recently increased experimental activity in the field of graphene quantum dots [1-2], the need of a theoretical description of these systems is apparent. In this work we study the symmetry classes of open and closed graphene quantum dots through the conductance and energy level statistics [3]. For an abrupt lattice termination, these properties are well described by the standard orthogonal and unitary ensembles of random matrix theory. For a smooth mass confinement, the Hamiltonian and the scattering matrix are block diagonal in the valley degree of freedom. While the effect of this structure is clearly visible in the conductance of open dots, it is suppressed in the spectral statistics of closed dots, because the intervalley scattering time is shorter than the time required required to resolve a level spacing in the closed systems but longer than the escape time of the open systems.

[1] L.A. Ponomarenko et. al., Science 320, 356 (2008)
[2] C. Stampfer, et. al., Appl. Phys. Lett. 92, 012102 (2008)
[3] J. Wurm, Adam Rycerz, Inanc Adagideli, M. Wimmer, K. Richter, H.U. Baranger, arXiv:0808.1008 (2008)

TT 26.17 Wed 18:45 HSZ 03

Few electrons in magnetic graphene quantum dots — •Wolfgang Häusler[1,2] and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany

We consider inhomogeneous magnetic fields to design quantum islands on graphene structures. Following the well known case of semiconducting quantum dots we investigate two interacting electrons. Without further consideration the Dirac Hamiltonian is ill defined for more than one particle. We solve this issue by projecting on positive energy states as physically justified by the presence of a chemical potential. Results of relatively demanding numerical diagonalizations will be presented for artificial graphene helium.

TT 27: Superconductivity: Vortex Dynamics, Vortex Phases, Pinning

Time: Wednesday 14:00–15:00 Location: HSZ 105

TT 27.1 Wed 14:00 HSZ 105

Vortex-vortex interaction in thin superconducting films — •Ernst Helmut Brandt — Max-Planck-Institut für Metallforschung, Stuttgart

The interaction between Pearl vortices in thin superconducting films is revisited. For infinitely extended films this problem was solved by Judea Pearl [1] who obtained the sheet current $J(r)$ around the vortex and the force $\Phi_0 J(r)$ on a second vortex with magnetic flux Φ_0 and at distance r in terms of the two rarely used Bessel functions S_1 and N_1. It is shown that the interaction potential $V(r)$ and force $-V'(r)$ can be approximated with high precision in the entire range of r by a simple logarithm. This expression directly shows the correct limits $V(r) = (\Phi_0^2/\mu_0)\ln(2.27\Lambda/r)/(2\pi\Lambda)$ for $r \ll \Lambda$ and $V(r) = \Phi_0^2/(\mu_0 \pi r)$ for $r \gg \Lambda$. Here $\Lambda = \lambda^2/d$ is the effective penetration depth, λ the London depth, and $d < \lambda$ the film thickness. The effect of finite film size on the vortex interaction is discussed. The interaction now depends not only on the distance r but on both vortex positions and on the film shape [2]. It is shown how the vortex interaction in finite films of any shape and size can be computed.

[1] J. Pearl, Appl. Phys. Lett. **5**, 65 (1964).
[2] E. H. Brandt, Phys. Rev. B **72**, 024529, 1-12 (2005).

TT 27.2 Wed 14:15 HSZ 105

Intrinsic bulk vortex lattice dynamics and tilt moduli revealed by time resolved small angle neutron scattering. — •Sebastian Mühlbauer[1,2], Christian Pfleiderer[1], Peter Böni[1], Albrecht Wiedenmann[3], Ted Forgan[4], and Günter Behr[5] — [1]Physik Department E21, Technische Universität München, D-85748 Garching — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, FRM II, D-85748 Garching — [3]Institut Laue Langevin, ILL, Grenoble, France — [4]School of Physics and Astronomy, University of Birmingham, Birmingham UK — [5]IFW Dresden, D-01069 Dresden,

In contrast to the local elasticity of crystal lattices, the elasticity of Vortex Lattices (VL) in superconductors is of non-local origin. The VL elasticity, thermal stability, pinning and transport properties can be described by the temperature, field and k-dependent elastic moduli c_{11}, c_{44} and c_{66}, hence yielding important informations on the microscopic nature of superconductivity. Measurements of the VL elastic moduli are traditionally limited to macroscopic transport measurements on bulk samples or microscopic surface sensitive methods such as decoration techniques. We report on a new method to measure the VL tilt modulus c_{44} by means of stroboscopic small angle neutron scattering, combined with a time varying magnetic field setup on an ultrapure niobium single crystal with vanishing pinning. This method allows the microscopic determination of the intrinsic VL elastic moduli in large bulk samples, unhampered by surface effects. We present first data, showing a clear change of the vortex-vortex interaction at the transition from the intermediate mixed state to the mixed state.

TT 27.3 Wed 14:30 HSZ 105

Interplay of thermomagnetic and nonequilibrium effects in nonlocal vortex transport in mesoscopic NbGe channels — •Florian Otto[1], Ante Bilušić[1,2], Dinko Babić[3], Christoph Sürgers[4], and Christoph Strunk[1] — [1]Inst. for Exp. and Appl. Physics, Univ. Regensburg, Germany — [2]Fac. of Nat. Sciences, Univ. of Split, Croatia — [3]Dept. Physics, Univ. Zagreb, Croatia — [4]Phys. Inst. and DFG CFN, Univ. Karlsruhe, Germany

Amorphous $Nb_{0.7}Ge_{0.3}$, a high-κ type-II superconductor with very low pinning, allows for measurements in the flux-flow regime over large parts of the B-T-phase diagram. When a transport current is driven through a narrow wire (width 250 nm) connected to remote voltage probes via a perpendicular channel (length 2 μm) in presence of an external (out-of-plane) magnetic field, the Transversal Flux Transformer Effect can be used to produce a nonlocal voltage drop on the remote contacts caused by vortex motion in the channel. In the simplest picture, the Lorentz force acting on the vortices in the local wire creates a pressure on the vortices in the channel, such that the mutual vortex repulsion can explain the nonlocal vortex motion. However, detailed measurements of nonlocal DC voltage-current characteristics taken across the whole B-T-plane show several new aspects, including abrupt sign reversals of the vortex motion. This can be understood in terms of an interplay between Lorentz force (low currents) and Nernst effect via local electron heating (high currents) for $T \ll T_c$, and between the Lorentz force (low currents) and a force due to the local suppression of the superconducting gap (high currents) for T close to T_c.

TT 27.4 Wed 14:45 HSZ 105

Observation of nanostripes and -clusters in NEG superconductors — •Michael R. Koblischka[1], Marc Winter[1], Pintu Das[1], Anjela Koblischka-Veneva[2], Miryala Muralidhar[3], Thomas Wolf[4], Nadendla Hari Babu[5], Steve Turner[6], Gustav van Tendeloo[6], and Uwe Hartmann[1] — [1]Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Functional Materials, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [3]SRL/ ISTEC, 1-10-13, Shinonome, Kotoku, Tokyo, 135-0062, Japan — [4]Forschungszentrum Karlsruhe GmbH, Institute of Solid State Physics, D-76021 Karlsruhe, Germany — [5]IRC in Superconductivity, University of Cambridge, Madingley Road, Cambridge, CB3 0HE, U. K. — [6]EMAT Research Group, University of Antwerp, B- 2020 Antwerp, Belgium

Nanostripes are observed in melt-textured and single-crystalline samples of the ternary light rare earth (LRE) compound $(Nd_{0.33}Eu_{0.33}Gd_{0.33})Ba_2Cu_3O_x$ (NEG) by means of atomic force mi-

croscopy, scanning tunnelling microscopy at ambient conditions, combined with TEM and electron backscatter diffraction. This enables the observation of several important features: Nanostripes are formed by chains of clusters, representing the LRE/Ba substitution. The periodicity of the nanostripes is found to range between 40 and 60 nm; the shape of the nanoclusters is elliptic with a major axis length between 300 and 500 nm and a minor axis length of about 30 to 150 nm. The dimensions of the nanostripes are similar for both types of NEG samples.

TT 28: Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

Time: Wednesday 15:15–18:00 Location: HSZ 105

Invited Talk TT 28.1 Wed 15:15 HSZ 105

Unconventional Superconductivity induced by Interfaces and Surfaces — •Matthias Eschrig — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe, Germany

Ordered many-body states in solids are often characterized by an order parameter that breaks one or more of the symmetries of the crystal. Such unconventional states lead to interesting new physics associated with the spontaneously broken symmetries. However, in order that such a symmetry breaking can occur it has to be energetically favored. Some of the most interesting symmetry broken states have never been found experimentally in bulk materials for that reason.

However, symmetries can be broken also by introducing interfaces with other materials. In this case, the evasive unconventional states might be induced locally near the interface, and can then penetrate as correlations into bulk materials. The properties of the induced states depend on the scattering characteristics of the interfaces and on the proximity induced states produced by the adjacent materials.

We discuss in particular interface-induced unconventional superconductivity in heterostructures with magnetically active materials, that may exhibit e.g. odd-frequency pairing or equal-spin triplet pairing states. We study the conditions under which such unconventional pairing amplitudes are induced and demonstrate how they can be tested in experiment and used for quantum devices.

TT 28.2 Wed 15:45 HSZ 105

Broken time-reversal-symmetry in triplet superconductor junctions — •Philip Brydon[1], Christian Iniotakis[2], Dirk Manske[3], and Manfred Sigrist[2] — [1]Technische Universität Dresden, Dresden, Germany — [2]ETH Zürich, Zürich, Switzerland — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

A rich variety of unconventional Josephson effects have been predicted for junctions combining magnetism and triplet superconductivity (e.g. P. M. R. Brydon *et al.*, Phys. Rev. B **77**, 104504 (2008); P. M. R. Brydon, D. Manske and M. Sigrist, J. Phys. Soc. Japan **77**, 103714 (2008)). Previous works assume, however, that the properties of the barrier material are independent of the two superconductors. We demonstrate that this assumption fails in a scenario where time-reversal symmetry is broken by the misalignment of the **d**-vectors of the triplet superconductors on either side of the junction. This allows the stabilization of a barrier magnetization, creating an exotic Josephson state distinguished by the existence of fractional flux quanta at the junction barrier. There is also a pronounced enhancement of the critical current through the junction at temperatures below the magnetic transition.

TT 28.3 Wed 16:00 HSZ 105

Non-local transport in normal-metal/superconductor hybrid structures: the role of interference and interaction — •Jakob Brauer[1], Detlef Beckmann[1], Florian Hübler[1], and Hilbert v. Löhneysen[2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, P.O.-Box 3640, D-76021 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.-Box 3640, D-76021 Karlsruhe and Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We present experimental results on non-local conductance in multiterminal hybrid structures, where two normal metal contacts are attached to a single superconductor. For contacts with an insulating tunnel barrier, and at energies below the energy gap of the superconductor, the non-local conductance is determined by the competition of crossed Andreev reflection (CAR) and elastic cotunneling (EC). The contributions of CAR and EC are expected to cancel each other in the tunneling limit. Recently [Russo et al., Phys. Rev. Lett. 95, 027002 (2005)], a non-vanishing signal has been observed in such structures, with an additional energy scale below the gap. So far, quantum interference and Coulomb interaction have been suggested to lift the cancellation of CAR and EC, but no established theory exists for this signal. We observe similar signals in our structures, and demonstrate that the origin is quantum interference.

TT 28.4 Wed 16:15 HSZ 105

Crossed Andreev reflection and dynamical Coulomb blockade — •Andreas Baumgartner, Andreas Kleine, Jelena Trbovic, and Christian Schönenberger — Institute of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

A natural source of entangled electrons is the nonlocal process of crossed Andreev reflection (CAR) [1]. In CAR the two electrons of a Cooper pair in a superconductor coherently tunnel into two spatially separated normal metal contacts. This process is expected to produce a negative nonlocal voltage, $U_{\rm nl}$, in a four terminal device with two normal (injector and detector) and two superconducting contacts. However, recent experiments have shown that elastic cotunneling (EC) and charge imbalance (CI) lead to $U_{\rm nl} > 0$ and can mask CAR [2]. In this contribution we show that $U_{\rm nl}$ can be negative for all subgap biases, which suggests that CAR can dominate all other processes, as required for a solid-state entangler. We fabricated a series of lateral multiterminal $Al/Al_2O_3/Pd$ hybrid structures with contact distances smaller than the superconducting coherence length and with different barrier resistances. We show that for a small window of injector and detector resistances CAR is the dominant nonlocal subgap process, and that for larger resistances the CAR and CI rates are reduced. We tentatively ascribe these systematic changes with barrier resistance to dynamical Coulomb blockade [1].

[1] Recher *et al.*, PRL 91, 267003 (2003).

[2] Cadden-Zimansky *et al.*, PRL 97, 237003 (2006), Russo *et al.*, PRL 95, 027002 (2005), Beckmann *et al.*, PRL 93, 197003 (2004)

15 min. break

TT 28.5 Wed 16:45 HSZ 105

Hybrid normal-superconducting systems comprising interacting quantum dots — •Michele Governale[1], Marco G. Pala[2], David Futterer[1], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]IMEP-LAHC, INP MINATEC, Centre National de la Recherche Scientifique, F-38016 Grenoble, France

Quantum dots tunnel-coupled to both normal and superconducting leads exhibit a very rich physics due to the presence of superconducting correlations, quantum fluctuations, strong electron-electron interaction, and non-equilibrium. In order to study these systems, we have developed a real-time diagrammatic expansion in the tunnel coupling to the leads [1], which describes both the equilibrium and non-equilibrium superconducting proximity effects in the quantum dot. In the limit of a large superconducting gap, all orders in the tunnel-coupling strength to the superconductors can be included within an exact resummation scheme. Corrections due to finite values of the gap are evaluated within a $1/\Delta$ expansion. This theory is applied to a single-level quantum dot tunnel coupled to two phase-biased superconducting leads and one voltage-biased normal lead. The normal lead is used to drive the dot out of equilibrium. We compute both the Josephson current between the two superconductors and the Andreev current in the normal lead, and analyze their switching on and off as well as transitions between 0- and π-states as a function of gate and bias voltage.

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

TT 28.6 Wed 17:00 HSZ 105

Spin-Supercurrents in SC/FM Heterostructures — •Roland Grein, Georgo Metalidis, Matthias Eschrig, and Gerd Schön — Institut für theoretische Festkörperphysik, Universität Karlsruhe and DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany

We consider a hybrid structure of a superconductor (SC) and a ferromagnet (FM) with a strong exchange field ($J \approx E_F$). To model this system, we use an extension of the quasiclassical theory of superconductivity. Recent experimental results indicate that spin-active scattering in the interface regions between the different materials is of crucial importance for understanding the transport properties of such systems. We use a microscopic model based on wave function matching to describe this spin-active scattering. It turns out that superconducting correlations, which are transmitted through such interfaces, acquire spin-dependent scattering phases. For a Josephson junction, these scattering phases lead to a renormalization of the current-phase relation. In particular, this leads us to the prediction of a spin-supercurrent in a FM layer which is coupled to only one superconducting electrode, provided that inter-band scattering is possible at the interface and the outer surface of the FM.

TT 28.7 Wed 17:15 HSZ 105

Superconducting spin valves based on epitaxial [Fe/V]-superlattices — •Gregor Nowak[1], Moreno Marcellini[2], Hartmut Zabel[1], Björgvin Hjörvarsson[2], and Kurt Westerholt[1] — [1]Experimentalphysik/Festkörperphysik, Ruhr Universität Bochum — [2]Department of Physics, University of Uppsala, Sweden

In superconducting spin valves of the type S/F1/N/F2 or F1/S/F2 with a superconducting layer S, two ferromagnetic layers F1 and F2 and a normal metallic layer N, the superconducting transition temperature T_S depends on the relative magnetization direction of the ferromagnetic layers F1 and F2. The difference of the transition temperature $\Delta T_S = T_S^{AP} - T_S^P$ with the magnetization direction of F1 and F2 either antiparallel or parallel is called the superconducting spin valve effect [1]. We observed a superconducting spin valve shift of up to ΔT_S=200 mK when aligning the sublattice magnetization in an external magnetic field in S/F1/N/F2 type of spin valves. In the F1/S/F2-type spin valves the ferromagnetic layer F1 was either a [Fe/V] or a [Fe_xV_{1-x}/V] superlattice, the F2 layer was a Fe-, a Co- or a Fe_xV_{1-x} film. Using weakly ferromagnetic Fe_xV_{1-x} alloy layers as F1 and F2 we find a spin valve effect of up to ΔT_S=24 mK. We also present experimental evidence for a drastic reduction or even a sign reversal of the superconducting spin valve effect in the presence of perpendicular magnetic stray fields from ferromagnetic domain walls.

[1] J.Y. Gu, C.-Y. You, J. S. Jiang, J. Pearson, Ya. B. Bazaliy, and S. D. Bader, Phys. Rev. Lett. 89, 267001 (2002)

TT 28.8 Wed 17:30 HSZ 105

Magnetic properties and local critical currents of cobalt covered MgB_2 films — •Sebastian Treiber[1] and Joachim Albrecht[2] — [1]Max Planck Institut für Metallforschung, D-70569 Stuttgart, Germany — [2]HTW Aalen, Beethovenstr. 1, D-73430 Aalen, Germany

At Temperatures below 10K the critical state in MgB_2 thin films gets unstable, the magnetic flux percolates filamentary into the superconductor. This state evolves due to chaotic motion of magnetic vortices and leads to dendritic flux density patterns. Since the critical current vanishes inside the dendrites this effect leads to a strong suppression of possible transport currents. We have found, that ferromagnetic cobalt cover layers can influence the flux pinning scenario in the superconductor. Therefore a heterostructure of MgB_2 and cobalt was investigated using SQUID magnetometry and magneto-optical (MO) imaging. Two different effects are observed. On the one hand the temperature for the occurrence of flux avalanches is shifted to lower temperatures as observed by MO studies. On the other hand magnetic hysteresis loops obtained by SQUID measurements show a significant asymmetry with respect to the $H_{ext} = 0$ axis attributed to magnetic effects on flux line pinning [1].

[1] S. Treiber, B. Stuhlhofer, H. - U. Habermeier and J. Albrecht, SUST (submitted)

TT 28.9 Wed 17:45 HSZ 105

Superconductivity and Magnetism in Cuprate Heterostructures Studied by Low Energy μSR — •Bastian M. Wojek[1,2], Elvezio Morenzoni[1], Dmitry G. Eshchenko[1,2], Andreas Suter[1], Thomas Prokscha[1], Edmond Koller[3], Emmanuel Treboux[3], Øystein Fischer[3], and Hugo Keller[2] — [1]Labor für Myonspinspektroskopie, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]Physik-Institut der Universität Zürich, 8057 Zürich, Switzerland — [3]DPMC, Université de Genève, 1211 Genève 4, Switzerland

Heterostructures consisting of magnetic/superconducting layers juxtaposed to each other are ideal systems to investigate the interplay of the two order parameters and to study possible interlayer coupling. Recently, so called giant proximity effects have been reported in Josephson devices consisting of HTS electrodes and a barrier of a cuprate in the pseudogap or AF state. Low energy μSR offers the unique possibility to measure on a nanometer scale local field distributions and identify superconducting and magnetic fractions. We used polarized low energy muons to investigate the local properties of single, bi- and tri-layers composed of superconducting $YBa_2Cu_3O_{7-\delta}$ and semiconducting $PrBa_2Cu_3O_{7-\delta}$. Zero field measurements show that the PBCO layers (thickness 50-75 nm) display in all structures the known AF ordering. However, measurements of the field profile $B(z)$ in the Meissner state show that below the critical temperature of YBCO, supercurrents flow without dissipation over the 50 nm thick AF barrier. The measurements indicate that a finite superfluid density may be induced in the AF layer adjacent to the superconducting layer.

TT 29: Correlated Electrons: Low-dimensional Systems - Materials 2

Time: Wednesday 14:00–18:15 Location: HSZ 301

TT 29.1 Wed 14:00 HSZ 301

Magnetic Structure and Interactions in the Quasi-1D Antiferromagnet CaV_2O_4 — •Oliver Pieper[1,2], Bella Lake[1,2], Aziz Daoud-Aladine[3], Manfred Reehuis[1,4], Karel Prokeš[1], Bastian Klemke[1], Klaus Kiefer[1], Jiaqiang Yan[5], Asad Niazi[5], David C. Johnston[5], and Andreas Honecker[6] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [3]ISIS Facility, Rutherford Appleton Lab, Chilton, UK — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [5]Ames Lab. and Departement of Physics and Astronomy, Iowa State University, Ames, USA — [6]Universität Göttingen, Institut für theoretische Physik, Göttingen, Germany

CaV_2O_4 is a spin-1 antiferromagnet where the magnetic vanadium ions are arranged on quasi-one-dimensional zig-zag chains with frustrated antiferromagnetic exchange interactions. Here we present high temperature susceptibility and single-crystal neutron diffraction measurements, which are used to deduce the magnetic structure, dominant exchange interactions and orbital configurations. The results suggest that at high temperatures of CaV_2O_4, the zig-zags behave as Haldane chains but at low temperatures, orbital ordering lifts the exchange frustration and the zig-zags become spin-1 ladders.

TT 29.2 Wed 14:15 HSZ 301

Strongly dispersive magnetic excitations in Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R. Kuzian[3], W. D. Stein[2], N. Wizent[1], A. Hiess[4], W. Schmidt[5], R. Klingeler[1], M. Loewenhaupt[2], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Institute for Problems of Materials Science Krzhizhanovskogo 3, 03180 Kiev, Ukraine — [4]Institut Laue Langevin, F-38042 Grenoble Cedex 9, France — [5]Jülich Centre for Neutron Science JCNS, Jülich, Germany

We report on recent inelastic neutron scattering experiments on Li_2CuO_2 which is considered to be the prototypical ferromagnetic $S = \frac{1}{2}$ spin chain compound. Although Li_2CuO_2 has been subject to many experimental and theoretical studies, its magnetic dimensionality is still discussed controversially. This open question is resolved by our spectroscopic study providing a set of magnetic exchange parameters. We find that the magnon excitation is strongly dispersive only for moment transfer along the chains. Analysis of our data by means of linear spin wave theory provides unequivocal evidence that

the compound is indeed a quasi-one-dimensional magnet. To be more specific, we find that the ferromagnetic nearest neighbor intra-chain coupling is the dominant magnetic interaction, but highly frustrated by competing antiferromagnetic next-nearest neighbor couplings. In comparison, the inter-chain exchange is relatively weak. Some of the magnetic properties of the material remain puzzling and will have to be discussed with respect to highly frustrated magnetism.

TT 29.3 Wed 14:30 HSZ 301

Ultrasonic investigations on the 1D diamond chain compound Azurite — •Cong T. Pham[1], Andreas Brühl[1], Mariano de Souza[1], Bernd Wolf[1], Jürgen Schreuer[2], Stefan Süllow[3], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, SFB/TR49, 60438 Frankfurt(M — [2]Institut für Mineralogie, Ruhr-Universität, 44780 Bochum — [3]Institut für Physik der kondensierten Materie, TU Braunschweig, 38106 Braunschweig

The natural mineral Azurite has been considered a model substance for the 1D distorted antiferromagnetic (AFM) diamond chain. The unusual magnetic properties were believed to arise from the competition between quantum fluctuations and spin frustration and have been modelled by assuming three AFM exchange-coupling constant J1,J2,J3 $>$ 0. However, the microscopic magnetic structure and the detailed phase diagram are unknown or disputed. Recent inelastic neutron scattering experiments suggest a non-frustrated structure with J3 $<$ 0 and J1 ˜ 0 below the Néel-temperature of 1.8 K. In this contribution, we present results of ultrasonic investigations on a high-quality single crystal. The longitudinal elastic constant has been studied as a function of temperature down to 80 mK and magnetic fields up to 12 Tesla. The data reveal clear signatures of the magnetic energy scales involved and disclose distinct anomalies at the magnetic phase transition. Based on these results a detailed B-T phase diagram is obtained which includes an additional phase boundary of unknown origin at low temperature (T $<$ 0.6 K). The latter is accompanied by a pronounced softening of the elastic constant.

TT 29.4 Wed 14:45 HSZ 301

Quantized Spin Waves in a Mesoscopic Antiferromagnetic Molecular Ring — •J. Dreiser[1], G. Carver[2], C. Dobe[2], H. U. Güdel[2], A. L. Barra[3], J. Taylor[4], and O. Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany — [2]Department of Chemistry and Biochemistry, University of Bern, 3012 Bern, Switzerland — [3]Grenoble High Magnetic Field Laboratory, CNRS, 38042 Grenoble Cedex 9, France — [4]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom

We present inelastic neutron scattering (INS) data as well as numerical simulations on the antiferromagnetic (AF) $CsFe_8$ molecule, in which eight spin-5/2 Fe(III) ions are arranged in a ring with nearest-neighbor AF Heisenberg interaction. In such even-numbered rings the lowest-lying excitations are formed by rotational modes of the Néel vector (L Band) while spin waves (E Band) occur at higher energies. This is in contrast to bulk antiferromagnets where spin waves are the lowest observed excitations. Further, spin waves become quantized, i.e., occur at discrete energies due to the mesoscopic size of the ring.

We recorded INS data up to high energies at the time-of-flight spectrometer MARI at ISIS, which clearly allowed us to observe the excitation of discrete spin waves. The data is modeled using a Heisenberg-exchange Hamiltonian together with a single-ion anisotropy term. Due to the molecules' symmetry, only two parameters J, D are needed and exact numerical diagonalization yields excellent agreement with the data.

TT 29.5 Wed 15:00 HSZ 301

Quantized Spin Waves in a Ferromagnetic Supertetrahedron: INS studies on Mn_{10} — •S. Stuiber[1], O. Waldmann[1], Y. H. Lan[2], N. Ghenadie[2], A. K. Powell[2], and T. Unruh[3] — [1]Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany — [2]Institut für Anorganische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [3]Technische Universität München, Forschungsneutronenquelle FRM-II, D-85747 Garching, Germany

Similar to extended systems also in a ferromagnetic cluster a spin-wave approach can be used to describe the low-lying magnetic excitations. In a cluster, however, it leads to quantized spin waves with discrete energies. In this work, we report inelastic neutron scattering (INS) experiments on a Mn_{10} cluster, performed at the direct time-of-flight spectrometer TOFTOF (FRM-II). This molecule is comprised of an octahedron of Mn^{3+} ions enclosed by a tetrahedron of Mn^{2+} ions, forming a supertetrahedron. Ferromagnetic couplings between the Mn ions lead to a ground state with total spin $S = 22$. The spin waves then correspond to the states in the $S = 21$ sector. INS is the experiment of choice to investigate this kind of excitations, because of its favorable selection rules. In our experiment we observed these excitations and used spin-wave calculations as well as exact diagonalization studies to model the data and infer values for the exchange coupling constants.

15 min. break

TT 29.6 Wed 15:30 HSZ 301

Fluctuation spectroscopy studies of the quasi–2D organic conductors κ−(BEDT−TTF)$_2$X — •Jens Brandenburg[1], Jens Müller[1], and John A. Schlueter[2] — [1]Max Planck Insitute of Chemical Physics of Solids, Dresden, Saxony, Germany — [2]Argonne National Laboratory, Argonne, Illinois, USA

The family of quasi–2D organic conductors κ−(BEDT−TTF)$_2$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 [1]. Fluctuation spectroscopy has been used to study the intrinsic charge carrier dynamics in this class of materials for the first time. Here, noise measurements as a function of temperature and magnetic field are presented for three compounds located at different positions of the phase diagram. A comparison with the resistance of the samples reveals additional features one of which can be assigned to the activation energy of the glass–like ordering of the ethylene endgroups of the ET–molecules [2]. For the materials close to the bandwidth controlled Mott transition we discuss a steep increase of the noise power upon decreasing temperature in the framework of percolation theory as due to the coexistence of antiferromagnetic insulating and superconducting phases [2].

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

[2] J. Müller, J. Brandenburg, J. A. Schlueter; to be published

TT 29.7 Wed 15:45 HSZ 301

Resistivity investigations on the X-ray irradiated Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl — •Ammar Naji[1], Ulrich Tutsch[1], Michael Lang[1], and Takahiko Sasaki[2] — [1]Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TRR49, D-60438 Frankfurt am Main — [2]Institute for Material Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi 980-8577, Japan

The compound κ-(ET)$_2$Cu[N(CN)$_2$]Cl is a two- dimensionally structured organic material with a rich pressure vs. temperature phase diagram including paramagnetic and antiferromagnetic Mott-insulating states as well as metallic, semiconducting and superconducting phases, see e.g., [1]. We used X-ray irradiation to induce defects in the material and by this change the charge distribution between anion- and ET-layers. The smaller resistivity of the irradiated samples compared to non-irradiated ones supports this idea [2]. As a consequence, X-ray irradiation may provide a means for doping the Mott-insulator away from half-filling. We will present resistivity data for the temperature range 5 K $\leq$ T $\leq$ 60K and pressures up to 50 MPa from which the p-T-phase diagram of X-ray irradiated κ-(ET)$_2$Cu[N(CN)$_2$]Cl will be extracted.

[1] S. Lefebvre *et al.*, Phys. Rev. Lett. **85**, 5420 (2000)

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

TT 29.8 Wed 16:00 HSZ 301

Thin films of charge transfer compounds of tetrathiafulvalene and its derivatives — •Vita Levitan and Michael Huth — Physikalisches Institut, Goethe-Universität, Frankfurt am Main, Germany

Thin films of the organic C(harge) T(ransfer) complex ET-TCNQ have been prepared by molecular beam epitaxy (MBE). We studied the growth of this compound by co-deposition and sequential deposition of two layers of ET and TCNQ molecules followed by a post growth annealing. At the layers' interface ET-TCNQ has been detected and characterized by x-ray diffraction and energy dispersive x-ray spectroscopy as the monoclinic phase of ET-TCNQ. The electrical properties of the bilayer (such as conductivity) were measured and analyzed.

We also prepared thin films of TTF-TCNQ with a preferred orientation of the microcrystals on the substrate along the b-axis of TTF-

TCNQ, being the highest conductivity axis of the compound. Various oxide-based substrate materials with orientations optimized for small layer-substrate lattice mismatch were chosen. We studied the influence of epitaxial clamping on the Peierls transition of TTF-TCNQ at about 60 K by means of temperature dependence transport measurement.

(TTF: tetrathiafulvalene, ET: bis(ethylenedithio)tetrathiafulvalene, TCNQ: tetracyanoquinodimethane)

TT 29.9 Wed 16:15 HSZ 301

Thermodynamic studies on the proposed 2D spin-liquid state in κ-$(ET)_2Cu_2(CN)_3$ — •Rudra Sekhar Manna[1], Andreas Bruehl[1], Mariano de Souza[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universitaet Frankfurt, SFB/TR49, D-60438 Frankfurt(M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

The charge-transfer salt κ-$(ET)_2Cu_2(CN)_3$, where ET = BEDT-TTF, is a spin S = 1/2 Mott insulator with a twodimensional (2D) triangular lattice structure. Because of the almost perfect geometrical frustration $\acute{t}/t \approx 1$ in this material, it has been proposed that quantum fluctuations destabilize long-range magnetic order and, instead, lead to liquid-like properties of the spin system [1]. Issues of high current interest include the nature of the low-lying elementary excitations of the spin liquid, particularly whether or not there is a spin gap, as well as the character of the anomaly observed around 6 K. The latter has been attributed to some "crossover"or "hidden order"[2]. Here we report on high-resolution thermal expansion and specific heat measurements focusing on the mysterious 6 K anomaly. We observe that this anomaly is accompanied by distinct and sharp features in the uniaxial-expansion coefficients suggestive of a second-order phase transition rather than a crossover. The data reveal a pronounced in-plane anisotropy corresponding to a significant distortion of the isotropic triangular lattice.

[1] Shimizu et al., Phys. Rev. Lett. 91, 107001 (2003).
[2] Yamashita et al., Nature Phys. 4, 459 (2008).

TT 29.10 Wed 16:30 HSZ 301

Spin-state polaron in lightly hole doped $LaCoO_3$ — •A. Alfonsov[1], E. Vavilova[1,2], V. Kataev[1], B. Büchner[1], A. Podlesnyak[3], M. Russina[3], A. Furrer[4], Th. Strässle[4], E. Pomjakushina[4,5], K. Conder[5], and D.I. Khomskii[6] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Hahn–Meitner–Institut, D-14109 Berlin, Germany — [4]Laboratory for Neutron Scattering, ETH Zürich & PSI, CH-5232 Villigen PSI, Switzerland — [5]Laboratory for Developments and Methods, PSI, CH-5232 Villigen PSI, Switzerland — [6]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

$LaCoO_3$ is nonmagnetic at low temperatures and shows a T-activated magnetism due to a change of the Co^{3+} spin state. Surprisingly, a very small Sr^{2+} (i.e. hole) doping yields a strong magnetic response already at low T. To establish its nature we performed electron spin- (ESR), nuclear magnetic resonance (NMR) and inelastic neutron scattering (INS) measurements of lightly doped $La_{1-x}Sr_xCoO_3$ single crystals ($x \sim 0.002$). ^{59}Co NMR data indicate the formation of extended magnetic clusters distributed over the entire sample volume. Low-T ESR spectra show up multiple lines with large g-factors suggesting that these clusters have a large spin multiplicity with a strong orbital contribution. From the Q-dependence of the INS intensity we conclude that the cluster comprises 7 magnetic Co ions. We propose a mechanism of how already a very light hole doping yields a formation of big spin polarons in $LaCoO_3$.

15 min. break

TT 29.11 Wed 17:00 HSZ 301

Anomalous dielectric response of the copper oxide chains in $LiCuVO_4$. — •Yulia Matiks, Peter Horsch, Reinhard Kremer, Bernhard Keimer, and Alexander Boris — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

Spectroscopic ellipsometry has been used to investigate the low-lying electronic excitations in the strongly correlated chain copper oxide $LiCuVO_4$ in the range 0.7 - 6.5 eV at temperatures 6 - 350 K. The Zhang-Rice singlet (ZRS) state has been evidenced in edge-sharing copper oxide chains for the first time. Temperature dependence of the ZRS peak identified in the dielectric response along the chains follows spin correlations within the chains that make ZRS apparent at 6 K but strongly suppressed and invisible at 300 K. This behavior is in a good agreement with recent cluster calculations within a pd-Hubbard model. [1] The integrated optical conductivity for polarization along the chains confirms the redistribution of the spectral weight between ZRS and non-bonding O2p states below 80 K. The corresponding effective number of charge carriers transferred between the states is 0.02 electrons per Cu atom indicating the kinetic energy gain of about 10 meV, which is of the same order of magnitude as the exchange integrals of the competing nearest J_1 = -2.1 meV and next-nearest J_2 = 4.3 meV neighbor interactions [2]. For polarization perpendicular to the chains, no spectral weight transfer between individual bands is observed.

[1] J. Málek et al., Phys. Rev. B 78, 060508 (R) (2008).
[2] M. Enderle et al., Europhys. Lett. 70, 237 (2005).

TT 29.12 Wed 17:15 HSZ 301

End states and singlet-triplet degeneracy in linear atomic chains — Antonio Monari[1], Valentina Vetere[2], Gian Luigi Bandazzoli[1], Stefano Evangelisti[2], and •Beate Paulus[3] — [1]Dipartimento di Chimica Fisica e Inorganica, Universita di Bologna, Bologna, Italy — [2]Laboratoire de Chimie et Physique Quantiques, Universite de Toulouse et CNRS, Toulouse Cedex, France — [3]Institut für Chemie und Biochemie, Frei Universität Berlin, 14195 Berlin

The electronic structure of linear beryllium chains has been theoretically studied by using ab initio methods. It turns out that, for internuclear distances close to the equilibrium structure, two partially filled edge orbitals ('edge states') localize at the chain ends. This gives rise to two low-lying states, a singlet ground state, $^1\Sigma_g$ and a quasi-degenerate triplet, $^3\Sigma_u$. the energy splitting goes rapidly to zero as the number of atoms in the chain is increased. Preliminary investigations indicate that this could be a general behavior shard by metals belonging to the groups 2 and 12.

TT 29.13 Wed 17:30 HSZ 301

Understanding magnetic properties of layered copper oxychloride $(CuCl)LaNb_2O_7$ — •Alexander Tsirlin[1,2] and Helge Rosner[1] — [1]Max-Planck Institute CPfS, Dresden, Germany — [2]Department of Chemistry, MSU, Moscow, Russia

The copper-containing oxychloride $(CuCl)LaNb_2O_7$ is one of the actively studied low-dimensional spin systems. Experimental data evidence the strong frustration of this compound, but the microscopic scenario of the frustration remains unknown. Initially, $(CuCl)LaNb_2O_7$ was considered as a promising realization of the spin-1/2 frustrated square lattice model. However, further studies suggested the sizable structural distortion, leading to a more complex spin physics. Experimental techniques fail to resolve the distorted structure, hence impeding the understanding of the magnetic properties. In this contribution, we present a computational study of $(CuCl)LaNb_2O_7$ and propose a valid miscroscopic scenario that accounts for all the experimental data available so far. Our results indicate orbital degeneracy as a primary origin of the structural distortion. The distorted structure is orthorhombic and includes CuO_2Cl_2 plaquettes instead of CuO_2Cl_4 octahedra in the regular structure. The distortion strongly modifies the exchange couplings in $(CuCl)LaNb_2O_7$ and leads to a three-dimensional spin model with pronounced one-dimensional features. Our findings propose a general scenario for the structural distortion and the spin physics of $(CuX)LaM_2O_7$ (X = Cl, Br; M = Nb, Ta) as well as an outlook for further experimental studies of these compounds.

TT 29.14 Wed 17:45 HSZ 301

Volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$: Orbital ordering on a distorted kagome geometry — •Oleg Janson[1], Johannes Richter[2], and Helge Rosner[1] — [1]MPI CPfS Dresden, Germany — [2]University of Magdeburg

The mineral volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$ has been recently claimed as a candidate for a real material realization of a spin-1/2 kagomé lattice. Despite the monoclinic distortion which allows non-frustrated magnetic couplings, experiments reveal the presence of frustration and no clear evidence for long-range order down to 50 mK. Here, we present a theoretical investigation of this interesting material. Based on DFT calculations, we estimate the relevant orbitals and couplings. Quite unusual for cuprates, we find different magnetically active orbitals for structurally different Cu(I) and Cu(II) atoms: while the latter has a hole in a $x^2 - y^2$ orbital (like in most cuprates), for Cu(I) the $3z^2 - r^2$ is half-filled like in $CuSb_2O_6$. This has a dramatic influence on exchange integrals, which have been estimated using the

LSDA+U approach. The magnetic degrees of freedom are mapped onto a Heisenberg model. We find that the orbital order leads to a picture of coupled frustrated chains rather than a kagomé model. For the proposed spin model we investigate the classical as well the quantum ground state. The possible influence of spin anisotropy and Dzyaloshinskii-Moriya interactions will be briefly discussed.
ZIH and IFW Dresden are acknowledged for support with computational resources.

TT 29.15 Wed 18:00 HSZ 301

Quantum phase transitions in $Ca_3Ru_2O_7$ — •Oliver Welzel[1], Patricia Alireza[1], Carsten Albrecht[2], Naoki Kikugawa[3], Andrew Mackenzie[3], and Malte Grosche[1] — [1]Cavendish Laboratory, Cambridge, UK — [2]Royal Holloway, University of London, Egham, UK — [3]School of Physics and Astronomy, University of St. Andrews, UK

The strongly correlated bilayer ruthenate $Ca_3Ru_2O_7$ undergoes first a magnetic transition ($T_N = 56$ K, $\mathbf{Q} = (0, 0, 1/2)$) and then a structural transition ($T_S = 48$ K) on cooling. At low temperature, this material exhibits very small Fermi surface pockets, consistent with its low carrier density.

We follow the evolution of the low temperature state of $Ca_3Ru_2O_7$ with pressure: The structural transition is rapidly suppressed, and T_S extrapolates to zero at $p_{c1} \simeq 35$ kbar. The magnetic transition is also suppressed. T_N extrapolates towards a critical pressure of $p_{c2} \simeq 55$ kbar, but above 40 kbar it is replaced by signatures of a new ordered phase with an onset temperature of about $T_X \simeq 25$ K. This new ordered phase, in turn, appears to be suppressed near $p_{c3} \simeq 80$ kbar.

We explore the nature of the high pressure state of $Ca_3Ru_2O_7$ in a series of high pressure measurements of the resistivity, magnetic susceptibility and magnetisation, and investigate, in particular, the vicinity of the quantum critical point, p_{c3}.

TT 30: Superconductivity: Cuprate High-Temperature Superconductors 2

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

TT 30.1 Wed 14:00 HSZ 304

Enhancement of the incommensurate magnetic order by an applied magnetic field in underdoped $YBa_2Cu_3O_{6.45}$ — •Daniel Haug[1], Vladimir Hinkov[1], Anton Suchaneck[1], Dmytro Inosov[1], Niels Christensen[2], Christof Niedermayer[2], Philippe Bourges[3], Yvan Sidis[3], Ji Tae Park[1], Alexandre Ivanov[4], Chengtian Lin[1], Joël Mesot[2], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Laboratoire Léon Brillouin, CEA-CNRS Saclay, France — [4]Institut Laue-Langevin, Grenoble, France

The discovery of quantum oscillations in the high-temperature superconductor $YBa_2Cu_3O_{6.5}$ above its critical magnetic field showed that the concepts of Fermi liquid theory are applicable to the strongly correlated electron system in the underdoped cuprates. However, the observation of small electron pockets in these experiments puts a new question as such pockets are incompatible with band structure calculations and the Fermi surface topology found in angle-resolved photoemission at zero magnetic field. Our recent neutron scattering experiments on $YBa_2Cu_3O_{6.45}$ reveal an enhancement of the static incommensurate magnetic signal at low temperatures when applying an external magnetic field. This field-enhanced magnetic order may lead to a Fermi surface reconstruction and thus provide a natural explanation for the unexpected Fermi surface topology observed in the quantum oscillation experiments at high magnetic fields.

TT 30.2 Wed 14:15 HSZ 304

Normal State Magnetotransport Properties of high quality $Nd_{2-x}Ce_xCuO_4$ single crystals — •Michael Lambacher, Toni Helm, Wolfgang Prestel, Mark Kartsovnik, Andreas Erb, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Str. 8, 85748 Garching, Germany

We present normal state magnetotransport data taken on a series of high quality $Nd_{2-x}Ce_xCuO_4$ single crystals grown by the TSFZ (traveling solvent floating zone) technique. We show that the unusual transport data of the optimally doped and overdoped crystals can be well explained within a two-band model using standard Boltzmann transport theory and anisotropic scattering rates. In particular, the observed sign change of the Hall effect with varying temperature is nicely reproduced. The presented model deviates from the general picture of the Fermi surface (FS) topology and doping dependent FS reconstruction deduced from ARPES measurements. This work has been supported by the DFG within the research unit FOR 538

TT 30.3 Wed 14:30 HSZ 304

Revealing the Fermi surface of $Nd_{2-x}Ce_xCuO_4$ by high-field magnetotransport — Toni Helm[1], •Mark Kartsovnik[1], Marek Bartkowiak[2], Michael Lambacher[1], Nikolaj Bittner[1], Ilya Sheikin[3], Andreas Erb[1], and Rudolf Gross[1] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Hochfeld-Magnetlabor Dresden, Germany — [3]High Magnetic Field Laboratory, Grenoble, France

Knowing the exact Fermi surface and its evolution with the doping level is one of the vitally important issues in the field of high-T_c superconducting cuprates. A promising tool to explore the Fermi surface is high-field magnetotransport which has been widely employed in studies of other layered systems, such as organic conductors. Recently, a breakthrough in the Fermiology of hole-doped cuprates was made by the observation of angular magnetoresistance oscillations (AMRO) and magnetic quantum oscillations. For electron-doped cuprates, however, no high-field magnetotransport data related to their Fermi surface has been reported so far. Here, we present results of high-field studies of the interlayer magnetoresistance of high-quality electron-doped $Nd_{2-x}Ce_xCuO_4$ single crystals. Samples with doping levels $x = 0.13$ to 0.17 have been studied at different temperatures and field orientations. We compare our data with those obtained on hole-doped cuprates and discuss them in terms of the Fermi surface geometry and its doping dependence.
This work is supported by DFG via Research Unit 538.

TT 30.4 Wed 14:45 HSZ 304

Effect of dopant atoms on local superexchange in cuprate superconductors: a perturbative treatment — •Kateryna Foyevtsova[1], Roser Valenti[1], and Peter Hirschfeld[2] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]University of Florida, Gainesville, FL 32611, USA

On the basis of the three-band Hubbard model for the cuprates, we calculate the magnetic superexchange between Cu ions in the presence of dopants up to fifth-order in perturbation theory. We find that fourth- and fifth-order contributions are equally important, and demonstrate that their sign depends on the relative dopant-induced spatial variation of the atomic levels in the CuO_2 plane, contrary to results obtained within the one-band Hubbard model. We discuss some realistic cases and their relevance for the pairing mechanism in the cuprate superconductors.

TT 30.5 Wed 15:00 HSZ 304

Doping by metal-oxygen complexes and phase separation in the superconducting solid solution $Bi_{2+y}Sr_{2-x}La_xCuO_{6+\delta}$ — •Jürgen Röhler[1], Christoph Trabant[1], Sebastian Standop[1], Helmut Dwelk[2], and Alica Krapf[2] — [1]Universität zu Köln, 50937 Köln — [2]Humboldt Universität zu Berlin, 12489 Berlin

Hole doping, $n_h(x)$, of the single-layer superconductor $Bi_{2+y}Sr_{2-x}La_xCuO_{6+\delta}$ (BLSCO) is shown from systematic x-ray absorption measurements at the Cu-, La- and Bi-sites to be controlled by formation of the metal-oxygen complexes [La^{3+}–O^{2-}], or/and [Bi^{3+}–O^{2-}]. It is not, as generally assumed, controlled simply by cationic La^{3+}/Sr^{2+} mixed valency. Interstitial excess oxygen atoms, taken up together with the substitution of Sr^{2+} by La^{3+} and partially also by excess Bi^{3+}, reside at two different sites in two different complex ion formations : [La–O] and/or [Bi–O] close to the faces of the CuO_6 octahedra, and [La_2–O] in between the Sr–O and Bi–O layers. The former dope holes into the CuO_2 planes. The latter do not, but break the van der Waals bonds

in the Bi-O double layers allowing for the stabilization of co-existing monoclinic and orthorhombic superstructures. The intricate competition between these three different complex formations is connected with the electronic inhomogeneities in the underdoped, and the macroscopic decomposition in the overdoped regimes. It may be also at the origin of the singular stability of BLSC around its optimum doped composition $x_{La} \simeq 0.35$, and of the hole saturation in the overdoped regime at $n_h \simeq 0.2$.

Supported by the ESRF through projects HE2644 and HE2955.

TT 30.6 Wed 15:15 HSZ 304

Nanomechanismus der Supraleitung in YBCO-Verbindungen — •Van Tri Nguyen — Hanoi University of Technology, Hanoi, Vietnam

Aus zahlreichen Untersuchungen kann es gezeigt werden, dass in der YBCO-Struktur, das Sublayer mit Y zwischen beiden (a,b)-CuO2-Ebenen, das leitungsentscheidende Layer, sich als ein moduliertes Nanolayer zeigt. Andererseits, aus den ESR-Ergebnissen wurden zwei Typen der stark superaustauschgekoppelten Elektronenspinpaaren [Cu-Y-Cu] in den orthorombischen Y-Einheitszellen dieser Nanolayer nachgewiesen: Ein antiferromagnetisches Paar entspricht der supraleitenden Phase und ein ferromagnetisches Paar entspricht der halberleitenden Phase. Diese Sachverhalte zeigen, dass der Leitungsmechanismus in YBCO in einem engen Innenzusammenhang mit den Eigenheiten der Electronendynamik seiner Nanostruktur sein muss. Die ungepaarten und hybridisierten Cu-Electronen verhalten sich im modulierten Nanolayer als quasi-freien Electronen (QFE) in einem Nanowellenleiter. Die QFE müssen dadurch komplizierte Quanteneffekte der Paarung in einem Quantum Well (Quantentopf) erfahren. Auf diseer Grundlage kann es zu erklären und ableiten einige grundsätzliche Probleme der Supraleitung in YBCO wie: Die Existenz des Spingaps Egs(T), einer Pseudoenergielücke; Die Rolle des [Cu-Y-Cu]- Singulettpaar als eine neue Art der Cooper-Paare und eine Gleichung zur Bestimmung der Übergangstemperatur Tc; Die Rolle des [Cu-Y-Cu]- Triplettpaars in der halbleitenden Phase. Die erreichten Ergebnisse sind in einer überraschenden Übereinstimmung mit den experimentellen.

TT 31: Matter at Low Temperature: Materials

Time: Wednesday 15:45–17:00 Location: HSZ 304

TT 31.1 Wed 15:45 HSZ 304

Modelling of the loss mechanisms in crystalline solids at low temperatures for future gravitational wave detectors — •Daniel Heinert[1], Alexander Grib[2], Christian Schwarz[1], Stefanie Kroker[1], Ronny Nawrodt[3], Wolfgang Vodel[1], Andreas Tünnermann[4], Sheila Rowan[3], Jim Hough[3], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Kharkov National University, Physics Department, 61077 Kharkov, Ukraine — [3]University of Glasgow, Institute for Gravitational Research, Kelvinbuilding, University Avenue, G12 8QQ Glasgow, Scotland — [4]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Mechanical losses play a crucial role in reducing thermal noise of future gravitational wave detectors. Low loss materials are needed at low temperatures to reduce thermal noise significantly.

We present a study of internal loss mechanisms in crystalline solids to understand the origin of dissipation. Exemplarily, the different loss contributions are described in crystalline quartz. The focus lies on thermoelastic losses and a contribution arising from the interaction of phonons. Then these results are applied to silicon as the most interesting material for the third generation of gravitational wave detectors.

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

TT 31.2 Wed 16:00 HSZ 304

Analysis of the electric field gradient in the perovskites $SrTiO_3$ and $BaTiO_3$: density functional and model calculations — •Katrin Koch[1], Roman Kuzian[2], Klaus Koepernik[3], and Helge Rosner[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden — [2]Institute for Problems of Materials Science, Kiev — [3]Leibniz Institute for Solid State and Materials Research, Dresden

We analyze recent measurements [1] of the electric field gradient on the oxygen site in the perovskites $SrTiO_3$ and $BaTiO_3$. We have performed density functional calculations within the local-orbital scheme FPLO using a recently implemented EFG module. The calculated values agree well with the experiment. We show that the electronic charge density around the oxygen ion is almost spherical for $SrTiO_3$ at the experimental volume, but surprisingly becomes more and more oblate with increasing lattice expansion. The same tendency in the density redistribution, that can be quantified as the increase of the difference in population of σ- and π- orbitals in the p shell, is found for $BaTiO_3$. Using a p-d like model Hamiltonian, we show that this counter-intuitive behavior can be explained by the contribution of oxygen $2s$ states to the crystal field on the Ti site. We argue that the surprisingly large difference between the observed electric field gradients of the two compounds in the cubic phase is mainly due to the difference in the on-site electronic density distribution. The proposed model description is of general relevance for all related transition metal oxides with similar crystal structure.

[1] R. Blinc et al. Condens. Matter **20**, 085204 (2008)

TT 31.3 Wed 16:15 HSZ 304

Experimental setup for investigation of mechanical losses of thin dielectric films at low temperatures — •Christian Schwarz[1], Stefanie Kroker[1], Ronny Nawrodt[2], Daniel Heinert[1], Stuart Reid[2], Iain Martin[2], Eleanor Chalkley[2], Ralf Neubert[1], Wolfgang Vodel[1], Andreas Tünnermann[3], Sheila Rowan[2], Jim Hough[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]University of Glasgow, Institute for Gravitational Research, Kelvinbuilding, University Avenue, G12 8QQ Glasgow, Scotland — [3]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Low mechanical loss materials are needed for enhanced future gravitational wave detectors in order to reduce thermal noise. The dielectric layers needed to form optical components play a crucial role. We present an experimental setup for the investigation of the mechanical losses of thin ($<1\,\mu$m) dielectric films on silicon cantilevers over a temperature range from 5 to 300 K. The experimental limits of the setup are investigated and discussed. First results on uncoated and coated cantilevers are presented. The cantilevers are coated with tantala (Ta_2O_5) by means of electron beam evaporation.

This work is in part supported by the German science foundation DFG under contract SFB TR7.

TT 31.4 Wed 16:30 HSZ 304

Effect of the spin-orbit interaction on the thermodynamic properties of Bi and Sb — •Reinhard K. Kremer[1], Manuel Cardona[1], Luis E. Díaz-Sánchez[2], Aldo H. Romero[2], Xavier Gonze[3], and Jorge Serrrano[4] — [1]Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]CINVESTAV, Departamento de Materiales, Unidad Querétaro, Querétaro, 76230, Mexico — [3]Unité de Physico-Chimie et de Physique des Matériaux Université Catholique de Louvain B-1348 Louvain-la-Neuve, Belgium — [4]ICREA-Dept. Física Aplicada, EPSC, Universitat Politécnica de Catalunya, Av. Canal Olímpic 15, 08860 Castelldefels, Spain

In the past years we have carried out a series of experiments as well as *ab initio* calculations of the dependence of the specific heat of semiconductors and insulators on T and isotopic masses. First results on the binary lead chalcogenides revealed marked differences between the calculated and the experimental heat capacities and the phonon dispersion relations. This finding raised the question of whether these discrepancies were due to the lack of spin-orbit (s-o) coupling in the *ab initio* electronic structure calculations. Using the ABINIT code which was recently extended to include s-o interaction we calculated the dispersion relations and the specific heat and compare it with our new low-temperature heat capacity measurements on Bi, Sb and PbX (X=S, Se, Te) and existing experimentally determined phonon dispersion relations. We find that agreement between measurements and calculations significantly improves when s-o interaction is included. Differences for the various investigated elements and binary systems

are discussed.

TT 31.5 Wed 16:45 HSZ 304

Far-infrared measurements on multiferroic $TbMnO_3$ — •Michael Schmidt, Christian Kant, Torsten Rudolf, Franz Mayr, Joachim Deisenhofer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany

Recently multiferroics with strongly enhanced magnetoelectric effects attracted considerable attention. Especially $TbMnO_3$ gained a lot of interest, as in this compound it has been documented that spin waves can be excited by ac electric fields. This novel excitations of multiferroics have been termed electromagnons [1].

Despite extensive experimental and theoretical efforts, the microscopic origin of these excitations is strongly debated and their coupling to phonons is not fully understood. New models aiming to explain the origin of these excitations have been developed [2,3].

We performed polarization dependent far-infrared spectroscopy on $TbMnO_3$ for wavenumbers ranging from 40 cm^{-1} to 8000 cm^{-1} and temperatures from 5 K to 300 K. We followed in detail the temperature dependencies of eigenfrequencies, strengths and damping constants of all IR-active phonon modes, with the main emphasis to study the coupling of phonons to spin excitations. We provide experimental evidence that the low energy phonon modes are strongly coupled to spin excitations, a characteristic feature of spin driven ferroelectricity.

[1] A. Pimenov et al., Nature Phys. **2**, 97 (2006)
[2] Y. Takahashi et al., Phys. Rev. Lett. **101**, 187201 (2008)
[3] R. Valdés Aguilar et al., arXiv:0811.2966v1 (unpublished)

TT 32: Postersession Superconductivity: Josephson Junctions, SQUIDs, Heterostructures, Andreev Scattering, Vortex Physics, Cryodetectors, Measuring Devices, Cryotechnique

Time: Wednesday 14:00–18:00 Location: P1A

TT 32.1 Wed 14:00 P1A

Investigation of self-heating in $Bi_2Sr_2CaCu_2O_8$ single crystals via low-temperature scanning laser microscopy — •M. Grünzweig[1], S. Guénon[1], H. B. Wang[2], J. Yuan[2], A. Iishi[2], S. Arisawa[2], T. Hatano[2], T. Yamashita[2], D. Koelle[1], and R. Kleiner[1] — [1]Physikalisches Institut &Center for Collective Quantum Phenomena,Universität Tübingen,Germany — [2]National Institute for Materials Science,Tsukuba 3050047, Japan

Recently, relatively strong emission of Terahertz radiation by large stacks of intrinsic Josephson junctions in $Bi_2Sr_2CaCu_2O_8$ single crystals has been discovered [1]. Perhaps surprisingly, the radiation occurs at dc input power levels where Joule heating already changes the temperature distribution in the sample considerably and thus affects the electric properties of the sample. To investigate this we have used low-temperature scanning laser microscopy (LTSLM) to image local electric field distributions in the stacks [2]. For high bias currents we discovered a feature that can be interpreted as a hot spot (i. e. an area of the stack which temperature is above the critical temperature of the superconductor). The fact that the hot spot is accompanied by a standing wave pattern is an indication that the hot spot might play an important role to stimulate Terahertz radiation. We present LTSLM results obtained from stacks with different geometries and with different current injection.

[1] L. Ozyuzer *et al.*, Science **318**, 1291 (2007)
[2] H. B. Wang, S. Guénon *et al.*, submitted to Phys. Rev. Lett.; arXiv:0807.2749v1 [cond-mat.supr-con]

TT 32.2 Wed 14:00 P1A

$YBa_2Cu_3O_7$ grain boundary junction dc SQUIDs for operation in high magnetic fields — •Konstantin Konovalenko, Joachim Nagel, Markus Turad, Matthias Bailer, Matthias Grünzweig, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut &Center for Collective Quantum Phenomena,Universität Tübingen,Germany

We investigate the suitability of dc SQUIDs for operation in high magnetic fields at 4.2 K. For this purpose, we fabricated small (micron-sized) $YBa_2Cu_3O_7$(YBCO) grain boundary junction dc SQUIDs on $SrTiO_3$ bicrystals with thin film Au shunt resistors. Fabrication was done by pulsed laser deposition of YBCO films, in-situ deposition of electron-beam evaporated Au films and Ar ion milling with photolithographically defined masks. For the fabricated SQUIDs we present results on electric transport properties, measured in a four-point arrangement, and on noise properties, measured with a Nb dc SQUID amplifier.

TT 32.3 Wed 14:00 P1A

Ramp-type Josephson junctions with $YBa_2Cu_3O_7$ and Nb electrodes — •Andreas Blank, Markus Turad, Christoph Maurer, Christoph Back, Reinhold Kleiner, and Dieter Koelle — PhysikalischesInstitut & Center for Collective Quantum Phenomena, UniversitätTübingen, Germany

We present our status of the development of an improved ramp-type Josephson junction technology for fabrication of all-high T_c junctions with $YBa_2Cu_3O_7$ (YBCO) electrodes and $PbBa_2Cu_3O_7$ (PBCO) barrier, and hybrid YBCO/Au/Nb junctions. The fabrication is done in a UHV cluster tool for the deposition of oxide thin films by pulsed laser deposition (PLD) using in-situ high-pressure RHEED for monitoring the thin film growth. Deposition of Nb and Au thin films is done by dc magnetron sputtering and electron beam evaporation, respectively, in two separate processing chambers. A milling chamber equipped with a high-frequency inductively-coupled plasma source allows surface cleaning and etching with argon and/or oxygen, reactive ion etching with SF_6 and removal of resist structures in an oxygen plasma. The substrate holder in the milling chamber allows in-situ adjustment and variation of the milling angle and additional rotation of the substrate about its normal axis, in order to realize an isotropic milling process, which is essential for the fabrication of 2-dimensional arrays of Josephson junctions. Initial results on the properties of fabricated ramp junctions will be shown.

TT 32.4 Wed 14:00 P1A

Thermal and Quantum Escape of Fractional Josephson Vortices — •Hanna Pöhler[1], Uta Kienzle[1], Kai Buckenmaier[1], Tobias Gaber[1], Michael Siegel[2], Dieter Koelle[1], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Physikalisches Institut, Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (KIT), Germany

By using a pair of tiny current injectors one can create an arbitrary κ discontinuity of the phase in a long Josephson junction (LJJ) and a fractional Josephson vortex (FJV), carrying a fraction $\Phi/\Phi_0 = \kappa/2\pi \leq 1$ of the magnetic flux quantum $\Phi_0 \approx 2.07 \cdot 10^{-15}$ Wb, which is pinned at the discontinuity [1]. If a bias current I, exceeds the critical value $I_c(\kappa)$ [2,3], an integer fluxon is torn off the discontinuity and the LJJ switches to the voltage state. Due to thermal or quantum fluctuations this escape event may occur at $I \lesssim I_c(\kappa)$.[4]

We have measured the critical current distribution $P(I)$ for different values of κ, temperature T and junction geometry. At low temperatures we see a saturation of the distribution width which is presumably due to the crossover from thermal activation to quantum tunnelling. The results are compared to numerical simulations based on the static sine-Gordon equation.

[1] E. Goldobin, et al., Phys. Rev. B **70**, 174519 (2004).
[2] A. V. Ustinov, Appl. Phys. Lett. **80**, 3153 (2002).
[3] B. A. Malomed and A. V. Ustinov, Phys. Rev. B **69**, 64502 (2004).
[4] P. Hänggi, et al., Rev. Mod. Phys. **62**, 251 (1990)

TT 32.5 Wed 14:00 P1A

A Josephson Vortex Ratchet climbs uphill — •Martin Knufinke[1], Kai Buckenmaier[1], Michael Siegel[2], Dieter Koelle[1], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Physikalisches Institut – Center for Collective Quantum Phenomena, University of Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (KIT), Hertzstr. 16, D-76187 Karlsruhe, Germany

A particle in a potential with broken reflection symmetry has a preferential direction of motion being driven by a deterministic or stochastic

force with zero time-average [1]. Josephson vortex ratchets (JVRs) offer a flexible way of implementing such a system in the underdamped regime [2]. In a long annular Josephson junction the particle is a fluxon that moves in a potential created by a suitable current injection profile [3,4]. Due to the asymmetry of the resulting potential an ac current drive leads to a dc voltage across the Josephson junction.

Being in the rectification regime we apply an additional bias current which tilts the potential and pushes the fluxon in the direction opposite to its motion, i.e. the fluxon moves uphill due to the ratchet effect. At some value I_{stop} of bias the fluxon stops. We determine I_{stop} both experimentally and numerically and obtain information about the loading capability of the ratchet.

[1] P. Hänggi *et al.*, Ann. Phys. (Leipzig) **14**, 51 (2004)
[2] G. Carapella *et al.*, Phys. Rev. Lett. **87**, 077002 (2001)
[3] E. Goldobin *et al.*, Phys. Rev. E **63**, 031111 (2001)
[4] M. Beck *et al.*, Phys. Rev. Lett. **95**, 090603 (2005)

TT 32.6 Wed 14:00 P1A

Effect of magnetic field on the escape rate in small Josephson junctions — •Kirill Fedorov[1], Alexey Feofanov[1], Ralf Dolata[2], Brigitte Mackrodt[2], and Alexey Ustinov[1] — [1]Physikalisches Institut, Universität Karlsruhe (TH), 76131 Karlsruhe, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

The escape of a point-like Josephson junction (JJ) from the superconducting state is reduced to the escape of a particle from a metastable state in the washboard potential. In the case of a finite size JJ, this problem becomes considerably more complex since the phase acquires a spatial dependence. We experimentally study the macroscopic quantum tunneling (MQT) and the thermal escape in a JJ, placed in an externally applied magnetic field and compare results with the recent theoretical paper by Yu. N. Ovchinnikov et al. [1]. It has been theoretically predicted that the magnetic field strongly changes the crossover temperature between MQT and thermal escape. The experiments were performed using 5 x 3 μm^2 niobium JJs with critical current density 1 kA/cm^2. We have found peculiarities in the escape statistics near the minima of Fraunhofer pattern of the switching current dependence on a magnetic field. A comparison of our experimental results with the Ovchinnikov et al. theory will be presented.

[1] Y. N. Ovchinnikov, A. Barone, and A. A. Varlamov, Phys. Rev. Lett. **99**, 037004 (2007).

TT 32.7 Wed 14:00 P1A

Two dimensional planar SQUID-Gradiometer on a $SrTiO_3$-bicrystal — •Uwe Schinkel[1], Christoph Becker[1], Alexander Steppke[2], Katharina Hoefer[1], Martin Pollithy[1], Veit Grosse[1], Sebastian Engmann[1], Frank Schmidl[1], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden, Germany

We designed a dc-SQUID-Gradiometer layout based on $YBa_2Cu_3O_{7-x}$ thin films on $SrTiO_3$ bicrystals and crossed bicrystals to detect the first order field gradient. In a planar configuration four galvanically coupled antenna structures can be read out by four dc-SQUIDs. Measuring the voltage modulation in an excitation coil changed magnetic field abnormal behaviour occurs. A redistribution of the screening current in the antennas can produce this disturbance. We present the layout, the preparation and the characteristics of each dc-SQUID. Especially the abnormal behaviours of the voltage modulation are analyzed. Therefore the influences of a homogenous magnetic field perpendicular to the gradiometer are studied.

TT 32.8 Wed 14:00 P1A

Investigation of superconducting thin film structures prepared by nanoscale wedge polishing — •Martin Pollithy[1], Katharina Höfer[1], Uwe Schinkel[1], Peter Michalowski[1], Veit Grosse[1], Frank Schmidl[1], Paul Seidel[1], Dagmar Meier[2], and Tanya Shapoval[2] — [1]FSU Jena, Institute of Solid State Physics, Helmholtzweg 5, D-07743 Jena, Germany — [2]IFW Dresden, Institute for Metallic Materials, PO Box 270116, D-01171 Dresden, Germany

The performance of dc-SQUID gradiometers depends very strong on the spread of the critical parameters Ic, Rn and Ls. After the preparation of high temperature superconducting devices it could be useful to tune the superconducting properties by decrease of the film thickness. On the other hand it is often helpful for sensor applications to realise a superconducting thin film structure with a smooth surface to avoid resistive or superconducting shunts in insulating layers on the top of the superconductor. In these investigations we use a mechanical wedge polishing procedure [1] to thin the superconducting devices (microbridges, dc-SQUIDs or dc-SQUID gradiometers) before and/or after the first measurements of the electrical properties. AFM and SEM measurements were done to characterise the film morphology. Temperature dependent measurements of the superconducting properties of microbridges, dc-SQUIDs and dc-SQUID gradiometer structures were realised. We discuss the possibilities and limitations of this procedure.

[1] T.Shapoval, S.Engel, M.Gründlich, D.Meier, E.Backen, V.Neu, B.Holzapfel, L.Schultz, Supercond. Sci. Tech. 21 (2008) 105015

TT 32.9 Wed 14:00 P1A

Superconducting properties of YBCO thin film structures with gold nanoclusters — •Marc Teichmann, Martin Pollithy, Katharina Höfer, Sebastian Engmann, Uwe Schinkel, Robert Hähle, Veit Grosse, Christoph Becker, Frank Schmidl, and Paul Seidel — FSU Jena, Institute of Solid State Physics, Helmholtzweg 5, D-07743 Jena, Germany

For our experiments we used laser ablation to prepare $YBa_2Cu_3O_{7-X}$ thin films with a film thickness of about 150 nm on (100) $SrTiO_3$ single crystalline substrates as well as on $SrTiO_3$ bicrystalls (24° and 30° grain boundary angle). X-ray, AFM and SEM investigations were done to determine the crystalline structure and morphology of the prepared thin films with and without gold nanoclusters. Ion beam etching with sample cooling was used to pattern microbridges as well as dc-SQUID and dc-SQUID gradiometer structures. The temperature dependence of the device and the contact resistance, the current-voltage characteristics at different temperatures and the magnetic field dependence were measured.

TT 32.10 Wed 14:00 P1A

Transport measurements on melt-textured SEG-123 superconductors exhibiting nanostripes — •Michael R. Koblischka[1], Marc Winter[1], Anming Hu[2], and Uwe Hartmann[1] — [1]Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Department of Physics, University of Waterloo, 200 Univ. Ave. West, Waterloo, ON, N2L 3P7, Canada

Transport measurements were performed on melt-textured, ternary light rare earth (LRE)-compounds $(Sm_{0.33}Eu_{0.33}Gd_{0.33})Ba_2Cu_3O_x$ (SEG) exhibiting self-organized nanostripes. The periodicity of these nanostripes ranges between 40 and 60 nm and extends over several tens of micrometers up to millimeters, as revealed by atomic force microscopy at ambient conditions [1]. Electrical contacts were prepared on the polished sample surface by means of electron-beam lithography, enabling the measurement of transport currents oriented parallel and perpendicular to the nanostripe direction. On decreasing the temperature from Tc, the data of the parallel direction deviate in intermediate fields (around 1 T) from the data of the perpendicular direction. At 85 K, there is a clear difference in jc between the two directions, with $j_c^{\mathrm{parallel}} > j_c^{\mathrm{perp}}$. Plotting the data in a scaling fashion shows that the peak positions are clearly different with $h_0^{\mathrm{parallel}} > h_0^{\mathrm{perp}}$, which indicates an increase of the δT_c pinning.

[1] M.R.Koblischka et al., Jpn. J. Appl. Phys. 45, 2259 (2006).

TT 32.11 Wed 14:00 P1A

Surface deformation caused by the Abrikosov vortex lattice — Pavel Lipavsky[1,2], •Klaus Morawetz[3,4], Jan Kolacek[2], and Ernst Helmut Brandt[5] — [1]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [2]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [3]Forschungszentrum Dresden-Rossendorf, PF 51 01 19, 01314 Dresden, Germany — [4]International Center for Condensed Matter Physics, 70904-910, Brasília-DF, Brazil — [5]Max Planck Institute for Metals Research, D-70506 Stuttgart, Germany

In superconductors penetrated by Abrikosov vortices, the magnetic pressure and the inhomogeneous condensate density induce a deformation of the ionic lattice. We calculate how this deformation corrugates the surface of a semi-infinite sample [1]. The effect of the surface dipole is included.

[1] Phys. Rev. B 77 (2008) 184509

TT 32.12 Wed 14:00 P1A

Surface superconductivity and capacitance of superconductors under electric and magnetic fields — •Klaus Morawetz[1,2], Pavel Lipavsky[3,4], Jan Kolacek[4], Ernst Helmut Brandt[5], and Michael Schreiber[1] — [1]Forschungszentrum Dresden-Rossendorf, PF

51 01 19, 01314 Dresden, Germany — [2]International Center for Condensed Matter Physics, 70904-910, Brasília-DF, Brazil — [3]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic — [4]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [5]Max Planck Institute for Metals Research, D-70506 Stuttgart, Germany

A superconducting layer exposed to a perpendicular electric and parallel magnetic field is considered within the Ginzburg-Landau (GL) approach. The GL equation is solved near the surface and the surface energy is calculated [1,2]. The nucleation critical field is shown to be changed in dependence on the magnetic and electric field. Special consideration is payed to the induced magnetic-field effect caused by diamagnetic surface currents. The latter effect constitutes the main contribution to the effective inverse capacitance which determines the effective penetration depth. The surface energy becomes strongly dependent on the width of the sample. An experimental realization is suggested for determining the change in the effective capacitance of the layer.

[1] Phys. Rev. B 78 (2008)054525
[2] arXiv 0804.0138

TT 32.13 Wed 14:00 P1A

The lateral S-(S/F)-S Josephson junctions — •Ondrej Vávra, Wolfgang Pfaff, and Christoph Strunk — Inst. for Exp. and Appl. Physics, Univ. Regensburg, Germany

Up to now the proximity effect at the superconductor-ferromagnet (S-F) interface was mainly demonstrated by the transport properties across the S-F interface [A.A. Golubov, M.Yu. Kupriyanov, and E. Ilichev, Rev. Mod. Phys. **76**, 411 (2004).]. We present the results on lateral transport along the S-F interface and its utilization as a Josephson junction. We have prepared Nb based Josephson junctions which consist of Nb micro bridges with a $Pd_{0.95}Fe_{0.05}$ or Fe strip deposited perpendicular to the bridge. The width of the ferromagnetic strip was varied between 50 and 800 nm. The critical current (I_C) of the Nb-$Pd_{0.95}Fe_{0.05}$ and Nb-Fe bi-layer, respectively, is found to be significantly reduced by the proximity effect with the ferromagnet.

We have studied the temperature and magnetic field (B) dependencies of the critical current. In magnetic field an interference pattern $I_C(B)$ is observed. In perpendicular magnetic field the junction exhibits $I_C(B)$ dependence similar to a Fraunhofer pattern which proves the dc Josephson effect. We also investigate the dependence of $I_C(B)$ oscillations on the orientation of the magnetic field. The control of the Josephson junction parameters is provided by third electrode connected to the F strip.

TT 32.14 Wed 14:00 P1A

Observation of absolute negative resistance in mesoscopic samples of a-NbGe — •Florian Otto[1], Ante Bilušić[1,2], Dinko Babić[3], Christoph Sürgers[4], and Christoph Strunk[1] — [1]Inst. for Exp. and Appl. Physics, Univ. Regensburg, Germany — [2]Fac. of Nat. Sciences, Univ. of Split, Croatia — [3]Dept. Physics, Univ. Zagreb, Croatia — [4]Phys. Inst. and DFG CFN, Univ. Karlsruhe, Germany

Local and nonlocal measurements on mesoscopic samples of amorphous NbGe, a high-κ type-II superconductor with very low pinning, reveal peculiar features in close vicinity of the transition temperature T_c: in absence of magnetic field, both local and nonlocal DC voltage current characteristics clearly display absolute negative resistance in a small interval around zero current and a small temperature range immediately below T_c . At the same time, a negative voltage is also observed in both local and nonlocal measurements of $R(T)$. The temperatures at which this occurs are consistently found to be around 0.95-0.96 T_c, which is clearly below the narrow superconducting transition region. Upon application of small external magnetic fields on the order of $B = 50\,\mathrm{mT}$, the effect can be suppressed. The origin of these completely unexpected features is not clear.

TT 32.15 Wed 14:00 P1A

Spin mixing at Superconductor Ferromagnet Interfaces probed by non-local transport — •Florian Hübler[1,2], Detlef Beckmann[1], Jakob Brauer[1], and Hilbert von Löhneysen[2,3] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, P.O.-Box 3640, D-76021 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.-Box 3640, D-76021 Karlsruhe — [3]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We present experimental results on non-local conductance in multiterminal hybrid structures, where two or more ferromagnetic (F) contacts are attached to a single superconductor (S). For contacts with an insulating (I) tunnel barrier, and at energies below the energy gap of the superconductor, the non-local conductance is determined by the competition of crossed Andreev reflection (CAR) and elastic cotunneling (EC). In FISIF structures, the contributions of CAR and EC are expected to depend on the orientation of the magnetisation of the F contacts. Recently, an asymmetric conductance signal as consequenc of a finite spin-mixing angle has been predicted [1]. We observe first signs for similar signals in our structures.

[1] Kalenkov and Zaikin, Phys. Rev. B 76, 224506 (2007)

TT 32.16 Wed 14:00 P1A

Crossover from 2D-3D behaviour in superconducting Nb/CuNi bilayers in a magnetic field — •Jan-Michael Kehrle[2], Vladimir Zdravkov[1,2], Günter Obermeier[2], Roman Morari[1], Eugen Antropov[1], Andrei Prepelitsa[1], Claus Müller[2], Achim Wixforth[2], Siegfried Horn[2], Reinhard Tidecks[2], and Anatolie Sidorenko[1,2,3] — [1]Institute of Electronic Engineering and Industrial Technologies ASM, Kishinev, MD2028, Moldova — [2]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [3]Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

A dimensional crossover in an external magnetic field, applied parallel to the layers, has been found for superconductor/ferromagnet (S/F) bilayers of Nb/CuNi. For decreasing temperature the square-root 2D-behaviour of the upper critical magnetic field, Bc2||(T) on the temperature, in the vicinity of the critical temperature Tc switches to the linear 3D-behaviour below the crossover temperature, Tcr. The 2D-3D crossover also occurs concerning the temperature dependence of superconducting fluctuations in the critical fluctuation regime. The fluctuation conductivity exhibits a 2D-behaviour in zero- and weak magnetic fields close to Tc, switching to a 3D-behaviour in strong magnetic fields at low temperatures. In a S/F bilayer the quasi-one dimensional Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) like state is realized, so that the superconducting properties are governed by interference effects of the pairing wave functions, i.e. by the pairing function flux through the S/F interface.

TT 32.17 Wed 14:00 P1A

Structure and local electronic properties of Ag and Co/Ag on Nb(110) — •Tihomir Tomanic[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe

The local variation of the superconductive order parameter in hybrid structures of a superconductor S with a normal metal N or ferromagnet F is a topic of current interest. We have started a study of Ag and Co islands on Nb via scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperatures.

As a prerequisite, we report on the surface structure of clean Nb(110) single crystals obtained after Ar^+ sputtering and flash heating up to 2300 °C in ultra-high vacuum. The atomic structure as well as the local superconducting properties have been explored by STM and STS at $T = 2.5$ and $T = 4.2\,\mathrm{K}$. We have studied the topography of a thin Ag overlayer (nominal thickness 5nm) on Nb(110) and of Co islands on top of the Ag overlayer. First results of the local electronic density of states derived from the current-voltage characteristics will be reported.

TT 32.18 Wed 14:00 P1A

Angle-dependent investigation of the upper critical field in NbN/Sm-Co bilayers — •Jan Engelmann, Silvia Haindl, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

The coexistence of superconductivity and magnetism leads to new interesting phenomena like domain-, domain-wall-superconductivity and stray field effects. To investigate thin film bilayers of hard-magnetic Sm-Co with very fine defined domain structure and superconducting NbN, we fabricated these bilayers using pulsed laser deposition. The Sm-Co thin film layer was prepared in UHV on a MgO(100)-substrate with a Cr-buffer, and subsequently the NbN was grown in a nitrogen-atmosphere. Epitaxy and texture were measured via x-ray diffraction, the magnetic properties were determined by VSM -measurements. The angle-dependent upper critical field, $\mu_0 H_{c2}$, of the bilayer was investigated in detail by a standard four probe technique using a PPMS.

TT 32.19 Wed 14:00 P1A

Turning a nickelate Fermi surface into a cuprate-like one through heterostructuring — •Philipp Hansmann[1,2], Xiaoping Yang[1], Alessandro Toschi[2], Giniyat Khaliullin[1], Ole Krogh Andersen[1], and Karsten Held[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Solid State Physics, Vienna University of Technology, Austria

Using the local density approximation and its combination with dynamical mean field theory, we show that electronic correlations induce a single sheet cuprate-like Fermi surface for $LaNiO_3/LaAlO_3$ heterostructures, even though both e_g orbitals contribute to it. This is possible because the correlations shift one of the two sheets above the Fermi level. As there are also strong antiferromagnetic fluctuations, the low-energy electronic and spin excitations resemble those of high-temperature cuprate superconductors.

[1] P.Hansmann, X. Yang, A. Toschi, G. Khaliullin, O.K. Andersen, K. Held, (arXiv:0710.2778) (2008)

TT 32.20 Wed 14:00 P1A

Decreasing excitation gap in Andreev billiards by disorder scattering — •Florian Libisch[1], Jürgen Möller[1], Stefan Rotter[1], Maxim Vavilov[2], and Joachim Burgdörfer[1] — [1]TU–Vienna, Austria — [2]University of Wisconsin, USA

We investigate the distribution of the lowest-lying energy states in a disordered Andreev billiard by solving the Bogoliubov-de Gennes equation numerically [1]. Contrary to conventional predictions we find a decrease rather than an increase of the excitation gap relative to its clean ballistic limit. We relate this finding to the eigenvalue spectrum of the Wigner-Smith time delay matrix between successive Andreev reflections. We show that the longest rather than the mean time delay determines the size of the excitation gap. With increasing disorder strength the values of the longest delay times increase, thereby, in turn, reducing the excitation gap.

[1] F. Libisch, J. Möller, S. Rotter, M. G. Vavilov, J. Burgdörfer, Europhys. Lett. 82, 47006 (2008).

TT 32.21 Wed 14:00 P1A

Behavior of the vortex-creep activation energy in $YBa_2Cu_3O_{7-\delta}/PrBa_2Cu_3O_{7-\delta}$ superlattices — •Ayman El Tahan[1], Lucica Miu[2], Gerhard Jakob[1], and Hermann Adrian[1] — [1]Institute of Physics, University of Mainz, 55099 Mainz, Germany — [2]National Institute of Materials Physics, 77125 Bucharest, Romania

$YBa_2Cu_3O_{7-\delta}/PrBa_2Cu_3O_{7-\delta}$ (YBCO/PBCO) superlattices with a different ratio of the superconducting and insulating layer thicknesses were prepared by high-pressure dc sputtering. The vortex-creep activation energy U was determined by analyzing the in-plane resistive transition of 200 μm- and 10 μm-wide bridges with the external magnetic field B oriented along the c axis. We found that U is proportional to the thickness of YBCO, and does not depend on the PBCO thickness, when the latter exceeds two unit cells. The U(B) dependence is well described by $U(B) \propto B^{(1/2)}$. The observed behavior can be explained in terms of 2D collective pinning. Financial support by the MWFZ Mainz, the Humboldt foundation, and the government of Egypt is gratefully acknowledged.

TT 32.22 Wed 14:00 P1A

Pinning investigation in NbN thin films — •Tetyana Shapoval, Silvia Haindl, Jan Engelmann, Volker Neu, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

NbN thin films with T_c=16 K and a thickness of 100 nm were fabricated on MgO(100) substrates by UHV pulsed laser deposition by using a Nb (99.95%) target in nitrogen gas atmosphere. Low temperature magnetic force microscopic (LT-MFM) images were performed after field cooling in a magnetic field of -2 mT to study the temperature dependence of vortex distribution. At low temperatures vortices are organized in a slightly disordered Abrikosov lattice with an average inter-vortex distance of 930 nm. Increasing the temperature to above $T = 75\%T_c$ leads to a movement of vortices during the MFM scan, which is interpreted as a thermally activated depinning process initiated by the stray field of the tip. The local pinning force has been estimated from MFM-images and compared with global VSM magnetization measurements. In addition, the temperature dependence of the penetration depth, λ, was extracted from the magnetic field profiles of single vortices.

The work is partially funded from the European Community under the Sixth Framework Programme Contract Number 516858: HIPERCHEM, and SFB 463/A4.

TT 32.23 Wed 14:00 P1A

Thermalization of energy in superconducting absorbers far from equilibrium: an experimental approach — •Loredana Fleischmann, Richard Weldle, Philipp Ranitzsch, Jan-Patrick Porst, Andreas Fleischmann, and Christian Enss — Universität Heidelberg, Kirchhoff Institut für Physik, INF 227, 69120 Heidelberg

The use of superconducting energy absorbers for low temperature micro-calorimeters offers several advantages like the possibility to have high stopping power together with low heat capacity. Due to a still not well understood thermalization of the energy released by the interacting particle, the use of superconducting absorbers is present only in special cases. We investigated by means of magnetic calorimeters the time response of the detector signal upon the absorption of x-rays in a superconducting absorber. Metallic magnetic calorimeters are low temperature energy dispersive detectors composed by an energy absorber well thermally connected to a paramagnetic temperature sensor which resides in a small magnetic field. The change of magnetization following the absorption of energy is measured as a change of flux in a low noise high bandwidth dc-SQUID. In particular we investigated absorbers made of rhenium, aluminum and aluminum doped with 600ppm manganese. The experiments using the Al and Al:Mn were performed in order to understand the role of magnetic impurities in the thermalization of energy. We discuss the temperature dependence of the energy thermalization in superconducting absorbers at the light of presently available theories.

TT 32.24 Wed 14:00 P1A

Low temperature metallic magnetic calorimeters for neutrino mass direct measurement — •Jan-Patrick Porst, Falk von Seggern, Loredana Fleischmann, Andreas Fleischmann, and Christian Enss — Universität Heidelberg, Kirchhoff Institut für Physik, INF 227, 69120 Heidelberg

In the last years the mixing of the three neutrino flavor eigenstates through a unitary matrix has been experimentally proved. Presently one of the greatest challenges in neutrino physics is to establish the absolute value of the masses of the three neutrino mass eigenstates. The kinematic determination of electron neutrino and antineutrino mass by means of the analysis of calorimetric spectra of isotopes which undergo a beta or electron-capture decay, with especially low energy available for the decay itself, represents an interesting method. In fact this method is less affected by theoretical models defining branching ratio among different decay modes. For the beta decay the isotope with the lowest Q-value present in nature is the 187-Re (Q about 2.5 keV) while for the electron capture decay the best candidate known is the 163-Ho (Q about 2.5 keV). Since those experiments need to be extremely precise, they might suffer from unexpected systematic errors. It is therefore important to investigate in detail the performance of the detectors and the calorimetric spectrum. We present our results obtained with low temperature magnetic calorimeters designed for measuring low energy beta and electron capture spectra. We also discuss problematic and the possibly present systematic uncertainties using this kind of detectors.

TT 32.25 Wed 14:00 P1A

Position Resolved High Resolution Particle Detection Using Magnetic Calorimeters — •Christian Pies, Christian Domesle, Sebastian Kempf, Andreas Fleischmann, Loredana Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

Low temperature micro-calorimeters are attractive x-ray and particle detectors for a large variety experiments due to their high resolving power and their energy dispersive character. With single pixel metallic magnetic calorimeters (MMC) an energy resolution of 2.7 eV for 6 keV x-rays was recently achieved. Quite some applications of MMCs would benefit greatly from the development of detector arrays, as they are position sensitive and allow for imaging, larger detection areas as well as the suppression of doppler-broadening in atomic spectroscopy at ion storage rings.

We recently developed two types of position sensitive MMC arrays. The first consists of 8 x-ray sensors, optimized for the energy range up to 100 keV, which are pairwise read-out by 4 dc-SQUIDs. The second prototype consists of a line of 8 large area absorbers for accelerated molecules, which are read-out by two dc-SQUIDs. To allow for this, two sets of paramagnetic sensors and pick-up coils are connected to the

absorbers, one with increasing, one with decreasing sensitivity along the line of absorbers. In this case, the sum of the two signal channels represents the deposited energy and the normalized difference the position. We present data for both detectors and discuss general design considerations as well as the achievable energy resolution.

TT 32.26 Wed 14:00 P1A

Towards MMC detector arrays: A microwave SQUID multiplexer — •Sebastian Kempf, Andreas Fleischmann, Loredana Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany.

Metallic magnetic calorimeters (MMCs) have shown to be suitable detectors for x-ray photons or massive particles in areas like astronomy, nuclear as well as atomic physics. They provide high energy resolution, high quantum efficiency, large energy bandwidth and linearity. However for many applications large detection areas, high count rates or imaging capabilities are crucial. These requirements can be satisfied by combining single detectors into large detector arrays. Due to constraints on cryogenic wiring, heat load and complexity, it is hardly possible to route thousands of wires from room temperature to the detector array. Thus a technique able to read out a large number of channels with a small number of wires has to be set up.

Recently a microwave SQUID multiplexer for the readout of low-temperature detector arrays was proposed. In such a setup every pixel consists of a superconducting $\lambda/4$-resonator inductively coupled to an unshunted rf-SQUID that is again inductively coupled to an input coil. A current through this coil is transduced to a change of magnetic flux in the SQUID and thus shifts the circuit's resonance frequency. By capacitively coupling many of those circuits to a common transmission line, injecting a frequency comb and monitoring the phase of each resonator, it is possible to infer the initial detector signal. We discuss an adaption of such a setup for the readout of MMC detector arrays.

TT 32.27 Wed 14:00 P1A

Coupling between coplanar waveguide resonators for multi-pixel kinetic inductance detectors — •Gerd Hammer, Martin Herold, Stefan Wünsch, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH), Karlsruhe, Deutschland

Coplanar resonators as core element of kinetic inductance detectors are suitable for large arrays in multi-pixel applications [1]. The readout of large arrays can be performed by simultaneous measurement of multiple channels using frequency domain multiplexing (FDM) [2]. We have studied the coupling of closely placed resonators for a multi-pixel design with a high packaging density. Superconducting resonators with niobium thin films on silicon substrates with different coupling to a transmission line have been designed, simulated and measured at liquid helium temperature. Results of the influence of coupling properties of closely placed resonators are presented and discussed in respect of a high packaging density.

[1] P. K. Day et al., Nature 425, 817 (2003).

[2] B. A. Mazin et al., Nucl. Instrum. Methods Phys. Res. A 558, 799 (2006).

TT 32.28 Wed 14:00 P1A

Investigation of energy relaxation processes in NbN thin film using optical and IR irradiation — •Dagmar Rall[1], Matthias Hofherr[2], Konstantin Ilin[2], Michael Siegel[2], Uli Lemmer[1], Alexei Semenov[3], and Heinz-Wilhelm Hübers[3] — [1]LTI, University of Karlsruhe, Germany — [2]IMS, University of Karlsruhe, Germany — [3]DLR Institute of Planetary Research, Berlin, Germany

Superconducting radiation detectors made from ultra-thin Niobium Nitride (NbN) films show high sensitivity (down to single-photon) and short response times (some ten ps), making them suitable for applications like astrophysics, spectroscopy and telecommunications. The electron energy relaxation processes and responsivity of thin NbN films and their dependence on the stoichiometry of NbN films and the critical dimensions of a device are investigated for further improvement and optimisation of the detection efficiency and speed. We present results on the study of the response of NbN thin film samples to optical and infra-red radiation. The NbN thin films with thickness from 3nm to 15nm were deposited by DC reactive magnetron sputtering onto heated sapphire substrates and patterned into lines with critical dimensions from less than 100nm up to several micrometers. The samples were kept at helium temperatures, electrically biased and excited by fs laser pulses or amplitude modulated (up to 15GHz) laser radiation. The absorbed energy is redistributed by inelastic scattering processes among electron and phonon subsystems of the NbN film. These interaction processes result in a change of resistivity of the film, which is measured as a change of voltage across the sample.

TT 32.29 Wed 14:00 P1A

Superconducting NbN detectors for synchrotron radiation — Alexei Semenov[1], Konstantin Il'in[2], Michael Siegel[2], •Heiko Richter[1], and Heinz-Wilhelm Hübers[1] — [1]DLR Instiute of Planetary Research, 12489 Berlin — [2]Instutute of Micro- and Nanoelectronic Systems, University of Karlsruhe

We present development of a special type of hot-electron bolometers that is designed to optimally detect pulsed synchrotron radiation in the terahertz frequency range. The enlarged log-spiral antenna makes it possible to sense the low-frequency part of the spectrum in coherent and non-coherent regime. The device follows the layout of a typical HEB mixer. The radiation is coupled quasioptically with the 6-mm elliptical silicon lens. The bolometer has the noise equivalent power 2 nW per square root Hz and responds to a few picoseconds long radiation pulse with the electric pulse having full width at half maximum of 160 ps. We present results obtained with this type of detector at different synchrotron facilities and discuss possible improvements of the detector performance.

TT 32.30 Wed 14:00 P1A

Three dimensional near-field radiation imaging up to the THz-regime — •Christian Brendel, Felix Stewing, and Meinhard Schilling — TU Braunschweig, Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Hans-Sommer-Strasse 66, D-38106 Braunschweig, Germany

Microwave devices are operated at very high frequencies ranging up to the THz-regime. For characterization of transmission lines, filters and directional couplers at these very high frequencies new instruments are required. We present the set-up and applications of our scanning THz-electronics prober STEP. As scanning sensor we employ a Josephson junction from the high-temperature superconductor YBa2Cu3O7 on a vibrating cantilever prepared from a LaAlO3-bicrystal. This superconducting detector is cooled to a temperature of about 30 K by a cryocooler. Despite this low temperature of the cantilever, which is about 10 um above its surface, the microwave device under investigation remains at room temperature. Based on this set up in a vacuum chamber we investigate the microwave properties of devices at frequencies of up to 762 GHz with a spatial resolution of 10 um far below the corresponding wavelengths. For the higher frequencies we couple far-infrared laser radiation from a CO2-laser pumped molecular laser system into the chamber. Applications of this novel instrument to microwave devices are demonstrated.

TT 32.31 Wed 14:00 P1A

THz-range free-electron laser ESR spectroscopy: techniques and applications in high magnetic fields — •Mykhaylo Ozerov, E. Čižmár, D. Kamenskyi, S. Zherlitsyn, T. Herrmannsdörfer, J. Wosnitza, and S.A. Zvyagin — Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden - Rossendorf (FZD), Dresden, Germany

The successful use of picosecond-pulse free-electron-laser (FEL) radiation for the continuous-wave THz-range electron spin resonance (ESR) spectroscopy has been demonstrated. The unique combination of two linac-based FELs (covering the wavelength range of 4 - 250 μm) with high magnetic fields at the Research Center Dresden-Rossendorf (FZD) allows for tunable-frequency ESR spectroscopy in an extraordinary broad frequency range of 1.2 - 75 THz in magnetic fields up to $\sim$ 70 T. The new approach is of particular importance for studying magnetic excitations in materials exhibiting field-induced phenomena (including magnetic phase transitions) and in spin systems with a large zero-field splitting. The performance of the spectrometer is illustrated with ESR spectra obtained in the low-dimensional organic material $(C_6H_9N_2)CuCl_3$ and the multiferroic compound $YMnO_3$

This work was made in collaboration with R. Wünsch, W. Seidel, H.D. Zhou, C. Wiebe.

TT 32.32 Wed 14:00 P1A

Verfahren zur Messung anisotroper thermischer Ausdehnungskoeffizienten an großen Proben — •Matthias Schneider, Armin Binneberg, Bernhardine Schumann, Björn Grossmann und Jürgen Klier — Institut für Luft- und Kältetechnik gemeinnützige Gesellschaft mbH, Bertolt-Brecht-Allee 20, D-01309 Dresden

Es wurde ein neuartiges optisches Verfahren zur Messung des makroskopischen thermischen Ausdehnungskoeffizienten entwickelt, bei welchem dessen Verhalten in unterschiedlichen Richtungen gleichzeitig ermittelt werden kann. Zudem zeichnet es sich durch die Möglichkeit aus, Proben mit Abmessungen bis zu einigen Dezimetern zu vermessen. Hauptsächliches Anwendungsgebiet ist die Untersuchung neuer Verbundwerkstoffe für thermische Isolierungen mit meist stark anisotropem Ausdehnungsverhalten. Das Messprinzip kann für unterschiedliche kryogene Medien eingesetzt werden. Darüber hinaus wird mit einem Messgerät für die Wärmeleitfähigkeit, das auf der Ermittlung der Abdampfrate einer kryogenen Flüssigkeit basiert, ein weiteres Prinzip zu Messung einer thermodynamischen Größe an ausgedehnten Proben vorgestellt.

TT 32.33 Wed 14:00 P1A

A scanning tunneling microscope for low temperatures — •Michael Marz[1,2], Gernot Goll[1], and Hilbert v. Löhneysen[1,2,3] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]DFG-Centrum für Funktionelle Nanostrukturen der Universität Karlsruhe (TH), 76128 Karlsruhe — [3]Institut für Festkörperphysik Forschungszentrum Karlsruhe, 76021 Karlsruhe

Scanning tunneling microscopy (STM) and spectroscopy (STS) are widely used to study topological and electronic properties of conducting materials. We installed a home-built STM into a dilution refrigerator, where we can reach temperatures down to 30 mK and apply magnetic fields up to 13 T. Calibration of the piezo of the scanning head was done on HOPG and $NbSe_2$ at room temperature, on both we achieved atomic resolution. At low temperatures we imaged with atomic resolution the topography of $NbSe_2$ as well as the flux-line lattice in small magnetic fields. The lattice constant a of the Abrikosov lattice shows the expected field dependence $a \propto 1/\sqrt{B}$. Spectroscopy clearly shows the superconducting density of states and Andreev bound states in the vortex core. The energy gap determined from a fit of the dI/dV vs. V curves reveals a distribution of the gap values probably due to the presence of the charge-density wave in $NbSe_2$.

TT 32.34 Wed 14:00 P1A

Design of a 300 mK, UHV, 9 T scanning tunneling microscope — •Danny Baumann[1], Torben Hänke[1], Paul Sass[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]IFW Dresden, Bereich Forschungstechnik, P.O. Box 270116, D-01171 Dresden, Germany

We present our progress in assembling an ultra high vacuum (UHV) scanning tunneling microscope (STM). This STM is designed for operating temperatures down to 300 mK and magnetic fields up to 9 T. Our system comprises an in-situ tip exchange and coarse xy-sample positioning system. Furthermore, five electrical leads are available on the sample holder to combine STM with transport measurements. The STM is mounted on a ^{3}He UHV cryostat which is connected to a three-chamber UHV system. In this work we will present first measurements on standard samples at low temperatures and UHV conditions.

TT 32.35 Wed 14:00 P1A

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

We present the design of a Scanning Tunneling Microscope (STM) for measurements at variable temperatures from 300K down to 4K. The microscope will be placed in a ^{4}He cryogenic system with a superconducting coil. This will allow measurements in cryogenic vacuum and optionally in static magnetic fields up to 17 Tesla. The STM is equipped with a sample cleaving mechanism to prepare samples in vacuum and at low temperatures.

TT 32.36 Wed 14:00 P1A

Control of vibrational modes and dissipation in nanomechanical resonators — •Stefan Bächle, Clemens Müthing, Elke Scheer, and Artur Erbe — Department of Physics, University of Konstanz

Nanomechanical systems are of interest for a wide range of practical applications (e.g. sensors, actuators) as well as for basic research. The main topic of the latter is to get a better understanding of the processes taking place at the transition of the macro-mechanical and quantum-mechanical regime. Scaling down a resonator to a point when its eigenfrequency exceeds 1 GHz, $\hbar\omega$ can be larger than the thermal energy k_BT. To reach this limit resonators with very low dissipation and damping are required. Up to date the correlation between e.g. size and shape of a nanomechanical resonator is still not understood. We present a magneto-electrical and an optical measurement setup, the sample preparation, as well as Finite Element Simulations on nanomechanical resonators. The eigenfrequencies of these silicon cantilever resonators are between several hundred MHz and up to 5GHz. The measurement setup is based on a HF-signal applied to the resonator, which is placed in a cryostat at 4K. A magnetic field of 1T up to 10T is applied perpendicularly to the samples surface. As a result the resonator is excited and starts to oscillate due to the Lorentz force. The optical measurements are based on a method called ASOPS (Asynchronous Optical Sampling).

TT 33: Postersession Correlated Electrons: Metal Insulator Transition, Spin Systems and Itinerant Magnets

Time: Wednesday 14:00–18:00 Location: P1A

TT 33.1 Wed 14:00 P1A

Optical conductivity and correlated bands of $LaVO_3$ and YVO_3 — •David Heilmann and Eva Pavarini — Institut für Festkörperforschung, Forschungzentrum Jülich, 52425 Jülich, Germany

We calculate the optical conductivities and momentum-resolved spectral functions for the $3d^2$ vanadates $LaVO_3$ and YVO_2.

As a method we adopt the LDA+DMFT technique, using Quantum Monte Carlo as an impurity solver. We obtain the self-energy matrix on the real axis by means of the Maximum-Entropy technique and a self-consistent procedure. We use the self-energy matrix to calculate the correlated band structure and the optical conductivity of $LaVO_3$ and YVO_2 both for the high-temperature orthorhombic and the low-temperature monoclinic structure. The effects of orbital fluctuations are discussed.

TT 33.2 Wed 14:00 P1A

Thermodynamic and electrical properties of EuC_{2+x} — •Oliver Heyer[1], Derk Wandner[2], Nils Hollmann[1], Uwe Ruschewitz[2], Thomas Lorenz[1], and John A. Mydosh[1] — [1]II. Physikalisches Institut, Universiät zu Köln, D-50937 Köln — [2]Institut für Anorganische Chemie, Universität zu Köln, D-50939 Köln

We have investigated the magnetization M, specific heat c_p and resistivity ρ of high-purity EuC_{2+x} (-0.1≤ x ≤ 0.3) compounds. The magnetization of EuC_2 shows a ferromagnetic ordering at $T_C \simeq 14$K with a saturation moment of $\simeq 7\frac{\mu_B}{FE}$. This imply that EuC_2 is composed of Eu^{2+} and the acetylide ion (C_2^{2-}). T_C hardly changes with x. In the paramagnetic phase all compounds are semiconductors with small bandgaps ($10-20$meV). A very interesting feature is that the onset of the ferromagnetic order decreases the resistivity ρ over several orders of magnitude indicating a metal-insulator transition (MIT). Applying magnetic fields up to 14 tesla, we find a systematic shift of the MIT temperature to higher values, resulting in a colossal magnetoresistance with changes in the resistivity up to 6 orders of magnitude. This behaviour resembles the colossal magnetoresistance of the better known Eu-rich EuO. Furthermore we carried out magnetization and specific heat measurements of YbC_2. The data identify this compound as a diamagnet without structural phase transitions. On this account YbC_2 is used as a non magnetic reference system.

TT 33.3 Wed 14:00 P1A

Co-tunneling in two-dimensional lattices of EBID-nanoparticles — •Roland Sachser, Fabrizio Porrati, and Michael Huth — Physikalisches Institut, Johann Wolfgang Goethe-

University, Frankfurt am Main, Germany

W-based granular metals have been prepared by electron beam induced deposition (EBID) from the tungsten-hexacarbonyl-precursor $W(CO)_6$. In EBID the electron beam raster process is reflected in the deposit in the limit of large dwell times. This results in a two-dimensional lattice of mesoscopic granular metal islands, in which metallic nanocrystals are separated by an insulating matrix. The islands have a high tungsten-content and therefore a high intrinsic conductivity. To investigate the transport mechanism we performed transport measurements over a temperature range from 2K to 260K. For low temperatures we observe a $\sigma \sim exp(-(T_0/T)^{1/2})$ dependence of the conductivity. The current-voltage-characteristics do not show a Coulombblockade. We interpret our measurements for low temperatures as a fingerprint of co-tunneling. By changing the electron beam parameters the size of the islands and the lattice constant can be varied. In this way it is possible to adjust the coupling between the islands and influence the transport mechanism.

TT 33.4 Wed 14:00 P1A

Orbital and charge ordering in CuI_2S_4 thiospinel studied by Raman scattering — •Vladimir Gnezdilov[1,2], Peter Lemmens[2], Yurii Pashkevich[3], Kwang-Yong Choi[4], and Vladimir Tsurkan[5] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU Braunschweig, Germany — [3]Donetsk Phystech, Ukraine — [4]Chung-Ang Univ., Seoul, Korea — [5]IAP, Chisinau, Moldova

CuI_2S_4 displays a metal-insulator (MI) transition at 230 K with an abrupt decrease of the electrical conductivity and a loss of localized magnetic moments [1]. Below T_{MI} CuI_2S_4 undergoes a simultaneous charge ordering and spin-dimerization transition [2] – a rare phenomenon in three-dimensional compounds. Here we present a Raman scattering study of CuI_2S_4 through the MI transition showing drastic changes of the spectra below T_{MI} consistent with the formation of isotropic Ir^{3+} and Ir^{4+} octamers and spin dimerization [2].

[1] T. Furubayashi et al., J. Phys. Soc. Jpn. 63, 3333 (1994).
[2] P.G. Radaelli et al., Nature 416, 155 (2002).

TT 33.5 Wed 14:00 P1A

The Fermi Surface of MoO_2 as studied by photoelectron spectroscopy, de Haas-van Alphen measurements and electronic structure calculations — •Jörg Kündel[1], Judith Moosburger-Will[1], Siegfried Horn[1], Udo Schwingenschlögl[2], and Volker Eyert[3] — [1]Experimentalphysik II, Universität Augsburg — [2]Theoretische Physik II, Universität Augsburg — [3]Center for Electronic Correlations and Magnetism, Universität Augsburg

A comprehensive study of the electronic properties of monoclinic MoO_2 from both an experimental and a theoretical point of view is presented. We focus on the investigation of the Fermi body and the band structure using angle resolved photoemission spectroscopy, de Haas-van Alphen measurements, and electronic structure calculations. For the latter, the new full-potential augmented spherical wave (ASW) method has been applied. Very good agreement between the experimental and theoretical results is found. In particular, all Fermi surface sheets are correctly identified by all three approaches.

Our results underline the importance of electronic structure calculations for the understanding of MoO_2 and the neighbouring rutile-type early transition-metal dioxides. This includes the low-temperature insulating phases of VO_2 and NbO_2, which have crystal structures very similar to that of molybdenum dioxide and display the well-known prominent metal-insulator transitions.

TT 33.6 Wed 14:00 P1A

Lattice distortions in oxide heterostructures — •Cosima Schuster[1] and Udo Schwingenschlögl[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]ICCMP, Universidade de Brasilia, 70904-970 Brasilia-DF, Brazil

Perovskite heterostructures from transition metal oxides have attracted recent interest due to the discovery of metallic interlayers in an otherwise semiconducting system. For example, a metallic contact between two common band insulators is realized in the $LaAlO_3/SrTiO_3$ heterointerface. Nevertheless, it was shown experimentally that the $LaAlO_3$ surface layer must reach a critical thickness of 4 unit cells for the interface to become conducting. This surface effect can be explained by first-principles electronic structure calculations. On varying the thickness of the $LaAlO_3$-layer on a $SrTiO_3$-substrate with a vacuum layer of at least 12 Å thickness, we have found that the interface conduction states are subject to almost rigid band shifts due to a modified Fermi energy. In addition, we take into account structural relaxation at both the $LaAlO_3/SrTiO_3$ interface and the $LaAlO_2$ surface. Drastic alterations are obtained on variation of the layer thicknesses. The distortion of the TiO_6 octahedra in the four layer structure is comparable to the multi-layer system (without surface) and enhances the metallicity in the vicinity of the interface. Modified and enhanced lattice distortions in the two layer system support an insulating state. Cooperative effects induced by the interplay between the interface/surface lattice relaxation and the electrostatic charge depletion explain the matal insulator transition.

TT 33.7 Wed 14:00 P1A

Prediction of insulator to metal transition in rubidium sesquioxide (Rb_4O_6) under high pressure — •S. Shahabeddin Naghavi[1], Gerhard H. Fecher[1], Claudia Felser[1], Jürgen Kübler[2], and Klaus Doll[3] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

We report on theoretical predictions of the insulator-metal transition in rubidium sesquioxide (Rb_4O_6) under high pressure implemented by crystal06 code. Two types of oxygen molecules exist in the sesquioxide Rb_4O_6; these are the paramagnetic hyperoxide O_2^- (two times) and the peroxide O_2^{--} (one molecule). By choosing the ferromagnetic solution and distinguishing between the two different kinds of oxygen molecules, the symmetry is reduced from cubic structure with the symmetry $I\bar{4}3d$ to tetragonal ($I\bar{4}2d$). By increasing the pressure, the differences in the bond-lengths between paramagnetic hyperoxide and peroxide is reduced until finally at a pressure of 162 Gpa they become the same. Moreover, at this pressure, the insulating state becomes metallic and the magnetism disappears. Independent calculations indicate that the equalization of the bond-lengths is essential for loosing the magnetic properties.

TT 33.8 Wed 14:00 P1A

Electronic excitation spectra on undoped and electron doped TiOCl — •Roberto Kraus[1], Martin Knupfer[1], Michael Sing[2], and Ralph Claessen[2] — [1]IFW-Dresden, D-01069 Dresden, Deutschland — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg

TiOCl as a low dimensional Mott insulator and a spin-Peierls compound has reached a lot of interest in the last years. TiOCl is a $3d^1$ system with a half filled band. One way to reach a metal-insulator transition is a filling-controlled method by doping with electrons. In TiOCl exists a large van der Waals gap in the chlorine layers which can be intercalated easily, in our case with potassium. We present the electronic excitation spectrum of TiOCl measured by electron energy loss spectroscopy. For the undoped case we find no dispersion of the excitation above the Mott-gap. With increased doping this excitation splits into a lower and higher lying part. We also investigate the changes of the crystal structure with electron diffraction and find a complex behavior with different superstructures and an expanding lattice constant perpendicular to the Ti chains.

TT 33.9 Wed 14:00 P1A

Doping dependence of stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ — •Christoph Trabant[1], Hsueh-Hung Wu[1,2], Marcel Buchholz[1], Enrico Schierle[3], Mohammed Benomar[1], Agung Nugroho[4], Alexander Komarek[1], Ralf Feyerherm[3], Markus Braden[1], Liu Hao Tjeng[1], and Christian Schüssler-Langeheine[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]NSRRC, Hsinchu, Taiwan — [3]Helmholtz-Zentrum Berlin — [4]Bandun University, Indonesia

Stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ with a doping level $n_h = x + 2\delta$ between 0.2 and 0.33 exhibits an unusual temperature dependence of the correlation length, which goes through a maximum at intermediate temperatures and decreases not only upon heating but also upon cooling. While the integrated intensity of the charge and spin order peak is conserved, the system breaks into smaller and smaller domains when cooled.

We studied this behavior as a function of Sr and oxygen content using resonant diffraction at the Ni $2p \rightarrow 3d$ ($L_{2,3}$) and $1s \rightarrow 4p$ (K) thresholds. The goal is to understand the mechanism for the low-temperature broadening. Differences between commensurate and incommensurate order as well as the effect of the oxygen content will be discussed.

Supported by the DFG through SFB 608 and by the BMBF through

05 ES3XBA/5.

TT 33.10 Wed 14:00 P1A

The coupled electronic order of manganese and oxygen states in doped manganites — •Jochen Geck[1,2], David G. Hawthorn[3], Kyle M. Shen[4], Hiroki Wadati[2], Enrico Schierle[5], Liu H. Tjeng[6], Hsueh-Hung Wu[6], Christian Schüssler-Langeheine[6], and George A. Sawatzky[2] — [1]IFW Dresden, Germany — [2]University of British Columbia, Canada — [3]University of Waterloo, Canada — [4]Cornell University, USA — [5]Helmholtz-Zentrum Berlin, Germany — [6]University of Cologne, Germany

Comparing resonant soft x-ray scattering (RSXS) experiments and realistic many-body calculations, the nature of the electronic crystal formed in the low-temperature phase of $La_{7/8}Sr_{1/8}MnO_3$ is investigated. The analysis of the experimental data implies that the modulation of the Mn-valence must be very small and that the detected Mn-ordering is mainly of orbital nature. The emerging picture of manganese orbital order, which is coupled to charge and orbital order of the O 2p-states, seems to be a general feature of electronically ordered manganites.

TT 33.11 Wed 14:00 P1A

Investigation of Orbital-Ordering in Sr_2VO_4 — •Joseph M. Law[1,2], Eva Brücher[1], Sukanta Karmakar[1], Karl Syassen[1], and Reinhard K. Kremer[1] — [1]Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Dep. of Physics, Loughborough University, Loughborough, U.K.

Sr_2VO_4 is a Mott insulator which crystallizes with the tetragonal K_2NiF_4 structure. It hosts V^{4+}, ($3d^1$ configuration), is another layered S=1/2 afm with unusual ground state properties. Recently it was shown that tetragonal Sr_2VO_4 undergoes a phase transition (PT) near 104K evidenced by a sudden drop of the magnetic susceptibility and anomalies in the lattice parameters (c increases by 0.15%) but no change of the crystallographic symmetry. Based on *ab initio* calculations the PT was ascribed to an orbital-ordering transition which leads to a decreasing occupancy of the d_{xy} orbital balanced by an increasing electronic density along the c axis.[1] We have investigated the orbital-ordering PT by heat capacity, dc resistivity and dielectric measurements on polycrystalline samples of tetragonal Sr_2VO_4. The heat capacity measurements display an anomaly confirming a PT at 104 K. Additionally, a sluggish precursor regime extending up to 125K consistent with the lattice properties was found. Our resistivity and dielectric measurements prove a Mott gap of $\sim$ 100 meV as already seen in thin films, which reveals an increase of the activation energy below $\sim$ 125 K leading to a rapid growth of the electrical resistance below the PT.

[1] H. D. Zhou *et al.*, Phys. Rev. Lett. **99**, 136403 (2007).

TT 33.12 Wed 14:00 P1A

Interplay between superconductivity and charge order in 2D organic superconductors — •Stefan Kaiser[1], Natalia Drichko[1], Yaxiu Sun[1], Martin Dressel[1], Toomas Room[2], Dan Hüvonen[2], Urmas Nagel[2], Matteo Masino[3], Alberto Girlando[3], and John Schlueter[4] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]KBFI, Tallinn, Estonia — [3]Dip. Chimica G.I.F. and INSTM-UdR Parma, Italy — [4]Material Science Division, Argonne National Laboratory, U.S.A.

Theoretical study of systems with quarter-filled conductance band and strong electron-electron correlations propose superconductivity mediated by charge order fluctuations [1]. We present IR reflectivity of a 1/4-filled organic superconductor β"-(BEDT-TTF)2SF5CH2CF2SO3 (Tc=5 K) in the frequency range between 8 and 10000 cm-1 at temperatures down to 1.8 K. Our spectroscopic study reveals a splitting of the charge-sensitive phonons showing charge order while transport properties show metallic behavior. The narrow Drude response and its interplay with charge fluctuations, evident in an electronic band, is responsible for superconductivity, with a superconducting gap of 12 cm-1 at 1.8 K. A comparison with the isostructural metal β"-(BEDT-TTF)2SF5CHFSO3 reflects the close relation between superconductivity and charge order.

[1]. J. Merino et al. Phys. Rev. Lett 87, 237002 (2001)

TT 33.13 Wed 14:00 P1A

Dynamic Spin Excitations and Magnetism in the Hubbard Model — •Sebastian Schmitt — Theoretische Physik II, TU Dortmund

The static and dynamic magnetic susceptibility of the Hubbard model is calculated within the dynamical mean field theory (DMFT) using the enhanced non-crossing approximation (ENCA) as impurity solver. The magnetic properties are discussed for various dopings, temperatures and lattices with and without frustration. Special emphasis is laid on the interpretation in terms of the two fundamental pictures of magnetism, i.e. Stoner-type magnetism of itinerant electronic excitations and Heisenberg spin-magnetism of localized magnetic moments. The transition between these two opposing pictures is discussed. An interesting reentrant behavior is observed for the antiferromagnetic Néel temperature in the intermediate coupling region. Additionally, a dispersionless collective mode is observed in the dynamic magnetic susceptibility for large values of the Coulomb repulsion at very low temperatures, indicating a localized singlet-triplet excitation connected with the breakup of local Kondo-singlets.

TT 33.14 Wed 14:00 P1A

A Functional Approach for the Spin Chain — •Stephan Filor and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen

We set up a new approach to the physics of spin systems which uses a resolvent method originally proposed by Keiter and Kuramoto. In analogy to the Baym-Kadanoff formalism the latter introduced the partition sum of a system as a functional of the resolvent of the Hamiltonian and its so called generalized self-energy. This functional is the starting point for a variational cluster method which is based on Potthoffs self-energy functional approach. In a first step we apply our ansatz to a Heisenberg spin chain.

TT 33.15 Wed 14:00 P1A

Spin-1 anisotropic Heisenberg antiferromagnets — •David Peters[1], Ian McCulloch[2], and Walter Selke[1] — [1]RWTH Aachen University and JARA-SIM, Germany — [2]The University of Queensland, Australia

Intricate phase diagrams of spin-1 Heisenberg antiferromagnets with exchange and single-ion anisotropy are studied using mainly density matrix renormalization group techniques.

Various phases are identified, including antiferromagnetic, spin-liquid (or spin-flop), supersolid (or biconical), and ferromagnetic phases. Results are compared to recent findings on related quantum models and to properties of corresponding classical spin systems.

Funded by the Excellence Initiative of the German federal and state governments.

TT 33.16 Wed 14:00 P1A

Spin-Dynamics of the antiferromagnetic S=1/2-Chain at finite magnetic Fields and intermediate Temperatures — •Simon Grossjohann and Wolfram Brenig — Institut für theoretische Physik, Technische Universität Braunschweig

We present results for the dynamic structure factor of the antiferromagnetic spin-1/2 Heisenberg chain at finite temperatures and finite magnetic fields. Using Quantum-Monte-Carlo based on the stochastic series expansion and Maximum-Entropy methods we detail the evaluation of longitudinal and transverse dynamic structure factors $S^{\alpha\beta}(q,\omega)$ with $\alpha\beta \in \{zz, xx, +-, -+\}$ from vanishing magnetic fields up to and above the threshold B_c for ferromagnetic saturation, as well as for high and for intermediate temperatures. The field-induced redistribution of spectral weight was focus of our studies, contrasting longitudinal versus transverse excitations. At finite fields below saturation incommensurate low-energy modes are found to be consistent with zero temperature Bethe-Ansatz. The crossover between the field induced ferromagnet above B_c and the Luttinger liquid below B_c is analyzed in terms of the transverse spin-dynamics and compared to T_1-relaxation rates on CuPzN. Finally we assess the quality of the analytic continuations by evaluating sum-rules and detailed balance to demonstrate excellent consistency of the Maximum-Entropy results.

TT 33.17 Wed 14:00 P1A

Magnetic impurities in two-dimensional spin-1/2 antiferromagnets — •Björn Willenberg, Simon Grossjohann, and Wolfram Brenig — Institut für theoretische Physik, Technische Universität Braunschweig

Using Quantum Monte-Carlo methods based on the stochastic series expansion we investigate a single spin degree of freedom coupled to a two-dimensional Heisenberg antiferromagnet (HAFM). Results will be presented for thermodynamic and dynamic properties. In particular

the local susceptibility will be considered as a function of temperature, magnetic field, and local spin quantum number. Moreover we will contrast the case of antiferro- versus ferromagnetic coupling of the impurity to the HAFM. This analysis will be extended to real-space spin correlation-functions which will be evaluated in the vicinity of the quantum impurity including a detailed finite size analysis. Finally the impurity dynamics will be considered by calculating imaginary time spin-correlators and performing Maximum Entropy analysis.

TT 33.18 Wed 14:00 P1A

Effective Hamiltonians for Doped Spin-$\frac{1}{2}$ Ladders from Self-Similar Continuous Unitary Transformations — •Sebastian Duffe, Tim Fischer, and Götz S. Uhrig — Technische Universität Dortmund

Doped spin-$\frac{1}{2}$ ladder systems are important model systems for 2D high-T_C superconductors. Their one-dimensionality renders them more tractable to various analytic and numerical approaches. Experimentally such ladder systems are realized in the so-called telephone number compounds $Sr, Ca, La_{14}Cu_{24}O_{41}$.
Here we systematically derive effective Hamiltonians for the hole motion in such spin ladders. The technique of choice are continuous unitary transformations (CUTs) which are performed self-similarly for the coefficients of operator monomials in real space in second quantization. The proliferating number of terms is bounded by truncating far reaching processes which reach longer than the finite correlation length. The magnetic excitations are triplons on the rungs of the ladder; the charge excitations are holes with spin living also on the rungs of the ladder. The effective Hamiltonian allows us to read off the dispersions of single excitations directly. But it also contains their interaction.

TT 33.19 Wed 14:00 P1A

Thermodynamics of a one-dimensional frustrated spin-$\frac{1}{2}$ Heisenberg ferromagnet — •Moritz Härtel[1], Johannes Richter[1], Dieter Ihle[2], and Stefan-Ludwig Drechsler[3] — [1]ITP, OvG-Universität Magdeburg, D-39016 Magdeburg, Germany — [2]ITP, Universität Leipzig — [3]Leibniz-Institut IFW Dresden

The frustrated one-dimensional J_1-J_2 Heisenberg ferromagnet ($J_1 = -1$, $J_2 > 0$) has attracted much attention due to recent experiments on edge-shared chain-cuprates, e.g. $LiVCuO_4$ and Li_2CuO_2.
We use a second-order Green's function technique and the full exact diagonalization of finite systems of up to $N = 22$ lattice sites to calculate thermodynamic properties (correlations functions $\langle \mathbf{S}_0 \mathbf{S}_n \rangle$, correlation length ξ, isothermal spin susceptibility χ, and specific heat C_V). Although we restrict on the ferromagnetic ground state, i.e. $J_2 < 0.25$, the frustration influences the thermodynamics substantially. We find that the critical indeces of the susceptibility and the correlation length are not changed by a finite frustration in absence of a magnetic field, i.e. $\chi = y_0 T^{-2}$ and $\xi = x_0 T^{-1}$ at $T \to 0$. The coefficients y_0 and x_0 decrease linearly with increasing J_2 and vanish at the critical point $J_2 = 0.25$ due to the zero-temperature phase transition that is accompanied by a change in the critical behavior. In addition, we detect the existence of an additional low-temperature maximum in the specific heat when approaching the critical point. Including a weak magnetic field ($h \lesssim 0.07$) this additional maximum exists already at $J_2 = 0$ but gets more pronounced with increasing J_2.

TT 33.20 Wed 14:00 P1A

Thermodynamic properties of the ferromagnetic Kondo Lattice Model at finite temperatures for different magnetic phases — •Martin Stier and Wolfgang Nolting — Humboldt-Universität zu Berlin, Institut für Physik, Theoretische Festkörperphysik, Newtonstraße 15, 12489 Berlin, Germany

We investigate the ferromagnetic Kondo Lattice Model (KLM) at finite temperatures for different (anti)ferromagnetic phases. To compare the theory with real materials like the manganites we extend the pure KLM by terms describing the Coulomb interaction, the superexchange and a Jahn-Teller splitting. Using a modified RKKY method we determine the various transition temperatures and decide by calculating the free energy which phase is actually present at a given parameter set. Additionally, we can evaluate other important thermodynamic quantities like the entropy or the specific heat.

TT 33.21 Wed 14:00 P1A

The ground state phase diagram of the ferromagnetic Kondo-lattice model — •Sören Henning and Wolfgang Nolting — Humboldt Universität zu Berlin; Institut für Physik; AG Festkörpertheorie; Newtonstr.15; 12489 Berlin

The magnetic ground state phase diagram of the ferromagnetic Kondo-lattice model is constructed by calculating internal energies of all possible bipartite magnetic configurations of the simple cubic lattice explicitly. This is done in one dimension (1D), 2D and 3D assuming a local moment of $S = \frac{3}{2}$ and a saturated sub-lattice magnetization. As will be shown, it is possible to treat all higher local correlation functions appearing in the many-body problem exactly under these assumptions. A simple explanation for the obtained phase diagram in terms of bandwidth reduction is given. Regions of phase separation are determined from the internal energy curves by an explicit Maxwell construction.

TT 33.22 Wed 14:00 P1A

Spin waves in the Heisenberg and in the Kondo-lattice Model — •Andrej Schwabe and Wolfgang Nolting — Institut für Physik, Humboldt-Universität, Newtonstraße 15, 12489 Berlin, Germany

We present a new approach to the 3D ferromagnetic Heisenberg model being bosonized by the Dyson-Maleev transformation. Magnon excitation energies and line widths are derived by applying the method of moments with a broadened magnon spectral density.
Furthermore, we extend the investigation to the ferromagnetic Kondo-lattice model that can be mapped onto an effective Heisenberg model by using the modified RKKY interaction and the Interpolating Selfenergy Approach. Magnon energies and line widths are calculated for the limiting cases relevant to manganites and ferromagnetic semiconductors. The dependence on band occupation n, intra-atomic exchange J and temperature is investigated. Both zone boundary magnon softening and anomalous magnon damping are found.

TT 33.23 Wed 14:00 P1A

Manipulating magnetic structures in chiral metals by currents — •Karin Everschor[1], Achim Rosch[1], and Rembert Duine[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institute for Theoretical Physics, Department of Physics and Astronomy Faculteit Betawetenschappen, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We investigate how currents can modify 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 very weakly to disorder and the underlying crystalline lattice. We start from the Landau-Lifshitz-Gilbert equation including adiabatic and non-adiabatic spin transfer torques. We investigate a variational approach to determine equations of motion for different magnetic structures. Especially interesting is the influence of currents on the so-called "A-phase" of MnSi, where a lattice of skyrmions forms.

TT 33.24 Wed 14:00 P1A

Spectral weight of Mott-Hubbard excitations in YVO_3 studied by ellipsometry — •Julia Küppersbusch[1], Christina Hilgers[1], Agung Nugroho[2], Thomas Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

We investigate the optical conductivity of YVO_3 between 0.75 and 5.5 eV from T=15 to 300 K by means of ellipsometry. Different groups reported contradictory data sets, none of them succeeded in explaining the T dependence of the peak structure [1-3].
The compound YVO_3 undergoes a series of temperature-induced structural/electronic phase transitions. The different phases show different spin/orbital ordering patterns, leading to a pronounced anisotropy in the optical spectra. The Mott-Hubbard gap of insulating YVO_3 is located at 1.6 eV. The strong increase of the optical conductivity above 4 eV is attributed to the onset of charge-transfer (CT) excitations. Below the CT transitions, the optical spectrum shows a three-peak structure with a complex T dependence. This has been attributed to the different types of spin/orbital ordering, but a consistent description could not be achieved. Our data resolve the issue of the contradictory data sets. We discuss the multiplet assignment of the different peaks and obtain an excellent understanding of the T dependence of the optical conductivity.

[1] S. Miyasaka, Y. Okimoto, and Y. Tokura, J. Phys. Soc. Jpn. **71**, 2086 (2002).
[2] A.A. Tsvetkov *et al.*, Phys. Rev. B **69**, 075110 (2004).
[3] J. Fujioka, S. Miyasaka, and Y. Tokura, PRB **77**, 144402 (2008).

TT 33.25 Wed 14:00 P1A

Synthesis and properties of the filled skutterudites

$CePt_4Ge_{12}$ and $SmPt_4Ge_{12}$ — •Walter Schnelle, Roman Gumeniuk, Andreas Leithe-Jasper, Helge Rosner, Michael Nicklas, Michael Baenitz, Michael Schöneich, Marcus Schmidt, Ulrich Schwarz, and Yuri Grin — MPI für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany

While the ternary platinum-germanium skutterudites with the trivalent rare-earths La and Pr are superconductors the isostructural compounds with Ce, Nd^{3+} and Eu^{2+} order antiferromagnetically [1]. Recently, isotypic $SmPt_4Ge_{12}$ was prepared at high pressure and XAS measurements reveal that the valence of samarium is temperature-independent and close to 3+. Magnetization data show typical van-Vleck paramagnetic behaviour at elevated temperatures. The low-temperature specific heat displays a field-independent Schottky-type anomaly and a large linear coefficient γ. $CePt4Ge_{12}$ shows a typical valence fluctuation behaviour with an average Ce valence close to 3+. Together with electronic band structure calulations and NMR investigations [2] we discuss the low-temperature behaviour of these new compounds.

[1] R. Gumeniuk *et al.* Phys. Rev. Lett. 100 (2008) 017002.
[2] M. Baenitz *et al.* this conference.

TT 33.26 Wed 14:00 P1A

Spin-phonon scattering and heat transport in spin ladders — •Christina Seidler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study the spin-phonon dynamics and the heat transport of two-leg spin-1/2 ladders in the presence of a magnetoelastic deformation-potential coupling. In the limit of weak inter-rung exchange we employ a mapping of the spin degrees of freedom to a gas of non-interacting bond-bosons to describe the magnetic excitations. The coupled spin-phonon excitations are derived perturbatively and their spectra will be discussed as a function of momentum, frequency, temperature, system parameters and external magnetic fields. Both optical and acoustical phonons will be considered.

The heat transport will be investigated in the linear-response regime by evaluating the corresponding Kubo integrals. Results for the temperature and the magnetic field dependence of both, the magnetic and phononic heat conductance, will be presented. In particular the effect of the field-induced triplet softening will be regarded.

Our results will be put into the context of the anomalous magnetic heat transport of the spin-ladder compound $Sr_{14}Cu_{24}O_{41}$.

TT 34: Postersession Matter at Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-Cold Atoms

Time: Wednesday 14:00–18:00 Location: P1A

TT 34.1 Wed 14:00 P1A

Phase Diagram of a Bosonic Model on a Square Lattice with Competing Interactions — •Ansgar Kalz, Andreas Honecker, Sebastian Fuchs, and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen

The analysis of frustrated spin systems reveals a variety of interesting phenomena as for example quantum criticality and ordering processes in exotic phases. The antiferromagnetic spin-1/2-Heisenberg model with nearest and next nearest neighbour interaction J_1 and J_2 shows a strong frustration near the critical point $J_2 \approx J_1/2$. The simulation of this frustrated spin system via Quantum Monte Carlo methods is limited by the sign problem. Therefore we simulated a closely related bosonic model which can be applied to cold atoms in optical lattices. We present phase diagrams for the classical Ising limit and the quantum case at finite and zero temperature.

TT 34.2 Wed 14:00 P1A

Quantum Monte Carlo Simulation of Suprafluidity with Fermions in a Two Dimensional Optical Lattice — •Klaus Ferdinand Albrecht and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart, D-70550 Stuttgart, Germany

Based on a Projector Quantum Monte Carlo Simulation, we examine the ground state properties of the attractive 2D fermionic Hubbard model. The main focus is on the supersolid phase, where in a periodic system it is known that the superfluid phase coexists with a crystalline structure (CDW-phase) at density n=1. We obtain the conditions for such a phase when the system is confined in a harmonic trap. Furthermore, we consider the BCS-BEC crossover region in a periodic system.

TT 34.3 Wed 14:00 P1A

Real-space DMFT for inhomogeneous strongly correlated fermionic systems — •Irakli Titvinidze[1], Michiel Snoek[1], Csaba Toke[1], Krzysztof Byczuk[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt, Germany — [2]Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland

We introduce the real-space dynamical mean-field theory (R-DMFT) method to describe strongly interacting lattice fermions in the presence of an external, position dependent potential. This method relies only on the assumption that the self-energy is a local quantity, and is exact in infinite dimensions. Using R-DMFT we study an ultracold spin 1/2 fermionic atomic gas in an optical lattice. Using the numerical renormalization group (NRG) as an impurity solver we show that antiferromagnetic order is stable in spatial regions with total particle density close to one, but persists also in parts of the system where the local density significantly deviates from half filling. In systems with spin imbalance, we find that antiferromagnetism is gradually suppressed and phase separation emerges beyond a critical value of the spin imbalance.

TT 34.4 Wed 14:00 P1A

Bosonic Dynamical Mean Field Theory for the Bose-Hubbard model — •Andreas Huberer, Michiel Snoek, and Walter Hofstetter — Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany

We study the physics of strongly correlated bosonic particles in optical lattices. The conventional bosonic Gutzwiller approximation, in which the hopping is treated in mean field, is exact in infinite dimensions and qualitatively reproduces the phase diagram. However, it does not include the effect of the hopping of normal particles and underestimates the size of the Mott insulating domains. We therefore take into account the leading 1/z corrections (z being the lattice coordination number) to the Gutzwiller approximation, which corresponds to Bosonic Dynamical Mean Field Theory. We derive the self-consistency relations for the superfluid order parameter and the Green's function. In order to solve them we use Exact Diagonalization as an impurity solver. Using this method we calculate the phase diagram for a single species of bosons at zero and nonzero temperature and calculate corrections to the mean-field results for various quantities. Furthermore we investigate the phase diagram for a mixture of two different spin states with unit filling at both zero and nonzero temperature. We apply this model to the experimental relevant case of a Rubidium-Potassium-mixture.

TT 34.5 Wed 14:00 P1A

Entanglement Dynamics of Ultra-Cold Atoms in Optical Superlattices — •Andreas Wagner, Thomas L. Schmidt, and Christoph Bruder — Universität Basel

We study the dynamics of ultra-cold atoms in optical superlattices and entanglement in such multipartite systems. We investigate and compare different ways to quantify and manipulate entanglement of three to four atoms, which are trapped in such a lattice and form a subsystem of a larger amount of trapped atoms. By manipulating the lattice we get information about the dynamics of entanglement distribution.

TT 34.6 Wed 14:00 P1A

Mean-field dynamics of a non-hermitian Bose-Hubbard dimer — •Astrid Elisa Niederle[1], Hans Jürgen Korsch[2], and Eva Maria Graefe[2] — [1]Theoretical Physics, Saarland University, D-66041 Saarbrücken — [2]FB Physik, TU Kaiserslautern, D-67653 Kaiserslautern

We investigate an N-particle Bose-Hubbard dimer with an additional

effective decay term in one of the sites. A mean-field approximation for this non-hermitian many-particle system is derived, based on a coherent state approximation. The resulting nonlinear, non-hermitian two-level dynamics, in particular the fixed point structures showing characteristic modifications of the self trapping transition, are analyzed. The mean-field dynamics is found to be in reasonable agreement with the full many-particle evolution.

TT 34.7 Wed 14:00 P1A

Spectral functions in one-dimensional quantum systems at T>0 — •Thomas Barthel[1], Ulrich Schollwöck[1], and Steve R. White[2] — [1]Institute for Theoretical Physics C, RWTH Aachen — [2]Department of Physics and Astronomy, University of California, Irvine, USA

We demonstrate how a combination of finite-temperature time-dependent density-matrix renormalization-group (t-DMRG) calculations and time-series prediction allows for an easy and very accurate calculation of spectral functions in 1d quantum systems, irrespective of their statistics, for arbitrary temperatures.

This is illustrated with spin structure factors of XX and XXZ spin-1/2 chains where we compare, in the first case, against an exact solution and, in the second case, against Bethe ansatz (BA) at T=0 and Quantum Monte Carlo (QMC) for T>0. [arXiv:0901.2342]

TT 35: Postersession Transport: Nanoelectronics, Quantum Coherence and Quantum Information, Fluctuations and Noise

Time: Wednesday 14:00–18:00 Location: P1A

TT 35.1 Wed 14:00 P1A

Interference and interaction effects in adiabatic pumping through quantum dots — •Bastian Hiltscher, Michele Governale, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

In order to investigate the effects of interference and interaction in adiabatic pumping, we consider an Aharonov-Bohm (AB) interferometer with a quantum dot embedded either in one or in both arms[1]. We employ a real-time formalism and we perform an expansion both in the tunnel-coupling strengths between dot and leads and in the pumping frequency[2], taking into account the Coulomb interaction non perturbatively.

We find that pumping in the AB interferometer with only one dot has a peristaltic but at the same time phase-coherent character. The flux dependence of the pumped current clearly indicates the presence of coherent processes in this transport mechanism. In an AB interferometer with one dot in each arm, it is possible to pump with the gate voltages of the two different dots. In this case, pumping relies purely on quantum-mechanical interference and has no classical counterpart.

[1] J. König und Y. Gefen, Phys. Rev. B **65**, 045316 (2002).

[2] J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. B **74**, 085305 (2006).

TT 35.2 Wed 14:00 P1A

Non-local Andreev transport through an interacting quantum dot — •David Futterer[1], Michele Governale[1], Marco G. Pala[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]IMEP-LAHC-MINATEC (UMR CNRS/INPG/UJF 5130), 38016 Grenoble, France

We investigate sub-gap transport through an interacting quantum dot tunnel coupled to one superconducting lead and two normal conducting leads which can be either ferromagnetic or non-magnetic[1]. Despite the tendency of a large charging energy to suppress the equilibrium proximity effect on the dot, a finite Andreev current can be achieved in non-equilibrium situations. We propose two schemes to identify non-local Andreev transport. In one of them, we identify crossed Andreev reflection by the dependence of the Andreev current on the relative orientation and polarization of the ferromagnetic leads. In the second scheme, the presence of strong Coulomb interaction leads to negative values of the non-local conductance as a clear signal of non-local Andreev transport. For our calculation we apply a real-time transport theory[2,3] in the limit of a large pair potential Δ.

[1] D. Futterer, M. Governale, M. G. Pala, and J. König, arXiv:0806.0237(2008).

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

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

TT 35.3 Wed 14:00 P1A

Influence of spin waves on transport through a quantum-dot spin valve — •Björn Sothmann[1,2], Jürgen König[1,2], and Anatoli Kadigrobov[3,2] — [1]Theoretische Physik, Universität Duisburg-Essen, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, Germany — [3]Departement of Physics, Göteborg University, Sweden

A quantum-dot spin valve, i.e. a single-level quantum coupled to ferromagnetic leads with arbitrarily oriented magnetizations, reveals interesting transport properties as e.g. negative differential conductance due to an interplay between non-equilibrium spin accumulation on the quantum dot and spin precession due to an exchange field which is created by virtual tunneling to the leads.

In order to describe the influence of spin waves on transport through a quantum-dot spin valve, we generalize the real-time diagrammatic transport theory developed in Ref. [1] to include magnonic degrees of freedom in the leads. In the regime of large spin-wave energies, we find that the formation of a trapping state leads to a negative differential conductance. Moreover, we find that magnons will be pumped from the source to the drain lead. In addition, we observe that the magnons can pump a completely spin-polarized current at zero bias voltage. We also report on the zero- and finite-frequency current noise. We find the latter to be sensitive to the magnonic contributions to the exchange field.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B **70**, 195345 (2004).

[2] B. Sothmann, J. König, A. Kadigrobov, in preparation.

TT 35.4 Wed 14:00 P1A

Time-resolved Electron Transport through Quantum Dot Systems — •Alexander Croy and Ulf Saalmann — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

The investigation of *time-resolved* currents in mesoscopic devices has gained a lot of interest over the past few years. There has been a lot of experimental and theoretical progress in realizing, modeling and understanding time-dependent electron transport.

In this context we study theoretically the time-resolved electric currents flowing through single and double quantum dots that are subject to a voltage pulse. An established tool in this regard is the non-Markovian quantum master equation (QME) for the many-body density matrix describing the state of the quantum dot system. Usually the QME is taken up to second order in the dot-reservoir coupling. For QMEs of higher order in the coupling not as many results are available.

In the present work we numerically solve a QME including terms up to fourth order and give results of the time-resolved occupation and the currents flowing through the system. Complementary to that we present a new method for treating time-dependent non-equilibrium Green function calculations in the wide-band limit. We show a comparison of the results obtained from both methods for the non-interacting resonant level model, indicating that the additional terms are important to describe the electric current.

TT 35.5 Wed 14:00 P1A

Towards quantum dots on GaAs nanowires — •Johannes Mösl[1], Anna Fontcuberta i Morral[2,3], and Stefan Ludwig[1] — [1]Fakultät für Physik and Center for NanoScience, LMU Munich, Geschwister-Scholl- Platz 1, D-80539 München, Germany — [2]TU Munich, Walter Schottky Institut, Am Coulombwall 3, 85748 Garching, Germany — [3]EPF Lausanne, Switzerland

Semiconductor nanowires is an emergent research topic in the field of nanoelectronics, as they form an excellent building block for 0D and 1D applications and allow novel architectures and material combinations. We study electronic transport properties of catalyst-free MBE

grown GaAs nanowires, p-doped at a number of different doping levels. Detailed characterization of the wires including electronic contacts fabricated by e-beam lithography and based on palladium or annealed zinc-silver alloys are discussed. Contact properties and a pronounced hysteresis of the current through the nanowires, as a backgate-voltage is swept, are explained within tentative models. In addition we present first transport measurements on quantum dots, which are defined electrostatically as well as by etched constrictions.

TT 35.6 Wed 14:00 P1A

Nonequilibrium transport through a correlated quantum dot with magnetic impurity — •Daniel Becker[1], Stephan Weiss[2], Michael Thorwart[3], and Daniela Pfannkuche[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, D-20355 Hamburg, Germany — [2]Niels Bohr Instituttet, Nano-Science Centret, Universitetsparken 5, DK-2100 Copenhagen, Denmark — [3]FRIAS, Albert-Ludwigs-Universität Freiburg, Albertstr.19, 79104 Freiburg, Germany

The deterministic, non-perturbative scheme of iterative summation of path integrals (ISPI)[1] is adopted to a single-level quantum dot with one quantum spin-1/2 magnetic impurity interacting with the dot-electron spins. For two electrons on the dot, Coulomb interaction is taken into account. A generating function is obtained to calculate the dc tunneling current at finite bias voltages and the orientation of the impurity spin. This real-time path integral extends over all paths of (i) the magnetic impurity spin and of (ii) Ising-like fluctuating spin fields, which are introduced to decouple the interacting dot-electrons. With the use of the ISPI scheme, the sum over all these paths can be carried out numerically, while exactly accounting for all lead-induced self-energies within a sufficiently long, but finite coherence time. This allows to study real-time nonequilibrium transport through the considered system in the case of strong electron-impurity interaction as well as strong coupling to the leads, even at low temperatures and for a wide range of bias voltages. In particular, the mutual influence between tunneling current and the impurity spin dynamics is of interest.

[1] S. Weiss et al., Phys. Rev. B 77, 195316 (2008)

TT 35.7 Wed 14:00 P1A

Transport properties of smooth and rough interfaces — •Mohamed Fadlallah[1], Cosima Schuster[1], and Udo Schwingenschlögl[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany — [2]ICCMP, Universidade de Brasilia, 70904-970 Brasila-DF, Brazil

The functionality of nanoscale devices depends crucially on the transport properties across the interfaces. As devices are reduced in size, interfaces dominate the transport. Nanocontacts hence were studied intensively over the last years and many approaches to calculate the transport were developed. Most are based on electronic structure calculations to obtain the material specific aspects. Nevertheless the properties of simple distorted interfaces are not well understood. Distortions may occur due to orientation mismatch, vacancy sites, buckling of the interface layer, or impurities. We discuss the equilibrium and non-equilibrium properties of distorted interfaces between simple metals (Au, Al) using the SMEAGOL code which combines density functional theory (DFT) and non-equilibrium Green's functions (NEGF) by using Landauer formula. The transmission coefficient is proportional to the density of states (DOS). Only in the case of a vacancy, we see a substantial reduction of the transmission coefficient near the Fermi level. Other kinds of distortion influence only the transmission at lower energies. With increasing voltage the transmission coefficient of the d-band decreases linearly, but stays constant near the Fermi level in the gold system. For Aluminum it is reduced over the whole energy range. This work was done in the collaboration with Dublin group of SMEAGOL.

TT 35.8 Wed 14:00 P1A

Current without external bias and diode effect in shuttling transport of nanoshafts — •Klaus Morawetz[1,2], Sibylle Gemming[1], Regina Luschtinetz[3], Lukas Eng[4], Gotthard Seifert[3], and Anatole Kenfack[5] — [1]Forschungszentrum Dresden-Rossendorf, PF 51 01 19, 01314 Dresden, Germany — [2]International Center for Condensed Matter Physics, 70904-910, Brasília-DF, Brazil — [3]Institute of Physical Chemistry and Electrochemistry, TU Dresden, 01062 Dresden, Germany — [4]Institute of Applied Photophysics, TU Dresden, 01062 Dresden, Germany — [5]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

A row of parallel ordered and coupled molecular nanoshafts is shown to develop a shuttling transport of charges at finite temperature. The appearance of a current without applying an external bias voltage is reported as well as a natural diode effect allowing unidirectional charge transport along one field direction while blocking the opposite direction[1]. The zero-bias voltage current appears above a threshold of initial thermal and/or dislocation energy.

[1] New J. Phys. 10 (2008) 103014-1-8

TT 35.9 Wed 14:00 P1A

A Microscopic Model of Current-Induced Switching of Magnetization — •Niko Sandschneider and Wolfgang Nolting — AG Festkörpertheorie, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

We study the behaviour of the magnetization in a ferromagnetic metal/nonmagnetic insulator/ferromagnetic metal/paramagnetic metal (FM1/NI/FM2/PM) tunnel junction. It is calculated self-consistently within the nonequilibrium Keldysh formalism. The magnetic regions are treated as band ferromagnets, such as Co, and are described by the single-band Hubbard model. The left (FM1) and right (PM) lead are assumed to remain in equilibrium. We developed a nonequilibrium spectral density approach to solve the Hubbard model approximately in the switching magnet FM2. By applying a voltage to the junction it is possible to switch between antiparallel (AP) and parallel (P) alignment of the magnetizations of the two ferromagnets. The transition from AP to P occurs for positive voltages while the inverse transition from P to AP can be induced by negative voltages only. This behaviour is in agreement with the Slonczewski model[1] of current-induced switching and appears self-consistently within the model, i.e. without using half-classical methods like the Landau-Lifshitz-Gilbert equation.

[1] J. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)

TT 35.10 Wed 14:00 P1A

Electrical-physical characteristics of Si/SiO_2/Ni nanoelectronic systems with ion tracks in strong magnetic fields — •Alexander Petrov[1], Egor Kaniukov[1], Sergey Demyanov[1], Ivan Svito[2], Alexander Fedotov[2], and Eugene Belonogov[3] — [1]Scientific-Practical Materials Research Centre NAS of Belarus, Minsk, Belarus — [2]Belarusian State University, Minsk, Belarus — [3]Voronezh State Technical University, Voronezh, Russia

The present research deals with the swift heavy ion track technology, which includes irradiation of a material by Au ions (energy 350 MeV, fluence 10^8 cm^{-2}), chemical etching of resulting swift heavy ion tracks and precision electrochemical deposition of magnetic metals in the resulting nanopores.

In this way structures on the base of SiO_2/n-Si with nanopores in silicon dioxide layers, filled with Ni nanoclusters, have been prepared and studied. Investigations of current-voltage dependences and magnetic characteristics of the obtained structures with Ni nanoclusters at strong magnetic fields up to 8 T and at low temperatures in the range of 1.8 K - 150 K have shown a possibility of control of these nanostructures properties by the effect of magnetic fields.

The obtained results confirm a feasibility of the use of the Si/SiO_2/Ni nanoelectronic systems with swift heavy ion tracks in low-temperature spintronic sensor devices.

TT 35.11 Wed 14:00 P1A

Conductance oscillations of polyacetylene at finite temperature — •Davoud Pouladsaz[1,2], Thomas Gessner[2,3], Michael Schreiber[1], and Reinhard Streiter[2,3] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Zentrum für Mikrotechnologien (ZfM), Technische Universität Chemnitz — [3]Fraunhofer-Einrichtung für Elektronische Nanosysteme (ENAS), Chemnitz

The length-dependence of the differential conductance oscillations in *trans*-polyacetylenes, suspended between gold contacts, is investigated by employing the non-equilibrium Green's function technique within the density-functional-based tight-binding method (gDFTB) to study the electronic transport properties of the proposed system under the applied bias voltages at finite temperature. The results reveal the efficient influence of the sulfur atoms, as the strong bonding clips to gold atoms, in the quantum transport.

TT 35.12 Wed 14:00 P1A

Charge transport properties of highly conducting tetrathiafulvalene (TTF) based nano-wires — •Marius Bürkle[1], Fabian Pauly[1], Janne Viljas[1,2], Juan Carlos Cuevas[3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik and

DFG-Center for Functional Nanostructures — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany Condensada, Universidad Autònoma de Madrid, 28049 Madrid — [3]Departamento de Física Teórica de la Materia

In a recent experiment [1], an unexpectedly high conductance was observed for tetrathiafulvalene based nanowires, when contacted by gold electrodes. Using density functional calculations [2], we demonstrate that this is due to the highest occupied molecular orbital, which aligns such that it is located only slightly below the Fermi energy of gold. We study the robustness of our findings by an analysis of different types of tetrathiafulvalene based nanowires and contact geometries.

[1] F. Giacalon et. al., Chem. Commun., 2007, 4854 - 4856, DOI: 10.1039/b710739k

[2] F. Pauly et. al., arXiv:0806.4173 and New J. Phys. (in press)

TT 35.13 Wed 14:00 P1A

Fermi-edge singularities: Bulk vs. mesoscopic systems — •Martina Hentschel and Georg Röder — MPI für Physik komplexer Systeme, Dresden

Fermi-edge singularities are among the simplest many-body effects and have been a key interest in condensed matter physics for many years. They have been extensively studied, and are understood, for bulk systems such as metals. In contrast, our focus here is on small (mesoscopic) systems like quantum dots and graphene. We mainly address the Fermi-edge singularities in the photoabsorption cross section that are known as the x-ray edge problem. They comprise the phenomena of Anderson orthogonality catastrophe and Mahan's exciton (Mahan-Nozieres-DeDominicis response) and result from the system's many-body response to the sudden, localized perturbation given by the core hole that is left behind when the x-ray excites an electron. We show that the mesoscopic regime holds surprises in form of many-body responses that strongly deviate from the macroscopic (bulk, or metallic) case. The differences originate in the finite system size, the intrinsic mesoscopic fluctuations, and most importantly, the modifications of the electron dynamics in confined ballistic systems that are typically studied in the field of quantum chaos. A particularly interesting behavior is seen in graphene where the vanishing density of states at the Dirac point significantly modifies the system's many-body response.

TT 35.14 Wed 14:00 P1A

Density functional theory on a lattice: Transport through a small interacting region — Michael Dzierzawa, Ulrich Eckern, •Stefan Schenk, and Peter Schwab — Universität Augsburg

Density functional theory is the method of choice for calculations of the electronic structure of complex materials. In recent years the method has been applied to study charge transport through systems of molecular size. However it is clearly necessary to determine the limits of the approach to assess the obtained results. To this end we suggest to study simple lattice systems, where the comparison with exact calculations is possible.

Hence we investigate a one-dimensional system with spinless fermions consisting of a small interacting region between two noninteracting leads. In particular we study the linear conductance through the interacting region. We find that for this specific system a naive calculation of the conductance, i. e. by ignoring the exchange-correlation kernel, is often sufficient. The local density approximation performs rather badly even for weak interaction, whereas the so-called exact-exchange approximation gives sensible results. We also propose an exact diagonalization procedure to obtain a non-local exchange-correlation potential for strongly interacting systems.

TT 35.15 Wed 14:00 P1A

Geometry-Dependence of 0.7 Anomaly in Quantum Point Contacts: A Study Using the Functional Renormalization Group — •Jan Heyder, Florian Bauer, and Jan von Delft — Arnold Sommerfeld Center for Physics, Ludwig-Maximilians-Universitaet, Muenchen

We study the geometry-dependence of the 0.7 anomaly of the conductance through a quantum point contact at zero temperature as a function of magnetic field, using the functional renormalization group (fRG). We model a 1-D quantum wire using a tight-binding chain with short-ranged Coulomb interactions and a prescribed onsite potential to mimick the potential barrier caused by the 2-D constriction. We study the influence of various shapes of this potential barrier on the magnetic-field dependence of the conductance, finding that it indeed does show a significant geometry-dependence.

TT 35.16 Wed 14:00 P1A

Using wave packet propagation to calculate conductivities — •Christoph Kreisbeck[1], Viktor Krückl[1], and Tobias Kramer[1,2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

The solution of the time dependent Schrödinger equation contains a lot of information about the stationary properties of the system under consideration. To reveal these information we consider the time evolution of a single wave packet and perform the Fourier transform of the autocorrelation function leading to the local density of states (LDOS), which is a key ingredient for the calculation of currents through semiconductor devices. Another way to calculate transport properties is to use flux lines - kind of charge sensors - detecting the energy dependent flux. Using these lines we obtain transmission propabilities, which are closely connected to the conductance, for a whole range of energies from a single wave packet run. In this contribution we illustrate the described technique for a multi-terminal device.

TT 35.17 Wed 14:00 P1A

Multiple electron transfer and transport through a DNA dimer — •Sabine Tornow[1], Gertrud Zwicknagl[1], Ralf Bulla[2], and Frithjof Anders[3] — [1]Inst. math. Physik, TU Braunschweig — [2]Inst. th. Physik, U Köln — [3]Inst. th. Physik, U Dortmund

We investigate multiple electron transfer in a donor-bridge-acceptor system where the molecular bridge comprises a DNA dimer (AT-AT or GC-GC) strongly coupled to a bosonic bath. The time dependent population probabilities and transfer characteristics of multiple electrons is calculated with the time-dependent renormalization group method at low temperatures and kinetic equations at large temperatures. The related transport properties for a system where donor and acceptor are replaced by left and right leads is discussed in different temperature and coupling regimes.

TT 35.18 Wed 14:00 P1A

Laser excitation of atomic point contacts on silicon membranes — •Reimar Waitz[1], Olivier Schecker[1,2], and Elke Scheer[1] — [1]University of Konstanz, D-78457 Konstanz, Germany — [2]IMEP-LAHC, MINATEC-INPG, F-38016 Grenoble, France

Light-induced conductance changes in metallic atomic-sized contacts in the tunneling and in the contact regime are studied. For this purpose, a new type of mechanically controlled break-junction (MCBJ) has been used [1].

MCBJs are made of a metallic wire with a suspended constriction. This constriction, forming a 100 nm wide bridge, can be elongated until having - just before breaking - a diameter of one atom. The elongation is achieved by stretching the substrate, consisting of a 340 nm thin crystalline silicon membrane, in contrast to MCBJs on bulk substrates, which use the bending of the substrate.

Compared to MCBJs on bulk substrates, this new type is advantageous for measuring the conductance of atomic point contacts under laser irradiation. Both the very low absorption and the low reflectivity of the membranes for visible light, make it possible to separate effects caused by the metal from effects caused by the substrate.

On our Poster we present results on light-induced reversible conductance changes of gold contacts. The dependence on intensity, wavelength and polarisation of the incident light has been investigated.

[1] R. Waitz, O. Schecker, and E. Scheer, Rev. Sci. Instrum. 79, 093901 (2008)

TT 35.19 Wed 14:00 P1A

Magneto-resistance of atomic-sized contacts of magnetic metals — •Stefan Egle[1], Hans-Fridtjof Pernau[1], Cécile Bacca[1], Magdalena Hüfner[2], and Elke Scheer[1] — [1]University of Konstanz, Germany — [2]ETH Zürich, Switzerland

We report electronic transport measurements carried out on atomic-size contacts made of ferromagnetic metals or noble metals with ferromagnetic electrodes. The magneto-resistance (MR) curves show very rich behavior with strong magneto-resistance ratios (MRR) up to 1,000 %. We study the possible influence due to the micro-magnetic order of the domains in the vicinity of the contact, giant MR, tunnel MR, ballistic MR and magneto-striction by analyzing MR curves in different orientations of the applied magnetic field with respect to the film plane and current direction. In order to separate the influence of the large electrodes from the influence of the contacts themselves, we used different sample geometries. We used cobalt samples within a symmet-

ric and an asymmetric layout as well as combinations of nonmagnetic electrodes with magnetic bridges and vice versa. In all geometries the MRR is of comparable size and the MR traces show a rich behavior. The main conclusion which we draw from our results is that the micromagnetism of the electrodes as well as the precise atomic arrangement of the contact account for the large MR values.

TT 35.20 Wed 14:00 P1A

Formation of low conductive constrictions in nanostructures by electromigration — •Birgit Kiessig[1,2], Wanyin Cui[1,2], Kai Grube[1], Regina Hoffmann[2], and Roland Schäfer[1] — [1]Forschungszentrum Karlsruhe, IFP, Postfach 3640, 76021 Karlsruhe — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe

Exposure of metallic nanostructures to high currents leads to deterioration by melting or electromigration. Ref. 1 describes a method how to use the latter in a controlled way to form constrictions with conductances down to the conductance quantum $G_0 = 2e^2/h$. Below several G_0 conductance prefers to stabilize at material dependent values well known from conductance quantization experiments.
We apply the method described in Ref. 1 to different materials and extend it to nanostructures containing rings. The rings are connected to two leads at opposite sides and the electromigration-controlled constriction formation acts in a balanced way in both ring arms.
[1] R. Hoffmann, D. Weissenberger, J. Hawecker, and D. Stöffler, Appl. Phys. Lett. **93**, 0431118 (2008).

TT 35.21 Wed 14:00 P1A

Electron induced heating and molecular phonon cooling in single C_{60} junctions — Gunnar Schulze, Katharina J. Franke, and •Jose Ignacio Pascual — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The functionality of single molecules as electronic devices relies on its stability against large current densities. Electronic current generates heat in the molecular junction due to coupling of electrons with molecular vibrations. Using a scanning tunnelling microscope operated at 5 K, we thermally decompose single C_{60} molecules on a metal surface by passing current through them, and investigate the response of the degrading current (and power) to changes in electron energy. The power for decomposition results from the balance between heating and cooling efficiencies [1]. We find that heating varies with electron energy and reflects the molecular resonance structure participating in the transport. Through inelastic electron spectroscopy measurements, we identify those vibrations which are mostly excited when tunneling through the LUMO state, confirming that symmetry selection rules apply here. Cooling, on the other hand, is a non-resonant process, dominated by the decay of molecular vibrations into electron-hole pair excitations. We find that the partial occupation of molecular states enhance the molecular cooling due to an enhancement of density of states at the molecule-metal interface [2].
[1] G. Schulze, et al., Phys. Rev. Lett. 100, 136801 (2008)
[2] G. Schulze, et al., N. J. Phys. 10, 065005 (2008)

TT 35.22 Wed 14:00 P1A

Quantum Transport Through Gold Wires: Ab Initio Studies Using Plane Waves and Supercells — •Björn Oetzel[1,2], Martin Preuss[1,2], Frank Ortmann[1,2], Karsten Hannewald[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörperphysik 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 scheme for an *ab initio* implementation of the Landauer-Büttiker theory for quantum transport by means of supercells and plane-wave basis sets. The suggested method works entirely in **k** space which allows to circumvent the complicated projections onto tight-binding Hamiltonians necessary in the more common real-space approaches to quantum transport. Here we apply this method to DFT calculations of transmission functions for quasi-1D Au nanowires of various lengths and widths. The results are discussed with respect to the possible replacement of semi-infinite electrodes by short Au nanowires in future calculations of metal-molecule-metal junctions.

TT 35.23 Wed 14:00 P1A

Molecular Switches in Break Junction Metal-Molecule-Metal Contacts — •Bernd Briechle[1], Thomas Kirchner[1], Uta Eberlein[1], Simon Verleger[1], Marcel Mayor[2], Alfred Blaszczyk[2], Thomas Huhn[3], Jannic Wolf[3], Dima Sysoiev[3], Elke Scheer[1], and Artur Erbe[1] — [1]FB Physik, Universität Konstanz, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe — [3]FB Chemie, Universität Konstanz, Germany

Metal-molecule-metal contacts are established using the Mechanically Controllable Break Junction (MCBJ) technique at room temperature in a toluene solution. We investigate short oligo phenylene ethynylenes (OPE) with various nitrogen-based end groups as well as different thiol-terminated molecular switches. Analysis is based on statistics of conductance traces recorded during opening and closing the junction, and on current-voltage characteristics taken at a constant electrode distance. We show that the latter can be described by a simple transport model involving a single broadened molecular orbital. The molecular switches exhibit a pronounced hysteretic switching behavior when the bias voltage exceeds a certain value ($\approx 0.4V$).

TT 35.24 Wed 14:00 P1A

Optical Spectroscopy on Tuneable Nano Gaps — •Daniel Gerster[1], Joachim Reichert[1], Stefan Klein[2], Harald Fuchs[2], and Johannes V. Barth[1] — [1]Physik Department, TU München, Germany — [2]Physikalisches Institut, Universität Münster, Germany

Novel techniques to establish tuneable nano gaps designed to act as electrodes for single molecule charge transport measurements are required both for fundamental research and device oriented applications. Hereby, the implementation of additional control parameters to influence the properties of the functional molecule within the gap is of special interest. We present a method to fabricate tuneable nanoscale electrodes where an apertureless scanning nearfield tip (SNOM-tip) is employed to serve as a counter electrode in a molecular junction and simultaneously as a light source. The apertureless SNOM-tip acts as plasmonic waveguide to focus surface plasmon polaritons to the apex of the tip, where a strongly enhanced evanescent field is confined to only a few nanometers. First spectroscopic measurements of light absorption at the empty gap reveal distinct standing wave patterns of optical waves between the electrodes, indicating high field intensities in the gap region.

TT 35.25 Wed 14:00 P1A

Phase-dynamics in superconducting atomic and molecular point contacts — •Benjamin Obert — Institut für theoretische Physik, Universität Ulm, Germany

In the conventional theory for current biased superconducting atomic point contacts the dynamics of the phase difference across the contact is described on single adiabatic surfaces for the Andreev bound states. Here we consider

(i) non-adiabatic transitions between these surfaces relevant for highly transmitting channels and

(ii) energy dependent transmission channels which may occur in molecular junctions.

TT 35.26 Wed 14:00 P1A

Charge transport through an interference SET — •Georg Begemann, Dana Darau, Andrea Donarini, and Milena Grifoni — University of Regensburg, Germany

We study the charge transport through a benzene interference single electron transistor. The interplay between Coulomb interaction and orbital symmetry produces specific transport characteristics that can be considered as the fingerprints of the contacted molecule. Specifically we predict selective conductance suppression and the appearance of negative differential conductance and current blocking when changing the contacts from para to meta configuration[1,2]. All effects originate from destructive interference in transport involving states with orbital degeneracy.

The studied transport phenomena are also robust under the perturbation exerted by the anchor groups binding the contact atoms to the leads or by an external electrostatic field.

[1] G.Begemann, D.Darau, A.Donarini, and M.Grifoni, Phys. Rev. B 77, 201406(R) (2008).
[2] D.Darau, G.Begemann, A.Donarini, M.Grifoni, arXiv:0810.2461

TT 35.27 Wed 14:00 P1A

Electron Dynamics in Molecular Wires Studied by a Density Matrix Approach — •Lisa Mövius and Ulrich Kleinekathöfer — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Recent investigations in the field of molecular electronics [1-3] are targeted on controlling the current through single molecules by laser fields.

In the present work, as in [1], the metal-molecule-metal junction is described using a quantum master equation within second-order perturbation theory, since the wire-lead coupling is assumed to be weak. The dynamics of the system can be influenced by applying a laser field, leading to novel effects like coherent destruction of tunneling to effectively suppress the current through the molecular wire. Using a projection operator approach [3] an efficient reduction of dimensionality can be achieved to render effective calculations of longer wires possible.

[1] S. Welack, M. Schreiber, and U. Kleinekathöfer, J. Chem. Phys. 124, 044712 (2006).

[2] I. Franco, M. Shapiro, and P. Brumer, Phys. Rev. Lett. 99, 126802 (2007).

[3] U. Harbola, M. Esposito, and S. Mukamel. Phys. Rev. B 74, 235309 (2006).

TT 35.28 Wed 14:00 P1A

Noise Measurements of Cryogenic Amplifiers for Qubit Experiments — •Christian Schwemmer[1], Tobias Wirth[1], Alexander Lukashenko[1], Jürgen Lisenfeld[1], Michael Mück[2], and Alexey Ustinov[1] — [1]Physikalisches Institut, Universität Karlsruhe (TH), Germany — [2]Institut für Angewandte Physik der Justus-Liebig Universität Giessen, Germany

Ultra-low noise cryogenic amplifiers are a prerequisite for a variety of readout schemes of qubits based on Josephson junctions. Evaluation of the noise temperature of cryogenic amplifiers is an essential task for achieving high sensitivity and lowest back action. We developed a cryogenic noise source based on a 50 Ohm load located in vacuum with variable temperature between 8 K and 60 K. By measuring the output power of a cryogenic low noise HEMT-amplifier at different temperatures of the load using a standard spectrum analyzer we determine the amplification and the noise temperature of the amplifier. The advantage of our method compared to the conventional noise diode switching technique is that in our approach the noise source is heated up continuously providing many data points and thus offering better resolution. In our ongoing measurements we are using this approach to measure the noise temperature and amplification of microstrip SQUID amplifiers operated at 4.2 K.

TT 35.29 Wed 14:00 P1A

Microwave Spectroscopy on Superconducting Flux Qubits — •Thomas Niemczyk[1], Lars Eggenstein[1,2], Frank Deppe[1,2], Elisabeth Hoffmann[1,2], Edwin Menzel[1], Matteo Mariantoni[1,2], Achim Marx[1], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department E23, Technische Universität München, Garching, Germany

There is promising progress in the realization of solid-state based quantum information processing (QIP) systems. Up to now, there is a number of different realizations of qubits, the building blocks for future quantum computers. Among these, superconducting (SC) qubits are very promising candidates. Furthermore, coupling SC qubits to high quality factor SC cavities opens the fascinating field of circuit quantum electrodynamics (cQED) where matter-light interaction can be studied on a fundamental level. We have fabricated SC flux-qubits which consist of an Al loop interrupted by 3 nm-sized $Al/AlO_x/Al$ Josephson junctions. For readout, the qubit is inductively coupled to a dc-SQUID which detects the small flux signal ($10^{-3}\Phi_0$) induced by the circulating currents in the qubit loop. The energy gap Δ between the ground state and the first excited state of the flux-qubits has been determined by μ-wave spectroscopy at 30 mK. We reproducibly could fabricate flux qubits with Δ values ranging between 3 and 5 GHz.
This work is supported by the DFG through SFB 631 and the Excellence Cluster 'Nanosystems Initiative Munich (NIM)'

TT 35.30 Wed 14:00 P1A

The dissipative quantum Duffing oscillator — •Carmen Frammelsberger and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg

The knowledge about relaxation and dephasing properties of solid state qubits is essential for quantum computation. In this contribution we consider a qubit interacting with an intermediate driven quantum Duffing oscillator which is itself coupled to an Ohmic bath. This resembles the case of a flux qubit read out by a DC-SQUID acting as a nonlinear oscillator. We consider the oscillator to be part of the environment seen by the qubit. We generalize the concept of an effective spectral density introduced by [1] to the case, that the intermediate oscillator is nonlinear. This is done by mapping the whole system onto a spin-boson problem with an effective spectral density using linear response theory. Within this approach we relate the effective spectral density with the imaginary part of the susceptibility of the quantum Duffing oscillator.

We derive the nonlinear effective spectral density in the rotating wave approximation (RWA) and observe both Ohmic low frequency behaviour and for high damping the response of a linear oscillator with shifted eigenfrequency. Within the RWA the possible parameters are restricted to finite nonlinearity and weak driving amplitudes. We elaborate a time-dependent perturbation theory to consider both the exact Floquet states of the linear oscillator as well as the result for the undriven quantum Duffing oscillator.

[1] A. Garg et al., J. Chem. Phys. 83, 9 (1985).

TT 35.31 Wed 14:00 P1A

Josephson Phase Qubits with Submicron Nb Junctions — Ralf Dolata[1], •Jürgen Lisenfeld[2], Brigitte Mackrodt[1], Alexander Lukashenko[2], Alexander Zorin[1], and Alexey Ustinov[2] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), Karlsruhe, Germany

The microscopic properties of materials including insulating dielectrics and tunnel barriers play a significant role in engineering of Josephson qubits. The use of ultra-small Josephson tunnel junctions should reduce the probability that the macroscopic variable (Josephson phase) couples to parasitic microscopic quantum systems located inside the junction barrier of smaller volume and, therefore, improve the coherence of the qubit. We have fabricated phase qubits applying multilayer Nb technology with lateral dimensions of the junctions of 0.5 μm by 0.5 μm and external on-chip capacitors with either SiO_2 or Si_3N_4 dielectric material. Preliminary measurements of the Rabi oscillations show for the latter samples an increase of the qubit coherence by about a factor of two, whereas generally short coherence times of order 10 ns indicate further decoherence sources being active.

TT 35.32 Wed 14:00 P1A

Engineering Quantum States of Light in Coplanar Cavities — •Michael Wulf, Ralf Dolata, and Alexander B. Zorin — Physikalisch Technische Bundesanstalt

Recently it has become possible to detect single photons in the microwave-regime using tools developed by the Quantum Information community. We propose here an experiment to directly study the coherence times of confined photons. For this purpose we use Single-Cooper-Pair boxes as photon detectors for two coupled superconducting coplanar cavities, and show how a photon-coherence time much longer than the rather limited coherence-times of charge boxes operating in the qubit regime can be observed.

TT 35.33 Wed 14:00 P1A

Full Counting Statistics of Interacting Quantum Dots with Ferromagnetic Leads — •Stephan Lindebaum, Daniel Urban, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

We investigate the full counting statistics of electronic transport through a single-level quantum dot weakly coupled to two leads. In the systems under consideration either one or both leads are ferromagnetic. For both situations we study the influence of the two spin channels on the transport properties to identify several underlying transport processes.

Starting from a generalized master equation we use a diagrammatic real-time theory to calculate the cumulant generating functions to first order in the tunnel coupling strength [1]. In the case of two ferromagnetic leads and strong Coulomb interaction an exchange field between dot and leads exists, which leads to a precession of the accumulated dot spin [2].

The interaction of dot electrons crucially affects the cumulants. If both leads are ferromagnetic the cumulants show a non-trivial dependence on the angle between the magnetization directions of the leads. They become strongly super Poissonian and may even diverge for high polarizations. Furthermore, they exhibit sign changes in dependence of the polarization angle. With only a single ferromagnetic lead it turns out that the majority electrons govern the statistics of the system.

[1] A. Braggio *et al.*, Phys Rev. Lett. **96**, 026805 (2006).

[2] M. Braun *et al.*, Phys. Rev. B **70**, 195345 (2004).

TT 36: Focussed Session: Superconductivity and Magnetism in Ferropnictides and Related Materials

Time: Thursday 9:30–13:00 Location: HSZ 03

Topical Talk TT 36.1 Thu 9:30 HSZ 03

Superconductivity and Magnetism in $LaO_{1-x}F_xFeAs$ — •Bernd Buechner[1], Hans-Joachim Grafe[1], Christian Hess[1], Ruediger Klingeler[1], Guenter Behr[1], Agnieszka Kondrat[1], Norman Leps[1], Guillaume Lang[1], Hans-Henning Klauss[2], and Hubertus Luetkens[3] — [1]IFW Dresden — [2]TU Dresden — [3]PSI Villigen

Measuring NMR as well as muSR, transport and thermodynamic properties we have determined the phase diagram of $LaO_{1-x}F_xFeAs$ superconductors. In my talk, I will show experimental studies of the magnetic ordering, properties of the superconducting state and the normal state properties in the superconducting regions of the phase diagram. While the temperature dependence of the London penetration as determined from *SR points to an isotropic s wave state, our early NMR data suggest singlet pairing and nodes of the order parameter. In the paramagnetic normal state, NMR on all three nuclei shows that the local electronic susceptibility rises with increasing temperature. This had led to suggest the presence of a pseudogap, which I will discuss in detail. The scaling of all NMR shifts with respect to the macroscopic susceptibility indicates that there is no apparent multiband effect through preferential hyperfine couplings. Relaxation measurements indicate a similar temperature-dependence for $(T_1T)^{-1}$, and suggest that the dynamical susceptibility changes uniformly in q space with varying temperature. The transport properties show some striking similarities to the findings in cuprates and, finally, susceptibility as well as NMR studies point to the antiferromagnetic fluctuations.

Invited Talk TT 36.2 Thu 10:00 HSZ 03

Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors — •Andrey Chubukov — Dept . of Physics, University of Wisconsin, 1150 University ave., Madison WI 53706

I discuss the interplay between antiferromagnetism and superconductivity in novel Fe-based superconductors within the itinerant model of small electron and hole pockets. I argue that the effective interactions in both magnetic and pairing channels logarithmically flow towards the same values at low energies, i.e., antiferromagnetism and superconductivity are competing orders. The magnetic instability comes first for equal sizes of hole and electron pockets, but looses to superconductivity upon doping. I discuss the transition between the two ordered states and argue that it must be first order. The superconducting gap has no nodes, but changes sign between the two Fermi surfaces (extended s-wave symmetry). I discuss properties of such superconductors and the effects of non-magnetic impurities. I argue that the temperature dependencies of the spin susceptibility, the NMR relaxation rate and the superfluid density are exponential for the clean case, but become power-laws in the dirty limit. I discuss potential smoking-gun experiments to probe extended s-wave symmetry.

Topical Talk TT 36.3 Thu 10:30 HSZ 03

Structural and magnetic transitions of underdoped $(Ba_{1-x}K_x)Fe_2As_2$ — •Dirk Johrendt[1], Marianne Rotter[1], Marcus Tegel[1], Inga Schellenberg[2], Falko M. Schappacher[2], and Rainer Poettgen[2] — [1]LMU München, Department Chemie, Butenandtstr. 5-13 (Haus D), 81377 München, Germany — [2]WWU Münster, Institut für Anorganische und Analytische Chemie, Corrensstr. 30, 48149 Münster. Germany

$BaFe_2As_2$ is the parent compound of the 122-type family of iron arsenide superconductors. Superconductivity up to $T_c = 38$ K is induced by doping the barium site by potassium or the iron site by cobalt or even without chemical doping under high pressure. The structural and magnetic phase transition of the parent compound is completely suppressed at the optimal doping level in $(Ba_{1-x}K_x)Fe_2As_2$ around x = 0.4. But In the underdoped regime, superconductivity co-exists with the orthorhombically distorted lattice and it is debatable at the moment, to what extent the superconducting state may also co-exist with the antiferromagnetic order.

The talk will first briefly review the properties of $BaFe_2As_2$ and the doped Ba122-superconductors. Then recent results of studies in the underdoped regime will be reported. $(Ba_{1-x}K_x)Fe_2As_2$ ($x < 0.4$) has been studied in detail by low-temperature x-ray powder diffraction and ^{57}Fe-Mössbauer spectroscopy. Relationships between the evolution of magnetic ordering and the onset of the orthorhombic lattice distortion are discussed in connection with possible inhomogeneities of the potassium distribution in underdoped superconducting Ba122-materials.

15 min. break

Topical Talk TT 36.4 Thu 11:15 HSZ 03

Relation of structure, magnetism, doping and pressure in AFe_2As_2 — •Helge Rosner, Deepa Kasinathan, Alim Ormeci, Katrin Koch, Miriam Schmitt, Walter Schnelle, Corneliu Miclea, Michael Nicklas, Manoj Kumar, Christoph Geibel, Ulrich Schwarz, and Andreas Leithe-Jasper — MPI CPfS Dresden, Nöthnitzer Str. 40, 01187 Dresden

We present an overview of our recent experimental and theoretical studies on the AFe_2As_2 (A = Sr, Eu, K) compounds. Starting with thermodynamic measurements and band structure results for the undoped $SrFe_2As_2$ under ambient conditions, we report the influence of hydrostatic pressure and substitution on the A site as well as the Fe site on the magneto-structural and superconducting transitions: (i) $SrFe_2As_2$ orders antiferromagnetically at 205 K, intrinsically tied to a tetragonal-orthorhombic distortion. (ii) The magnetism is weakened upon application of pressure as indicated by resistivity, X-ray data and calculations. (iii) Similar to substitution on the A site, substitutions on the Fe-site quenches the magnetic transition and induces bulk superconductivity with T_c up to 20 K. (iv) For underdoped $SrFe_{2-x}Co_xAs_2$, superconductivity with T_c up to 27 K is observed for pressures of 2.6 GPa. The first observation of bulk superconductivity induced by electron doping in AFe_2As_2 compounds – despite strong disorder in the Fe-As layer – favors an *itinerant* electronic theory in contrast to the strongly correlated cuprates. Although discrepancies between experiment and calculated electronic structure remain, DFT band structure calculations provide a consistent overall picture of AFe_2As_2 compound.

TT 36.5 Thu 11:45 HSZ 03

DFT studies of Iron-based Superconductors — •Lilia Boeri[1], Oleg V. Dolgov[1], Alexander A. Golubov[2], and Ole Krogh Andersen[1] — [1]MPI-FKF, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente,7500 AE Enschede, The Netherlands

The discovery of superconductivity in iron pnicticides has generated considerable interest. So far, however, not only the pairing mechanism, but even the basic electronic structure of these materials is not well understood.

We use Density Functional Theory to understand the electronic and vibrational properties of LaOFeAs, which can be considered a prototype for iron pnictides.

First, we calculate the phonon dispersions and electron-phonon coupling using linear response and show that standard Migdal-Eliashberg theory cannot explain the experimental T_c. Then we derive ab-initio an accurate tight-binding Hamiltonian, using downfolding + N-ization (NMTO), which allows us to elucidate the origin of the complicated band structure of iron pnicticides. As a first application of our model, we study itinerant magnetism.

Topical Talk TT 36.6 Thu 12:00 HSZ 03

Quasiparticle renormalization effects in the normal-state optical properties of iron pnictides — •Alexander Boris[1], N.N. Kovaleva[1,2], P. Popovich[1], Y. Matiks[1], C.T. Lin[1], R.K. Kremer[1], L. Boeri[1], O.V. Dolgov[1], I.I. Mazin[3], and B. Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — [2]Department of Physics, Loughborough University, Loughborough, United Kingdom — [3]CCMS, Naval Research Laboratory, Washington, D.C. 20375, USA

We report a comprehensive spectroscopic ellipsometry study on iron pnictides, $LaFeAsO_{1-x}F_x$ and $Sr_{1-x}K_xFe_2As_2$, over a wide range of temperatures (10 - 350 K) and photon energies extending from the far infrared (IR) into the deep ultraviolet (UV), 0.01 - 6.5 eV. The optical

conductivity spectra are dominated by a sequence of interband transitions which agree very well with those predicted by LDA calculations. The free charge carrier response is, however, heavily damped. This implies that the electronic states near the Fermi surface are strongly renormalized. From our optical measurements we address

i) electron-electron correlation effects [1],

ii) electron-phonon coupling, and

iii) dynamic charge and spin ordering [2]

as possible renormalization factors.

[1] A.V.Boris et al., preprint at arXiv:0806.1732;

[2] I.I. Mazin and M.D. Johannes, Nature Physics (in press), preprint at arXiv:0807.3737.

Topical Talk TT 36.7 Thu 12:30 HSZ 03

C-axis transport of pnictide single crystals — •Paul Müller[1], Yuri Koval[1], Günter Behr[2], and Bernd Büchner[2] — [1]Department of Physics, Universität Erlangen-Nürnberg — [2]IFW Dresden

Mesa structures were fabricated on the (ab) plane of small $LaO_{0.9}F_{0.1}FeAs$ single crystals. Resistance vs. temperature measurements showed metallic behavior with a residual resistance ratio higher than 10. Both magnetic susceptibility and c-axis transport measurements showed the same value for the critical temperature, i.e. ∼20K. Current-voltage characteristics are typical for overdamped Josephson junctions with a critical current density of $\sim 10^5$ A/cm^2. Moreover, the critical current vs. temperature dependence follows the Ambegaokar-Baratoff relation for the maximum dc Josephson current. One possible explanation could be that we have observed an intrinsic Josephson effect in <c>-direction. This is supported by recent measurements of radiation emission between 11 and 12 GHz. Finally, we discuss current injection effects on Josephson critical current and T_c.

TT 37: Transport: Nanoelectronics II - Spintronics and Magnetotransport

Time: Thursday 9:30–13:00 Location: HSZ 105

TT 37.1 Thu 9:30 HSZ 105

Anisotropic magnetoresistance in ferromagnetic atomic-sized metal contacts — •Michael Häfner[1,2], Janne Viljas[1,3], and Juan Carlos Cuevas[2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid — [3]FZ Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe

Recent experiments in ferromagnetic atomic-sized contacts have shown that the anisotropic magnetoresistance (AMR) is greatly enhanced and has an asymmetric angular dependence as compared with that of bulk samples. The origin of these effects is still under debate. In this work [1] we present a theoretical analysis of the AMR in atomic contacts of the 3d ferromagnetic materials. Our results strongly suggest that the anomalous AMR stems from the reduced symmetry of the atomic contact geometries. We also present calculations supporting the idea that the pronounced voltage- and temperature dependence in some experiments can be attributed to impurities near the constrictions.

[1] M. Häfner et al., arXiv:0811.4491.

TT 37.2 Thu 9:45 HSZ 105

Spin-Polarized Conductance in a Single Magnetic Atom? — •Cormac Toher and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany.

Single atom conductance measurements can be performed by forming nanocontacts using a scanning tunnelling microscope (STM). In the case of fully spin-polarized transport, a spin resolved conductance quantum of $0.5G_0 = \frac{e^2}{h}$ is expected, in contrast to the value of $G_0 = \frac{2e^2}{h}$ expected in normal atomic nanocontacts with one full spin degenerate open channel. A spin-resolved conductance has been observed in the experiments carried out by Néel *et. al.* [1] on cobalt atoms. When the cobalt atom is placed on a copper surface and contacted by a tungsten tip, a conductance of G_0 is observed, whereas when it is placed on a cobalt island and contacted by a nickel tip, a conductance of $0.5G_0$ is observed. Here we present the results of calculations to explore the mechanism underlying this effect, investigating whether or not spin-polarized transport is actually present. These calculations were performed using the ab initio transport method SMEAGOL [2], which combines the non-equilibrium Green function formalism with the DFT implementation SIESTA [3].

[1] N. Néel, J. Kröger, and R. Berndt, Phys. Rev. Lett. (submitted).

[2] A. R. Rocha *et. al.*, Phys. Rev. B **73**, 085414 (2006).

[3] J. M. Soler *et. al.*, J. Phys. Cond. Matter **14**, 2745 (2002).

TT 37.3 Thu 10:00 HSZ 105

Transport through an interacting quantum dot tunnel coupled to a ferromagnet with time-dependent magnetisation — •Nina Winkler, Michele Governale, and Jürgen König — Theoretische Physik · Universität Duisburg-Essen

We study adiabatic pumping through a system consisting of a quantum dot coupled to a normal and a ferromagnetic lead. 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. Here, we consider a different pumping scheme. By changing slowly in time the lead properties, e.g. the magnetisation, we can generate a pumped DC current. To this aim, we generalise a diagrammatic real-time approach for adiabatic pumping through quantum dots with ferromagnetic leads [1, 2] to account for a time-dependent magnetisation.

We consider two different pumping situations: First, we choose the amplitude of the magnetisation of the ferromagnetic lead and the level position of the dot or the tunnel coupling to the normal lead as pumping parameters. Second, we pump by periodically changing the direction of the magnetisation. We investigate the adiabatic charge and spin transport through the system by performing a systematic perturbative expansion in powers of the tunnel-coupling strengths but treating the on-site Coulomb interaction on the quantum dot exactly.

[1] J. Splettstoesser *et al.*, Phys. Rev. B **74**, 085305 (2006).

[2] J. Splettstoesser *et al.*, Phys. Rev. B **77**, 195320 (2008).

TT 37.4 Thu 10:15 HSZ 105

Spin-Electric Coupling in Molecular Magnets — •Mircea Trif[1], Filippo Troiani[2], Dimitrije Stepanenko[1], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]CNR-INFM National Research Center S3 c/o Dipartimento di Fisica via G. Campi 213/A, 41100, Modena, Italy

We study the triangular antiferromagnet Cu3 in external electric fields, using symmetry group arguments and a Hubbard model approach. We identify a spin-electric coupling caused by an interplay between spin exchange, spin-orbit interaction, and the chirality of the underlying spin texture of the molecular magnet. This coupling allows for the electric control of the spin (qubit) states, e.g., by using an STM tip or a microwave cavity. We propose an experimental test for identifying molecular magnets exhibiting spin-electric effects.

TT 37.5 Thu 10:30 HSZ 105

Magnetic and transport properties of ferromagnet / semiconductor Heterostructures (Ga,Mn)As/GaAs — •S R Dunsiger[1], T Goko[2,3], J P Carlo[2], G Nieuwenhuys[4], T Prokscha[4], E Morenzoni[4], D Chiba[5], T Tanikawa[5], F Matsukura[5], H Ohno[5], R H Heffner[6], and Y J Uemura[2] — [1]Physik Dept E21, TU München, Garching, Germany — [2]Dept of Physics, Columbia University, New York, USA — [3]TRIUMF, Vancouver, Canada — [4]PSI, Villigen, Switzerland — [5]Laboratory for Nanoelectronics and Spintronics, RIEC, Tohoku University, Sendai, Japan — [6]LANL, Los Alamos, USA

Ferromagnet-Semiconductor heterostructures show immense promise for device applications, in particular in the injection of polarised spins into a semiconducting substrate. More fundamentally, the III-V semiconducting materials (Ga,Mn)As exhibit unusual long range indirect exchange interactions between Mn ions, where the Mn atoms simultaneously act as a magnetic species and charge donors. An intriguing link between the magnetic and transport properties is hence implied.

Low-energy μSR, in addition to magnetization and transport measurements on specimens with Mn concentrations between 1.0 and 3.4 % are reported. Ferromagnetism with a sharp onset temperature and

nearly 100 % volume fraction is observed, at odds with debate over the rather inhomogeneous nature of the phase transitions. In addition, the semiconductor-to-metal transition and paramagnetic-to-ferromagnetic transitions occur at different Mn concentrations, while unusually, even a semiconducting film shows static ferromagnetism developing.

TT 37.6 Thu 10:45 HSZ 105

Anomalous Hall effect in granular ferromagnetic metals and effects of weak localization — •Hendrik Meier, Maxim Kharitonov, and Konstantin Efetov — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum

We theoretically investigate the anomalous Hall effect in a system of dense-packed ferromagnetic grains in the metallic regime. Using the formalism recently developed for the conventional Hall effect in granular metals, we calculate the residual anomalous Hall conductivity σ_{xy} and resistivity ρ_{xy} and weak localization corrections to them for both skew-scattering and side-jump mechanisms. We find that, unlike for homogeneously disordered metals, the scaling relation between ρ_{xy} and the longitudinal resistivity ρ_{xx} does not hold. The weak localization corrections, however, are found to be in agreement with those for homogeneous metals.

TT 37.7 Thu 11:00 HSZ 105

Anisotropy of the intrinsic anomalous Hall effect in FePt, FePd and FeNi ordered alloys — •Yuriy Mokrousov[1,2], Eric Roman[1], and Ivo Souza[1] — [1]University of California at Berkeley, USA — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

We calculate from first principles the intrinsic anomalous Hall conductivity (AHC) of the layered $L1_0$ alloys FePt, FePd and FeNi. We find large intrinsic contributions (comparable to those of bulk Fe, Co, and Ni), in apparent disagreement with a recent experimental work (K.M. Seemann *et al.*, arXiv:0811.1258) which attributed the anomalous Hall effect in FePd and FePt entirely to skew-scattering from impurities. We propose that a clear signature of the intrinsic effect in these materials is its strong dependence on the orientation of the magnetization with respect to the uniaxial direction, while skew-scattering is expected to be largely isotropic. The calculated anisotropy has opposite signs for FePt (where the AHC is reduced by almost a factor of two as the magnetization direction is changed from the [001] to the [110] direction) and for FePd and FeNi, where instead it increases, but by a smaller amount. By selectively turning off the spin-orbit interaction on the Fe and X atoms (X=Pt,Pd,Ni), we investigate their individual contributions to the AHC.

15 min. break.

Invited Talk TT 37.8 Thu 11:30 HSZ 105

Quantum dissipative spin ratchets — •Milena Grifoni — University of Regensburg, Regensburg, Germany

Rather than fighting it, so-called quantum Brownian motors take advantage of thermal noise and quantum tunneling to move efficiently microscopic entities, as e.g. electrons, along predetermined directions. Here we focus on a particular class of quantum Brownian motors, i.e., quantum ratchets which, due to broken spatial symmetry, produce movement in one direction from a force that may be acting at random. We shall discuss, in particular, how the ratchet effect can be used to produce pure spin currents, i.e., a finite spin current and the absence of charge transport. To this extent we consider electrons moving in a quasi-one-dimensional asymmetric periodic structure with Rashba spin-orbit interaction, strong dissipation and subject to ac-driving. We show that under a finite coupling strength between the orbital degrees of freedom the electron dynamics at low temperatures exhibits a pure spin ratchet behaviour with in-plane polarization. Moreover, the equilibrium spin currents are not destroyed by the presence of strong dissipation.

TT 37.9 Thu 12:00 HSZ 105

Spin-orbit ratchet mechanism: correlation between dissipation and magnetic field effects — •Sergey Smirnov[1], Dario Bercioux[2], Milena Grifoni[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Physikalisches Institut and Freiburg Institute for Advanced Studies, Universität Freiburg, D-79104 Freiburg, Germany

We investigate ratchet-like behavior of electron spin transport in a periodic quasi-one-dimensional system with Rashba spin-orbit interaction [1]. The orbital longitudinal electron degree of freedom is coupled to orbital degrees of freedom of an external environment which is the source of dissipation. The spin ratchet effect appears when the periodic potential is asymmetric and the electron orbital degrees of freedom are coupled [2]. We additionally apply an in-plane magnetic field which is transverse to the transport direction. The magnetic field does not break the existence conditions of the spin ratchet effect. However, it has an impact on the spin current when the effect is present. Theoretically it is interesting that the magnetic field is correlated only with the friction part of the dissipation and not with the noise part [3]. What is important for applications is that in particular the magnetic field can both reduce and enhance the spin current, produce the spin current reversals and affect the dependence on the electric field driving.

[1] S. Smirnov, et al., EPL 80, 27003 (2007).
[2] S. Smirnov, et al., Phys. Rev. Lett. 100, 230601 (2008).
[3] S. Smirnov, et al., arXiv:0809.1296v1 (accepted in Physical Review B).

TT 37.10 Thu 12:15 HSZ 105

Universal Spin and Charge Fluctuations in Quantum Dots with Rashba Spin-Orbit Interaction — •Juan-Diego Urbina[1], Diego Espitia[1,2], Dominik Bauernfeind[1,3], and Klaus Richter[1] — [1]Universitaet Regensburg — [2]Universidad Pedagogica y Tecnologica de Colombia — [3]Harvard University

We present a novel approach to study spin and charge fluctuations in quantum dots subject to Rashba spin-orbit interaction. From the numerical side we present a spinorial implementation of the Plane Wave Decomposition Method (widely used in non-spin billiards) which allows us to efficiently construct eigenstates and energies of Rashba billiards. The method can be applied to dots with arbitrary shape and with spin-orbit interaction of any strength. With this technique we calculate exact spatial correlations for a dot with irregular shape. The results are then used to test the universal prediction given by a spinorial version of the celebrated Berry's ansatz presented here for the first time.

Our results fully support the claim that the spin-spin, charge-charge and spin-charge correlations in typical quantum dots with Rashba interaction are described by a spinorial Gaussian Random Field universally characterized by its two-point correlation matrix, which is presented in closed analytical form.

TT 37.11 Thu 12:30 HSZ 105

Effective spin-orbit coupling in a benzene interference SET — •Andrea Donarini, Georg Begemann, Dana Darau, and Milena Grifoni — University of Regensburg, Germany

Electronic transport through a benzene single electron transistor is dominated by the interplay between Coulomb interaction and interference between degenerate molecular states. The presence of spin polarized leads induces a novel spin accumulation effect explained in terms of an effective coupling between the orbital and spin degrees of freedom of the molecule.

TT 37.12 Thu 12:45 HSZ 105

Single electron transport in exchange-coupled spin systems — •Gerold Kiesslich, Clive Emary, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin

We study a single electron transistor setup where the localized electron spin is exchange-coupled to another spin. We utilize a quantum master equation approach with the exact dynamics for the spin system in nonequilibrium and the coupling to the electronic reservoirs in Born-Markov-Secular approximation. We discuss the spin-resolved magnetotunneling properties (e..g electron counting statistics) and present a novel spin blockade effect.

TT 38: Correlated Electrons: Low-dimensional Systems - Models 1

Time: Thursday 9:30–13:00 Location: HSZ 301

TT 38.1 Thu 9:30 HSZ 301

Thermally Activated Peierls Dimerization in Ferromagnetic Spin Chains — •Jesko Sirker[1], Alexander Herzog[1], Andrzej M. Oles[1,2], and Peter Horsch[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland

We demonstrate that a Peierls dimerization can occur in ferromagnetic spin chains activated by thermal fluctuations [1]. The dimer order parameter and entanglement measures are studied as functions of the modulation of the magnetic exchange interaction and temperature, using a spin-wave theory and the density-matrix renormalization group. We discuss the case where a periodic modulation is caused by spin-phonon coupling and the case where electronic states effectively induce such a modulation. The importance of the latter for a number of transition metal oxides is highlighted.

[1] Phys. Rev. Lett. 101, 157204 (2008)

TT 38.2 Thu 9:45 HSZ 301

A real-time study of diffusive and ballistic transport in spin-1/2 chains using the adaptive time-dependent DMRG method — •Stephan Langer[1], Fabian Heidrich-Meisner[1], Jochen Gemmer[2], Ian McCulloch[3], and Ulrich Schollwoeck[1] — [1]Institut für Theoretische Physik C, RWTH Aachen University, Germany — [2]Institut für Theoretische Physik, Universität Osnabrück, Germany — [3]The University of Queensland, Brisbane, QLD 4072, Australia

We study spin transport and dynamics in one-dimensional quantum spin-1/2 systems at zero temperature. Using the time-dependent adaptive Density Matrix Renormalization Group (DMRG) method, we follow the time evolution of the magnetization starting from inhomogeneous initial states. Our goal is to distinguish between ballistic and diffusive transport. This is achieved by looking at the long-time behavior of the spatial variance of the magnetization, where, for instance, a quadratic increase in time is indicative of ballistic transport. Applying this to the spin-1/2 XXZ chain, we confirm the established picture of ballistic transport in the critical phase. In the massive phase, strong perturbations are required to drive the dynamics, which show diffusive behavior. Then we turn to two non-integrable models, the two-leg spin-ladder and the frustrated spin chain, for which we find diffusive behavior in all massive phases, but ballistic transport in the gapless phase of the frustrated chain. Since our analysis does not rely on linear-response theory, we can explore the full range of perturbation strength, and, in particular, out-of-equilibrium physics.

TT 38.3 Thu 10:00 HSZ 301

Ground State Properties of the 1D t-J Model with Density Matrix Renormalization Group — •Alexander Moreno[1], Alejandro Muramatsu[1], Salvatore Manmana[2], and Reinhard Noak[3] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institute of Theoretical Physics, Condensed Matter Theory, Lausanne, Switzerland — [3]Philipps Universität Marburg, Germany

We study the ground state properties of the one-dimensional t-J model by using the Density Matrix Renormalization Group (DMRG). On the basis of spin-spin, density-density, and pairing correlation functions we study the possible phases, like Luttinger liquid, superconducting, spin-gap and phase separated regions and clarify the contradictions between different studies[1-3].

[1] M. Ogata, M. U. Luchini, S. Sorella, and F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).

[2] C. S. Hellberg and E. J. Mele, Phys. Rev. B. **48**, 1 (1993).

[3]M. Nakamura, K. Nomura, and Kitazawa, Phys. Rev. Lett. **79**, 3214 (1997).

TT 38.4 Thu 10:15 HSZ 301

Local density of states of 1D Mott insulators and CDW states with a boundary — •Dirk Schuricht[1], Fabian H. L. Essler[1], Akbar Jaefari[2], and Eduardo Fradkin[2] — [1]The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK — [2]Department of Physics, University of Illinois at Urbana-Champaign, USA

We determine the local density of states (LDOS) of one-dimensional incommensurate charge density wave (CDW) states in the presence of a strong impurity potential, which is modeled by a boundary[1]. We find that the CDW gets pinned at the impurity, which results in a singularity in the Fourier transform of the LDOS at momentum $2k_F$. At energies above the spin gap we observe dispersing features associated with the spin and charge degrees of freedom respectively. In the presence of an impurity magnetic field we observe the formation of a bound state localized at the impurity. All of our results carry over to the case of 1D Mott insulators by exchanging the roles of spin and charge degrees of freedom. We discuss the implications of our result for scanning tunneling microscopy experiments on spin-gap systems such as two-leg ladder cuprates.

[1] D. Schuricht, F. H. L. Essler, A. Jeafari, and E. Fradkin, Phys. Rev. Lett. **101**, 086403 (2008).

15 min. break

TT 38.5 Thu 10:45 HSZ 301

Temperature dependent optical conductivity in frustrated chain cuprates near the ferromagnetic-spiral critical point — •Stefan-Ludwig Drechsler[1], Jiri Malek[1,2], Satoshi Nishimoto[1], Helge Rosner[3], Ulrike Nitzsche[1], Roman Kuzian[1,4], and Helmut Eschrig[1] — [1]IFW-Dresden, Germany — [2]Inst. Phys. ASCR, Czech Republic — [3]MPI-CPfS Dresden, Germany — [4]Inst. of Mat. Sci. Problems, Kiev, Ukraine

The optical conductivity $\sigma(\omega)$ [1] and the loss function of EELS are calculated at finite temperature T for CuO_2 chain clusters within a five-band O2pCu3d-Hubbard model using exact diagonalizations and the DMRG-technique. Data at $T = 300$ K for Li_2CuO_2 are reanalyzed within this approach. The relative weights of Zhang-Rice singlet and triplet charge excitations near 2.7 and 4 eV, respectively, depend strongly on T, and a rather dramatic dependence of $\sigma(\omega)$ on the ratio of the 1^{st} to 2^{nd} neighbor exchange integrals is predicted. From our results information about exchange interactions for frustrated edge-shared cuprates can be obtained from T-dependent optical spectra. The obtained exchange integrals compare well with results of LDA+U calculations. Our results are also relevant for magnetically weakly coupled unfrustrated wide-gap insulators in general.

[1] J. Málek *et al.*, PRB **78** 060508(R) (2008).

TT 38.6 Thu 11:00 HSZ 301

Density Matrix Renormalization Group in the Heisenberg picture — •Michael Hartmann[1,2,3], Javier Prior[2,3], Stephen Clark[4], and Martin Plenio[2,3] — [1]Technische Universität München, Physik Department, 85748 Garching, Germany — [2]Institute for Mathematical Sciences, Imperial College London, United Kingdom — [3]QOLS Blackett Laboratory, Imperial College London, United Kingdom — [4]Clarendon Laboratory, University of Oxford, United Kingdom

In some cases the state of a quantum system with a large number of subsystems can be approximated efficiently by the density-matrix renormalization group (DMRG), which makes use of redundancies in the description of the state. Here we show that the achievable efficiency can be much better when performing DMRG in the Heisenberg picture (H-DMRG), as only the observable of interest but not the entire state is considered. In some non-trivial cases, H-DMRG can even be exact for finite bond dimensions.

TT 38.7 Thu 11:15 HSZ 301

Disorder-induced stabilization of pseudogap in the electronic spectral density of the two-dimensional Anderson-Hubbard model — •Prabuddha Chakraborty[1,2], Simone Chiesa[2], Richard Scalettar[2], and Warren Pickett[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]University of California, Davis, CA 95616, USA

In this talk, we present the observation of a pseudogap in the electronic spectral density in the two-dimensional Anderson-Hubbard model on a square lattice. We show the behaviour of the pseudogap when the electronic density, the disorder strength and the Hubbard correlation are varied. In particular, we show that the disorder stabilizes the pseudogap across a wide range of electron densities and correlation strengths. The numerical methods we use are exact diagonalization and Determinant quantum Monte Carlo. We also demonstrate that

our observations are completely consistent with recent experimental results on disordered high temperature Cuprate superconductors.

TT 38.8 Thu 11:30 HSZ 301

Correlation and impurities in carbon nanotubes: A DMRG approach — •Alexander Struck[1], Sebastian A. Reyes[1,2], and Sebastian Eggert[1] — [1]Department of Physics and Reserch Center OPTIMAS, Univ. Kaiserslautern, Kaiserslautern, Germany — [2]Departamento de Física Pontificia Universidad Católica de Chile, Santiago de Chile, Chile

Carbon nanotubes (CNTs) are well suited to study strong electronic correlations in quasi-one-dimensional systems experimentally and theoretically. Of particular interest is the interplay of interactions between the conducting electrons and impurities in the nanotube. Impurities include the boundaries of short tubes as well as structural imperfections such as the Stone-Wales lattice distortion. Interactions can lead to different phases of the electron liquid, depending on their range and strength, and can produce quasi-localized ground states of e.g. the Mott insulator type or a charge density wave. In this talk, we introduce effective lattice models to describe armchair and zigzag nanotubes with different types of impurities at low energies. The models are quasi-one dimensional and allow straightforward use in 1D techniques like the density-matrix renormalization group (DMRG). We discuss impurity effects in armchair CNTs and the influence of electron-electron interaction using DMRG calculations.

15 min. break.

TT 38.9 Thu 12:00 HSZ 301

Quantum oscillations from Fermi arcs — •Heidrun Weber[1,2] and Marcel Franz[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T 1Z1

When a metal is subjected to a strong magnetic field B, nearly all measurable quantities exhibit oscillations periodic in $1/B$. Such strong quantum oscillations represent a canonical probe of the Fermi surface, a defining property of a metal. We will discuss a new mechanism for quantum oscillations which requires only finite segments of a Fermi surface to exist, terminated by a pairing gap. We consider a real-space version of a BCS-like model Hamiltonian, whose hopping amplitude includes the usual Peierls factor and whose superconducting order parameter takes into account the existence of an Abrikosov vortex lattice. By a fully quantum mechanical treatment of the model we show that the density of states at the Fermi level exhibits an oscillatory behavior. Our results reconcile the recent breakthrough experiments showing quantum oscillations in a cuprate superconductor $YBa_2Cu_3O_{6.51}$, with a well-established result of many angle resolved photoemission (ARPES) studies which consistently indicate Fermi arcs - truncated segments of a Fermi surface - in the normal state of cuprates.

TT 38.10 Thu 12:15 HSZ 301

Momentum dependence of the spin-susceptibility in two dimensions: nonanalytic corrections in the Cooper channel — Stefano Chesi[1], •Robert Zak[1], Pascal Simon[1,2,3], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Laboratoire de Physique et Modelisation des Milieux Condenses, CNRS and Universite Joseph Fourier, BP 166, 38042 Grenoble, France — [3]Laboratoire de Physique des Solides, CNRS UMR-8502 Universite Paris Sud, 91405 Orsay Cedex, France

We consider the effect of rescattering of pairs of quasiparticles in the Cooper channel resulting in the strong renormalization of second order corrections to the spin susceptibility in a two-dimensional electron system. We use the Fourier expansion of the scattering potential in the vicinity of the Fermi surface to find that each harmonic becomes renormalized independently. Since some of those harmonics are negative, the slope of the spin susceptibility is bound to be negative at small momenta, in contrast to the lowest order perturbation theory result, which predicts a positive slope. We present in detail an effective method to calculate diagrammatically corrections to the spin susceptibility to infinite order.

TT 38.11 Thu 12:30 HSZ 301

Quantum Hall ferromagnetic states and spin-orbit interactions in the fractional regime — •Stefano Chesi and Daniel Loss — Department of Physics, University of Basel, CH-4056 Basel, Switzerland

The competition between the Zeeman energy and the Rashba and Dresselhaus spin-orbit couplings is studied for fractional quantum Hall states. A transition of the spin-polarization direction is predicted to occur at a small value of the Zeeman energy. For a given fractional state, the phenomenon can be accurately described in the perturbative limit of high magnetic fields. We consider the Laughlin wavefunctions and the Pfaffian state as specific examples and show that this phenomenon allows one to obtain valuable information about the nature of the correlated ground-state, and in particular about its pair-correlation function. We discuss indications of non-analytic features around the fractional states and include significant effects of the nuclear bath polarization in the relevant regime of temperatures and magnetic fields.

TT 38.12 Thu 12:45 HSZ 301

Weak-coupling CT-QMC and it's application to the Peierls transition in the quarter filled Holstein model. — •Fakher F. Assaad and Thomas C. Lang — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

After briefly reviewing the weak coupling CT-QMC approach we show how to generalize it to include phonon degrees of freedom[1]. The efficiency of this approach is tested in the framework of the one-dimensional Holstein model at quarter-band filling. We show that for adiabatic phonons, a phase transitions from a Luttinger to Luther Emery liquid is triggered by the electron phonon coupling. The Luther-Emery phase is characterized by dominant $2k_f$ charge correlations[2]. Those results stem from a detailed study of the temperature dependence of the single particle spectral function, the optical conductivity, as well as charge and spin dynamical structure factors.

[1] F.F. Assaad and T. Lang, Phys. Rev. B 76, 035116 (2007)
[2] F.F. Assaad, Phys. Rev. B 78, 155124 (2008).

TT 39: Correlated Electrons: Heavy Fermions 1

Time: Thursday 9:30–13:00 Location: HSZ 304

Invited Talk TT 39.1 Thu 9:30 HSZ 304

Electron spin resonance in Kondo systems — •Peter Wölfle — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe

Well-defined electron spin resonance (ESR) lines have been detected recently in several heavy fermion compounds, in which ferromagnetic correlations appear to be present [1]. We first discuss [2] the theory of ESR for the Kondo impurity system at temperatures T<<TK (Kondo temperature) , where the local spin ESR line has a width of order TK and is therefore unobservably broad.. By contrast, in the Anderson lattice system in the Kondo regime the ESR linewidth is narrow, and gets broadened by spin lattice relaxation and quasiparticle interaction processes. We show [2] that the spin lattice induced ESR linewidth is greatly reduced by an effective mass factor. The quasiparticle induced linewidth is small in the Fermi liquid regime, proportional to max(T^2,B^2) (T=temperature, B=Zeeman energy). The total ESR linewidth is reduced by exchange narrowing induced by a ferromagnetic exchange interaction. This explains the available ESR data.

[1] C. Krellner et al., Phys. Rev. Lett. 100, 066401 (2008).
[2] E. Abrahams and P. Wölfle, Phys. Rev. B78, 104423 (2008).

TT 39.2 Thu 10:00 HSZ 304

Tuning the Kondo Effect in $YbRh_2Si_2$: Electron Spin Resonance under Pressure and Doping — •Jan Wykhoff[1], D. V. Zakharov[2], H.-A. Krug von Nidda[2], I. Fazlizhanov[3], J. Sichelschmidt[1], C. Krellner[1], C. Geibel[1], A. Loidl[2], and F. Steglich[1] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden — [2]EP V, EKM, University of Augsburg, D-86135 Augsburg — [3]E. K. Zavoisky Physical Technical Institute, 420029 Kazan, Russia

The observation of a well defined Electron Spin Resonance (ESR) sig-

nal below the Kondo temperature T_K in the heavy-fermion compound $YbRh_2Si_2$ refutes a common believe that concentrated rare earth ions in Kondo-lattice intermetallic compounds would be ESR silent in the Kondo regime. The signal shows distinct properties of the Yb^{3+} $4f$ spin and, hence, should contain valuable microscopic information on the dynamical Kondo coupling to the conduction electrons [1]. We investigated the effect of tuning the $4f$ - conduction electron hybridization strength by Co-doping and hydrostatic pressure up to 3 GPa. Both stabilize antiferromagnetic order, lead to a reduction of T_K, and yield pronounced changes in the ESR parameters. By comparing the quantitatively different effect of pressure and Co doping on the ESR parameters we found a relation of the zero temperature residual ESR linewidth to the residual resistivity and the linear in temperature slope of the linewidth as was similarly reported for the La-doping case [1].

[1] J.W. *et al.* Physica C 460-462, 686 (2007); J.Sci.Tech.Adv.Mat. 8 389 (2007); J.S. *et al.* Phys. Rev. Lett. 91 156401 (2003).

TT 39.3 Thu 10:15 HSZ 304

Do heavy charge carriers entail a large Nernst coefficient? — •Ulrike Köhler[1,2], Cornelius Krellner[1], Niels Oeschler[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]present address: Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany

The Nernst effect is the development of a transverse thermal voltage in a magnetic field perpendicular to a heat current. During the past years unusually large Nernst coefficients ν have been observed in several Ce- and U-based heavy-fermion (HF) compounds. It has been speculated, that the huge Nernst signals are related to the enhanced effective charge carrier masses $m^\star$ of these systems. So far, however, investigations on Yb-based HF metals are lacking to corroborate this picture. We therefore studied the Nernst effect in $YbRh_2Si_2$, an archetype non-Fermi-liquid compound with a Kondo temperature T_K of 20 K. The Nernst coefficient is presented between 6 K and 200 K, i.e. covering the crossover from low effective charge carrier masses above T_K to the HF regime at $T \ll T_K$. ν is found to be negative with a minimum close to T_K, thus supporting the speculation about a relation between large ν and enhanced $m^\star$. The absolute values of the Nernst coefficient, however, are more than one order of magnitude smaller than in other HF systems. We discuss our findings in consideration of recent investigations on the correlated semiconductor CeNiSn, which point to a predominant importance of a low charge carrier density instead of a large $m^\star$ for the occurrence of a strong Nernst effect.

TT 39.4 Thu 10:30 HSZ 304

Concentration tuning of magnetic order in $CePd_{1-x}Ni_xAl$ compounds — •Nadezda Bagrets[1], Veronika Fritsch[1], Gernot Goll[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

The intermetallic alloys $CePd_{1-x}Ni_xAl$ are examples of antiferromagnetic (AF) heavy-fermion compounds which can be tuned to quantum critical point (QCP). CePdAl is well known as geometrically frustrated Kagomé-like lattice [1]. The substitution of Pd with Ni in CePdAl induces chemical pressure. The transition temperature decreases with increasing Ni content [2]. We performed specific-heat measurements on $CePd_{1-x}Ni_xAl$ compounds down to 30 mK. The AF transition is still visible for x=0.1. From the T_N vs. x dependence we expect the QCP at about $x = 0.12 - 0.13$. Surprisingly, our measurements show that the magnetic moment per formula unit at low temperature increases with increasing Ni content (chemical pressure) in contrast to a hydrostatic pressure [3]. We will present the specific heat and susceptibility measurements at very low temperatures as well as magnetization measurements up to a room temperature.

[1] H. Kitazawa, *et al.*, Physica B **199/200**, 28 (1994).
[2] Y. Isikawa, *et al.*, Physica B **281/282**, 365 (2000).
[3] S. Hane, *et al.*, Physica B **281/282**, 391 (2000).

TT 39.5 Thu 10:45 HSZ 304

Magnetic Anisotropy in Tetragonal Rare Earth Compounds — •Veronika Fritsch[1], Michael Marz[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

We have investigated single crystals of RAu_2Ge_2 with R = Ce and Pr as well as Ce_2MGa_{12} with M = Ni, Pd and Pt, grown by a flux growth method with Au-Ge flux for RAu_2Ge_2 and Ga flux for Ce_2MGa_{12}. The latter crystallizes in a tetragonal structure with layers of Ce atoms separated by segments of Ga only alternating with $GaPd_6$ segments [1]. Measurements of the dc susceptibility χ revealed a strong magnetic anisotropy. For the magnetic field along the c-axis, antiferromagnetic order sets in at 9.6 K (Ni), 10.6 K (Pd) and 5.7 K (Pt), as evidenced by sharp maxima in $\chi(T)$, for the magnetic field perpendicular to the c-axis $\chi(T)$ continues to increase monotonically down to 2 K. In RAu_2Ge_2 compounds, crystallizing in the considerably simpler $ThCr_2Si_2$ structure [2], a similar situation was found: with the magnetic field parallel to the c-axis antiferromagnetic order was found at 11.9 K (Ce) and 10.8 K (Pr), but with the magnetic field aligned perpendicular to the c-axis, no evidence for magnetic order is found down to 2 K. We will present measurements of magnetization and electrical resistivity exploring the possible proximity of these systems to a field-induced quantum critical point.

[1] R. T. Macaluso *et al.*, J. Sol. State Chem. **178** (2005) 3547.
[2] A. Loidl *et al.*, Phys. Rev. B **46** (1992) 9341.

15 min. break

TT 39.6 Thu 11:15 HSZ 304

Low-energy optics of the heavy-fermion compound UNi_2Al_3 — •Marc Scheffler[1], Julia Ostertag[1], Katrin Steinberg[1], Martin Dressel[1], and Martin Jourdan[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany

Heavy-fermion materials are intermetallic compounds with unusual metallic behavior at low temperatures. From the optical point of view, the Drude response (the transport relaxation time is enhanced in the same way as the effective mass) and the so-called hybridization gap (a signature of the peculiar band structure due to electronic interactions) are of particular interest. The low energy scales of heavy fermions call for optics at very low frequencies and in a broad range, but the only material studied in detail so far is UPd_2Al_3, where we found an extremely narrow Drude response (around 5GHz) and an optical excitation at 100GHz in the antiferromagnetic state.

To generalize those previous results, we focus here on the related heavy-fermion compound UNi_2Al_3. We have grown high-quality thin films and studied them with a combination of microwave and optical techniques in a very broad frequency range. At temperatures below 30K, we find a strongly frequency-dependent optical conductivity: the Drude roll-off resides below 20GHz, but above 100GHz another broad conductivity maximum occurs. In addition to the frequency and temperature dependence of the conductivity, we also present its anisotropy, and we discuss them in the context of the different energy scales of this material.

TT 39.7 Thu 11:30 HSZ 304

Superconductivity in $CeCu_2Si_2$: evidence of fermisurface change — •Enrico Faulhaber[1], Oliver Stockert[2], Wolfgang Schmidt[3,4], Karin Schmalzl[3,4], Christoph Geibel[2], Frank Steglich[2], and Michael Loewenhaupt[1] — [1]TU Dresden; Institut für Festkörperphysik; D-01062 Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe; D-01187 Dresden — [3]Forschungszentrum Jülich GmbH; Institut für Festkörperforschung; D-52425 Jülich — [4]Institut Laue-Langevin; F-38042 Grenoble

The first discovered heavy fermion superconductor $CeCu_2Si_2$ has been investigated for nearly 30 years now. Key properties of the material are an antiferromagnetic order below 1 K dominated by a nesting of the Fermi surface and a superconducting phase below ≈0.6 K. This phase seems to depend on the magnetism in the material, possibly pointing towards a magnetically mediated superconductivity.

In a recent experiment we investigated the delicate relationship between the magnetic and superconducting phases. We used the neutron scattering technique to observe the magnetic propagation vector. Also, the instrument was complemented with a unique in-situ *ac*-susceptibility setup to record the superconductivity of the sample during the neutron diffraction. Applying a magnetic field, we found an unexpected change of the magnetic propagation vector which correlates well with the superconducting volume. This shift is absent in non-superconducting samples, indicating a strong entanglement of both phenomena (superconductivity and magnetism) and might point to a change of the Fermi surface caused by the superconductivity.

TT 39.8 Thu 11:45 HSZ 304

Investigation of $Yb_2Pt_6AL_{15}$ single crystals: heavy fermion

system with a large local moment degeneracy — •Micha Deppe, Stefanie Hartmann, Monica E. Macovei, Niels Oeschler, Michael Nicklas, and Christoph Geibel — Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Possible new Cerium or Ytterbium based heavy fermion compounds for the study of a quantum critical point (QCP) are of high interest. We studied $Yb_2Pt_6AL_{15}$ because it exhibits an interesting quasi 2D crystal structure. It crystallizes in the hexagonal structure type $Sc_{1.2}Fe_4Si_{9.8}$ and this structure presents RE_2Al_3 - layers separated by two Pt-Al layers in a large distance $c/2 = 8.18$ Å between the RE_2Al_3 - layers and a large c/a ≈ 4 ratio.
Here we present our investigations of the magnetic properties by means of susceptibility $\chi(T)$, specific heat $C(T)$, resistivity $\rho(T)$ and thermoelectric power $S(T)$ measurements. While all properties follow in general the behavior typical for Kondo-lattice systems, $\chi(T)$ and $C_p(T)/T$ present broad maxima in the T range 17-35 K, which matches nicely the prediction of the Coqblin-Schrieffer model for $J = 7/2$. A large degeneracy of the local moment is also supported by a reduced Kadowaki-Woods ratio. Thus, the analysis of all investigated properties evidences $Yb_2Pt_6Al_{15}$ to be a paramagnetic Kondo-lattice system with the whole $J = 7/2$ multiplet involved in the formation of the Kondo state, a Kondo temperature of the order of 60 K, and a heavy Fermi-liquid ground state with a Sommerfeld coefficient $\gamma_0 = 0.33\ J/mol{-}Yb\ K^{-2}$ corresponding to a mass enhancement of the order of 30.

TT 39.9 Thu 12:00 HSZ 304

Normal state magnetoresistance in the heavy fermion superconductor $CeCo(In_{0.925}Cd_{0.075})_5$ — •Sunil Nair[1], S. Wirth[1], M. Nicklas[1], A. D. Bianchi[2], Z. Fisk[3], and F. Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Départment de Physique, Université de Montréal, Montréal, Quebec H3C 3J7, Canada. — [3]University of California, Irvine, California 92697, USA.

The $CeMIn_5$ (where M: Co,Ir) family of heavy fermion systems is currently in vogue due to the delicate interplay between unconventional superconductivity and magnetism observed in these systems. A putative quantum critical point – which lies in the vicinity of the superconducting regime in the temperature-magnetic field phase space of these systems – manifests itself in a host of novel properties. An additional ambient pressure phase space was opened up by Cd substitution on the In site, which acts as an efficient electronic tuning agent and shifts the ground state from a superconducting to an antiferromagnetic one. Here, we present sensitive measurements of the magnetoresistance in the $CeCo(In_{0.925}Cd_{0.075})_5$ system in the temperature range 0.05 K $\leq T \leq$ 4 K and with magnetic fields of up to 15 T. At fields larger than the superconducting upper critical field, features corresponding to a possible destabilization of the antiferromagnetic order are observed. Measurements performed with the magnetic field applied along different crystallographic directions indicate that this feature is strongly anisotropic. The implications of our results are discussed in the context of the crystallographic and magnetic anisotropy of these systems.

TT 39.10 Thu 12:15 HSZ 304

μSR-studies on the Heavy-Fermion-Superconductor $CeCoIn_5$ at high magnetic fields — •Johannes Spehling[1], Hans Henning Klauss[1], Jeff Sonier[2], Eric Bauer[3], and Robert Heffner[3] — [1]Institut für Festkörperphysik, Technical University Dresden, D-01069 Dresden, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, BC, Canada — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A

In strong magnetic fields the Heavy Fermion superconductor $CeCoIn_5$ shows a first order transition from the normal state into the superconducting phase [1]. It is suggested that a specifically modulated superconducting state is formed, the FFLO state, theoretically predicted by Fulde, Ferrell, Larkov and Ovchinnikov in 1964/1965 [2]. We have carried out transverse field μSR-measurements between 2T and 5T ($\hat{c} \parallel H$) on single-crystalline $CeCoIn_5$ in a temperature range between 25mK and 7K. In addition to the standard modulation perpendicular to the applied field due to the flux line lattice, a longitudinal modulation is expected. In that case an additional broadening of a local probe spectrum due to hyperfine fields should occur. The data clearly evidence the fielddriven change from second to first order-like transition at an external field of 4.8T. On the other hand no additional line broadening is observed at very low temperatures below T_c, which disagrees with the assumptions of a static FFLO state.

[1] A. Bianchi *et al.*, Phys. Rev. Lett. **91**, 187004 (2003).
[2] P. Fulde and R. A. Ferrell, Phys. Rev. **135**, A550 (1964).

TT 39.11 Thu 12:30 HSZ 304

Electronic transport properties of c-axis oriented $CeCoIn_5$ thin films — •Oleksandr Foyevtsov and Michael Huth — Johann Wolfgang Goethe University, Frankfurt am Main, Germany

We report results of the growth of c-axis oriented thin films of the heavy-fermion superconductor $CeCoIn_5$ prepared by molecular beam epitaxy. The films were grown by co-deposition of the constituent elements on chemically cleaned a-plane α-Al_2O_3 substrates. X-ray (XRD) diffraction, atomic force (AFM) and scanning electron microscopy (SEM) were used for film characterization. The films show a pronounced c-axis growth preference with a moderate tendency for epitaxial in-plane order driven by substrate crystallographic planes. In general the films' morphology is rough, which we assume is driven by the weak wetting tendency of the In component. Comparative growth studies done on the parent compound $CeIn_3$ support this assumption. By optimization of the growth process, samples with improved surface morphology were obtained. Electronic transport measurements (resistivity, magneto-resistivity, Hall effect) were performed in the temperature range from 1.8 K to 270 K in magnetic fields up to 9 T. We prepared superconductor-insulator-superconductor tunnel junctions on selected thin films using thin amorphous AlO_x layers as insulating barrier and In layers as counter electrode. These tunnel diodes were prepared in-situ by a stencil mask technique. First results on the tunneling spectroscopy of these diodes will be presented.

TT 39.12 Thu 12:45 HSZ 304

The magnetisation dynamics in the superconducting state of UBe_{13} investigated by inelastic neutron scattering — •Arno Hiess[1], Oliver Stockert[2], and Zachary Fisk[3] — [1]Institut Laue - Langevin, Grenoble, France — [2]MPI-CPfS, Dresden, Germany — [3]Univ. California, Irvine, USA

Inelastic neutron scattering experiments continue to shed light on the interplay of magnetism and superconductivity. Previously such experiments established that the magnetisation dynamics of several high-temperature superconductors differs in the superconducting and in the normal state. Such an effect has also been reported in three intermetallic superconductors, e.g., UPd_2Al_3, $CeCoIn_5$ and $CeCu_2Si_2$. We here report high-resolution inelastic neutron scattering experiments on a large UBe_{13} single crystal using the cold neutron three-axis spectrometer IN14 at ILL, Grenoble. UBe_{13} is a cubic material which at low temperatures exhibits a large electronic contribution to the specific heat and becomes superconducting below $T_{sc} = 0.85$ K. In agreement with previous experiments and below about 30 K we observed short-lived and short-ranged magnetic fluctuations at selected momentum space positions. The measurements in the normal state show a quasi-elastic signal. Upon entering the superconducting state a reduction of magnetic intensity is observed below 0.5 meV, suggesting the magnetic response becomes inelastic below T_{sc}. Our results will be compared to those obtained in other superconductors and rationalised within a simple scenario of superconductivity.

TT 40: Superconductivity: Ferropnictides 1

Time: Thursday 14:00–19:00 Location: HSZ 03

TT 40.1 Thu 14:00 HSZ 03

Antiferromagnetic correlations in the normal state of $LaFeAsO_{1-x}F_x$ with $0 \leq x \leq 0.125$ — •Rüdiger Klingeler, Norman Leps, Liran Wang, Christian Hess, Günter Behr, Vladislav Kataev, and Bernd Büchner — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

We have studied the interplay of magnetism and superconductivity in $LaFeAsO_{1-x}F_x$ with $0 \leq x \leq 0.125$. For low doping with $x \leq 0.04$, our data confirm a moderate suppression of both the structural transition and the antiferromagnetic spin density wave formation. For $x \geq 0.05$,

both anomalies are completely suppressed and superconductivity is observed. Remarkably, the temperature dependence of the normal state susceptibility well above T_C is almost independent of doping, i.e. both the absolute value and the slope are nearly unchanged compared to the undoped case [1]. This implies at least local antiferromagnetic interactions which barely depend on hole doping although the ground state changes entirely from an orthorhombic antiferromagnetic poor metal ($x \leq 0.04$) to a tetragonal superconductor ($x \geq 0.05$). These surprising results are discussed in terms of (i) - pseudogap formation, (ii) - antiferromagnetic correlations, and (iii) - preformed bipolarons which might be relevant to the pairing mechanism.

[1] R. Klingeler et al., Preprint at http://arxiv.org/abs/0808.0708

TT 40.2 Thu 14:15 HSZ 03

Electronic phase diagram of the $LaO_{1-x}F_xFeAs$ superconductor: A muon spin relaxation study — •H. Luetkens[1], H.-H. Klauss[2], F.J. Litterst[3], T. Dellmann[3], R. Klingeler[4], C. Hess[4], R. Khasanov[1], A. Amato[1], C. Baines[1], M. Kosmala[5], O.J. Schumann[5], M. Braden[5], J. Hamann-Borrero[4], N. Leps[4], A. Kondrat[4], G. Behr[4], J. Werner[4], M. Kraken[3], and B. Büchner[4] — [1]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland — [2]Institut für Festkörperphysik, TU Dresden — [3]Institut für Physik der Kondensierten Materie, TU Braunschweig — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden — [5]II. Physikalisches Institut, U Köln

The structural and electronic phase diagram of $LaO_{1-x}F_xFeAs$ and, in particular, the exact nature of the change from the magnetically ordered to the superconducting state that was determined by means of x-ray scattering, muSR and Mössbauer spectroscopy will be presented [1-3]. A discontinuous first-order-like change of the Néel temperature, the superconducting transition temperature, the sublattice magnetisation and the superfluid density is found between x=0.04 and x=0.05. While these results strongly question the relevance of quantum critical behaviour in iron pnictides they prove an important role of the structural orthorhombic distortion disappearing exactly at the SDW magnetism and superconductivity phase boundary.

[1] H. Luetkens et al., Phys. Rev. Lett. 101, 097009 (2008).
[2] H.-H. Klauss et al., Phys. Rev. Lett. 101, 077005 (2008).
[3] H. Luetkens et al., arXiv:0806.3533 (2008).

TT 40.3 Thu 14:30 HSZ 03

Functional renormalization group study of the iron pnictides — •Christian Platt, Carsten Honerkamp, and Werner Hanke — Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Recently, a new class of superconductors (sc) - Fe-based sc - was discovered. These sc iron pnictides are most likely less correlated than the high-T_c cuprates but present again a challenging case of competing magnetic and superconducting orders at low temperatures. Therefore, perturbative functional renormalization group (fRG) methods appear adequate for the theoretical modelling of the phase diagram. Here, we apply the fRG to a four-band (Fe-d-orbital) model including intra- and interband couplings as well as interband pair hoppings. We compute the leading instabilities, i.e. spin-ordered phase in the "underdoped"situation and the leading pairing instability as a function of the electron density and interaction parameters.

TT 40.4 Thu 14:45 HSZ 03

Thermodynamic study of the Co-doped Ba-122 iron pnictide — •Frédéric Hardy[1], Christoph Meingast[1], Thomas Wolf[1], Rolf Heid[1], Peter Adelmann[1], Peter Schweiss[1], Doris Ernst[1], and Hilbert v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany

Since the discovery of the new high-T_c iron pnictides, many scenarios were put forward to describe the symmetry of the order parameter including d-wave and unconventional s-wave. Early heat capacity measurements suggested that the electron-doped 1111 compounds show a nodal gap, while K-hole-doped 122 materials are fully gapped. Here we present a critical analysis of our own specific-heat data on Co-doped 122 single crystals, in which we pay particular attention to the details of the phonon background subtraction as well as to the contribution of impurity phases. We also discuss an interesting field-dependence of the thermal expansivity below T_c(H).

TT 40.5 Thu 15:00 HSZ 03

Strong coupling of superconductivity to c/a in $Ba(Fe,Co)_2As_2$ — •Christoph Meingast[1], Frederic Hardy[1], Peter Adelmann[1], Peter Schweiss[1], Doris Ernst[1], Hilbert v. Löhneysen[1,2], and Thomas Wolf[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany.

Just as in the cuprates, magnetism and superconductivity occur in close proximity to each other in the newly discovered FeAs-based materials. Here, using high-resolution thermal expansion and specific heat measurements, we study the thermodynamic response of the lattice parameters to superconducting and magnetic order in $Ba(Fe,Co)_2As_2$ single crystals. We show that there is a strong coupling of the c/a ratio to both the superconducting and magnetic/structural phase transitions. According to the Ehrenfest relationship, the ordering temperatures of both ordered states are expected to increase with increasing c/a. This suggests that the occurrence of superconductivity is strongly linked to the magnetic/structural transition.

TT 40.6 Thu 15:15 HSZ 03

Electronic phase separation in the slightly underdoped iron pnictide superconductor $Ba_{1-x}K_xFe_2As_2$ — •Ji Tae Park[1], D. S. Inosov[1], Ch. Niedermayer[2], G. L. Sun[1], D. Haug[1], N. B. Christensen[2], R Dinnebier[1], A. V. Boris[1], A. J. Drew[3], L. Schulz[3], T. Shapoval[4], U. Wolff[4], V. Neu[4], X. Yang[1], C. T. Lin[1], B. Keimer[1], and V. Hinkov[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, Stuttgart, Germany — [2]ETHZ & PSI, Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, Chemin du Musée 3, Fribourg, Switzerland — [4]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

We performed a combined study of the slightly underdoped novel iron pnictide superconductor $Ba_{1-x}K_xFe_2As_2$ by means of X-ray powder diffraction, neutron scattering, muon spin rotation (μSR), and magnetic force microscopy (MFM). Commensurate static magnetic order sets in below $T_m \sim 70$ K as inferred from the emergence of the magnetic (1 0 3) reflection in the neutron scattering data and from the observation of damped oscillations in the zero-field-μSR asymmetry. Transverse-field μSR below T_c shows a coexistence of magnetically ordered and non-magnetic states, which is also confirmed by MFM imaging. This coexistence could be explained by electronic phase separation into antiferromagnetic and superconducting/normal state regions on a scale of several tens of nanometers indicating that such mesoscopic phase separation can be considered an intrinsic property of some iron pnictide superconductors.

15 min. break

TT 40.7 Thu 15:45 HSZ 03

The intrinsic electronic phase diagram of iron-pnictide superconductors — •C. Hess, A. Kondrat, A. Narduzzo, J. E. Hamann-Borrero, R. Klingeler, H. Grafe, G. Lang, F. Hammerath, D. Paar, A. Alfonsov, V. Kataev, J. Werner, G. Behr, and B. Büchner — Leibniz-Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany

We present a detailed study of the intrinsic electronic phase diagram of the oxypnictide superconductors in the normal state based on the analysis of the electrical resistivity ρ of both $LaO_{1-x}F_xFeAs$ and $SmO_{1-x}F_xFeAs$ for a wide range of doping. Our data give clear-cut evidence for unusual normal state properties in these new materials. As a function of doping ρ of $LaO_{1-x}F_xFeAs$ shows a clear transition from pseudogap to Fermi liquid-like behavior, mimicking the phase diagram of the cuprates. Moreover, our data reveal a correlation between the strength of the pseudogap signatures and the stability of the superconducting phase. The pseudogap signatures, which are clearly connected with the structural and magnetic transitions of the parent material, become stronger in $SmO_{1-x}F_xFeAs$ where superconductivity is enhanced and vanish when superconductivity is reduced in the doping region with Fermi liquid-like behavior [1]. We further present evidence for the connection between the pseudogap signatures in electrical transport and the slowing-down of spin fluctuation.

[1] C. Hess et al., Preprint at http://arxiv.org/abs/0811.1601

TT 40.8 Thu 16:00 HSZ 03

Magnetic properties of $LaO_{1-x}F_xFeAs$ — •Sangeeta Sharma[1,2], John Kay Dewhurst[1,2], Sam Shallcross[3], Christophe Bersier[1,2], Francesco Cricchio[4], Antonio Sanna[2,5], Sandro

Massidda[5], E. K. U Gross[2], and Lars Nordstroem[4] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [3]Lehrstuhl für Theoretische Festkörperphysik, Staudstr. 7-B2, 91058 Erlangen, Germany. — [4]Department of Physics, Uppsala University, Box 530, SE-75121 Uppsala, Sweden. — [5]Dipartimento di Fisica, Universita' di Cagliari, Cittadella Universitaria, I-09042 Monserrato(CA), Italy

Using state-of-the-art first-principles calculations we have elucidated the complex magnetic and structural dependence of LaOFeAs upon doping. Our key findings are that (i) doping results in an orthorhombic ground state and (ii) there is a commensurate to incommensurate transition in the magnetic structure between $x = 0.025$ and $x = 0.04$. Our calculations further imply that in this system magnetic order persists up to the onset of superconductivity at the critical doping of $x = 0.05$. Finally, our investigations of the undoped parent compound reveal a small itinerant moment and orthorhombic structure with both moment and distortion angle in excellent agreement with experiments.

TT 40.9 Thu 16:15 HSZ 03

Doping dependence of the charge distribution of iron pnictides — •Guillaume Lang[1], Hans-Joachim Grafe[1], Katarina Manthey[1], Franziska Hammerath[1], Dalibor Paar[1,2], Katrin Koch[3], Helge Rosner[3], Günther Behr[1], Jochen Werner[1], and Bernd Büchner[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Dept. of Physics, Fac. of Science, Univ. of Zagreb, P. O. Box 331, HR-10002 Zagreb, Croatia — [3]Max Planck Inst. for Chem. Phys. of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany

We have investigated the evolution, on doping, of the charge distribution in the new $LaO_{1-x}F_xFeAs$ superconductor. This is done using ^{75}As Nuclear Quadrupole Resonance (NQR), which is a sensitive local probe of the electric field gradient generated by the charge distribution. A significant increase of the quadrupole frequency is observed when going from the undoped situation to the superconducting region of the phase diagram, reflecting the change in density or spatial distribution of the electrons ([1], and subsequent measurements to be published). This increase cannot be properly accounted for by LDA calculations, even though there is good agreement between theory and experience for the undoped case. We discuss this discrepancy as well as the relation to the superconductivity, i.e., the link to the doping-dependence of the critical temperature.

[1] H.-J. Grafe, G. Lang et al., arXiv:0811.4508, submitted to New Journal of Physics (invited paper, special issue on iron pnictides superconductors)

TT 40.10 Thu 16:30 HSZ 03

Observation of the many body satellite in $Ba_{1-x}K_xFe_2As_2$ single crystals by resonant x-ray photoemission spectroscopy — Andreas Koitzsch[1], Thomas Kroll[1], Roberto Kraus[1], Martin Knupfer[1], Bernd Büchner[1], David Batchelor[2], Guoli Sun[3], Dunlu Sun[3], and •Chengtian Lin[3] — [1]IFW Dresden, Postfach 270116, 01171 Dresden — [2]Forschungszentrum Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Valence band and core level measurements of $Ba_{1-x}K_xFe_2As_2$ single crystals with photon energies across the Fe L_3 absorption edge are reported. Within the resonance regime of the photon energy profile an intensity enhancement centered at E = 3.6 eV is observed which can be identified as the many body satellite. The energy position of the satellite matches the expectations based on previously extracted parameters from Fe L x-ray absorption spectroscopy and Fe 2p x-ray photoemission spectroscopy. The results show, that the Hubbard repulsion U, although smaller than the bandwidth, preserves a clear physical meaning giving rise to local electron phenomena in an otherwise itinerant environment.

TT 40.11 Thu 16:45 HSZ 03

Momentum dependence of the superconducting gap in $Ba_{1-x}K_xFe_2As_2$ — •D. V. Evtushinsky[1], D. S. Inosov[1,2], V. B. Zabolotnyy[1], A. Koitzsch[1], M. Knupfer[1], B. Büchner[1], G. L. Sun[2], V. Hinkov[2], A. V. Boris[2], C. T. Lin[2], B. Keimer[2], A. Varykhalov[3], A. A. Kordyuk[1,4], and S. V. Borisenko[1] — [1]Institute for Solid State Research, IFW Dresden, P. O. Box 270116, D-01171 Dresden, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [4]Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

The precise momentum dependence of the superconducting gap in the iron-arsenide superconductor with $T_c = 32$ K (BKFA) was determined from angle-resolved photoemission spectroscopy (ARPES) via fitting the distribution of the quasiparticle density to a model. The model incorporates finite lifetime and experimental resolution effects, as well as accounts for peculiarities of BKFA electronic structure. We have found that the value of the superconducting gap is practically the same for the inner Γ-barrel, X-pocket, and "blade"-pocket, and equals 9 meV, while the gap on the outer Γ-barrel is estimated to be less than 4 meV, resulting in $2\Delta/k_BT_c = 6.8$ for the large gap, and $2\Delta/k_BT_c < 3$ for the small gap. We also observe that below T_c photoemission signal contains large non-superconducting part.

TT 40.12 Thu 17:00 HSZ 03

Correlations in Ferropnictides — •Klaus Koepernik and Helmut Eschrig — IFW Dresden, Germany

The strenght of correlations in the ferropnictide superconductors is still under debate. While arguments for an electron-electron interaction U of 5eV have been made, some experimental results support a U of merely 1eV. Density functional theory in the local spin density approximation (LSDA) seems to describe several aspects of the electronic structure quite reasonably, which would also support a smaller U. However, the unusually large error of the calculated lattice structure remains a puzzle. We discuss the influence of correlations on the electronic structure and the properties of the ferropnictides in the framework of LSDA+U calculations.

15 min. break

TT 40.13 Thu 17:30 HSZ 03

Theory for magnetic excitations in Fe-pnictide superconductors — •Maxim Korshunov[1,2] and Ilya Eremin[1,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany — [2]L.V. Kirensky Institute of Physics, Siberian Branch of RA, 660036 Krasnoyarsk, Russia — [3]Institute für Mathematische und Theoretische Physik, TU Braunschweig, D-38106 Braunschweig, Germany

We analyze the spin response in the normal and superconducting states of the Fe-pnictide High-T_c superconductors. While the normal state spin excitations are dominated by the continuum of the interorbital antiferromagnetic (AFM) spin density wave fluctuations (SDW) and the incommensurate intraband SDW fluctuations, the unconventional superconductivity yields different feedback: the resonance peak in form of the well-defined spin exciton occurs *only* for the interband scattering at the AFM momentum Q_{AFM} for the extended s-wave ($s_\pm$) superconducting order parameter and it is extremely weak for the d-wave order parameter due to the specific Fermi surface (FS) topology. We discuss this essential difference in the context of neutron scattering experiments used for determination of the superconducting wave function symmetry.

For the non-superconducting state, we show that the commensurate AFM SDW transition disappears already at the doping concentration $x \sim 0.04$ reflecting the evolution of the FS. Correspondingly, with further increase of the doping the AFM fluctuations are suppressed for $x > 0.1$ and the $\mathrm{Im}\chi(Q_{AFM}, \omega)/\omega$ becomes nearly temperature independent, in agreement with recent NMR experiments.

TT 40.14 Thu 17:45 HSZ 03

Interplay between crystal structure and magnetism in the superconducting AFe_2As_2 (A = Ca, Sr, Ba and Eu) Systems: A First-principles Study — •Alim Ormeci, Deepa Kasinathan, Katrin Koch, Miriam Schmitt, and Helge Rosner — MPI CPfS, Dresden

Although the recently discovered FeAs-based superconducting compounds crystallize in different structures, they have the same Fe-As substructure and display very similar electronic properties including similar patterns of structural and magnetic transitions. However, experimentally important differences are also found between the REOFeAs (RE = rare-earth) and the AFe_2As_2 families. Because sample composition and quality are easier to control in the latter family, we focus on the AFe_2As_2 systems. Using all-electron full-potential calculations, we study the relation between the onset of spin-density wave (SDW) and the tetragonal-to-orthorhombic transition. We find that the SDW pattern is necessary for the structural transition to take

place. We also explore how electronic structure and magnetic behavior change when all free structural parameters, As-z, c/a and a/b, are optimized at different unit cell volumes (pressures). All four systems are compared with each other based on the calculation results. Most calculated properties agree well with the measured properties, but several of them are rather sensitive to the As z position. For a microscopic understanding of the electronic structure of this new family of superconductors this structural feature is crucial, but its correct ab initio treatment still remains an open question.

TT 40.15 Thu 18:00 HSZ 03

Renormalized in-plane plasma frequencies and insight into the superconductivity of iron pnictides from optical studies and low-temperature μSR data — •Stefan-Ludwig Drechsler[1], Helge Rosner[2], Klaus Koepernik[1], Mandy Grobosch[1], Guenter Behr[1], Roman Schuster[1], Friedrich Roth[1], Saad Elgazzar[3], Bernd Buechner[1], and Martin Knupfer[1] — [1]IFW-Dresden, D-01171 Dresden, Germany — [2]MPI-CPfS Dresden, Germany — [3]Menoufia Univ., Shebin El-kom, Egypt & Uppsala Univ., Sweden

Theoretical values for the unscreened plasma frequencies of several Fe pnictides from DFT-LDA based calculations are compared with experimental plasma frequencies obtained from reflectivity measurements on both polycrystalline samples [1] and single crystals. The sizable renormalization observed for all considered compounds points to the presence of significant many-body effects beyond the LDA. From the measured large empirical background polarizabilities $\varepsilon_\infty \gtrsim$ 10-15 we discard a sizable value of the Coulomb repulsion $U \sim 4$ eV on Fe sites as proposed in the literature. From the extrapolated μSR (muon spin rotation) penetration depth data at very low-temperature and the experimental unscreened plasma frequency the total coupling constant λ_{tot} for the electron-boson interaction is estimated within the framework of the Eliashberg-theory within an effective single band approximation. For $LaFeAsO_{0.9}F_{0.1}$ a weak to intermediately strong coupling regime is found whereas in the pronounced multiband case a constraint for various intraband coupling constants is obtained.

[1] S.-L. Drechsler, M. Grobosch *et al.*, PRL **101** in press (2008).

TT 40.16 Thu 18:15 HSZ 03

Pressure-induced structural and magnetic transitions in the 122 iron arsenide compounds — •Yuzhong Zhang, Hem Kandpal, Ingo Opahle, Harald Jeschke, Claudius Gros, and Roser Valenti — Institut für Theoretische Physik, Goethe Universität Frankfurt, Germany

The parent compounds of the new superconductor family (Ca, Sr, Ba)Fe_2As_2 under hydrostatic pressure at low temperature are investigated within the framework of ab initio molecular dynamics. Structural phase transitions from orthorhombic to tetragonal phase are detected in all these materials. These transitions are simultaneously accompanied by magnetic phase transitions from a stripe-type antiferromagnetic state to a paramagnetic state. While the obtained first-order phase transition in $CaFe_2As_2$ is consistent with the experimental results, we predict from our calculations that the phase transitions in $SrFe_2As_2$ and $BaFe_2As_2$ are of weak first order and continuous order, respectively. Analysis of Fermi surfaces, partial density of state as well as bandstructures as a function of chemical and hydrostatic pressure reveals the differences among these compounds. Finally we discuss, out of our calculations, the possible mechanism of the superconducting states.

TT 40.17 Thu 18:30 HSZ 03

Investigation of superconductivity and magnetism in $EuFe_2As_2$ — •Hirale S. Jeevan and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We present an investigation of superconductivity and magnetism in $EuFe_2As_2$ by doping of K, Ni,Co and P. The recent discovery of superconductivity in FeAs and related systems has a great impact in the field of superconductivity research. Superconductivity is found close to a magnetic and non-magnetic phase transition suggesting an unconventional pairing mechanism. We have synthesized single crystals and powder samples of both doped and undoped samples of $EuFe_2As_2$ and investigated their physical properties. We found rather unique behavior due to the additional ordering of Eu^{2+}, which is absent in other systems like $BaFe_2As_2$,$SrFe_2As_2$ etc. The heat capacity, resistivity and magnetization measurements carried out at ambient pressure on the parent compound show an antiferromagnetic spin-density-wave (T_{SDW}) at $\approx$ 190K related to the Fe_2As_2 layers and magnetic ordering of Eu^{2+} (T_N) moments at $\approx$ 20K. Upon doping Eu with K >30%, T_{SDW} gets suppressed and superconductivity appears at $\approx$ 32K and also Eu^{2+} ordering suppressed to the low temperature. On the other hand,doping of Co and Ni to the Fe site suppresses the SDW transition but no SC is found, possibly due to Eu ordering which appears unchanged at $\approx$ 19K.We will also discuss the effect of P doping to the As site.

Collaboration with: C.Geibel, Z.Hossain, Deepa Kasinathan, C. F. Miclea, M. Nicklas and H. Rosner

TT 40.18 Thu 18:45 HSZ 03

ESR spectroscopy on (Gd,La)$O_{1-x}F_x$FeAs superconductors — •A. Alfonsov, F. Murányi, V. Kataev, N. Leps, R. Klingeler, A. Kondrat, C. Hess, A. Köhler, J. Werner, G. Behr, and B. Büchner — IFW Dresden, Institute for Solid State Research, D-01171 Dresden, Germany

We present results on electron spin resonance (ESR) spectroscopy of polycrystalline samples of the (Gd,La)$O_{1-x}F_x$FeAs superconductor with different levels of fluorine and gadolinium doping. The ESR signal of a small amount of Gd spins doped to the parent compound LaOFeAs is sensitive to the structural and in particular to the magnetic phase transition occurring in this material at temperatures $\sim 130 - 150$ K. Fluorine doping suppresses both transitions and leads to superconductivity. Correspondingly, the Gd ESR response shows no signatures of the magnetic order in the FeAs planes of samples with a superconducting ground state. In the concentrated compound GdOFeAs the Gd ESR response is sensitive to the magnetism of the FeAs planes, too. Doping of this material with ~ 15 % of fluorine yields superconductivity with $T_c \approx 21$ K. Surprisingly, Gd ESR gives clear indications of the enhancement of (quasi)-static magnetic correlations in the superconducting samples which set in below ~ 80 K and continue to develop even in the superconducting state. We compare ESR data with results of thermodynamic and transport measurements on these samples and discuss a possible role of magnetic rare-earths for the magnetism of the FeAs-planes in which the superconductivity evolves upon the fluorine doping.

TT 41: Matter at Low Temperature: Quantum Liquids, Bose-Einstein-Condensates, Ultra-cold Atoms

Time: Thursday 14:00–19:00 Location: HSZ 105

TT 41.1 Thu 14:00 HSZ 105

Dynamics of Interacting Bose-Bose Mixtures in an Optical Lattice — •Julia Wernsdorfer, Michiel Snoek, and Walter Hofstetter — Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt, Germany

We investigate a bosonic quantum gas consisting of two interacting species in a two-dimensional optical lattice. The equilibrium properties and dynamics of this system are obtained by means of the Gutzwiller method. In particular we study the ramp-up of the optical lattice, which occurs on a time scale comparable to the tunneling time of the bosons. We investigate the adiabaticity of this process with respect to the many body quantum states to analyze whether the bosonic gas is in an equilibrium state when time-of-flight measurements are carried out. The effect of finite temperature is investigated by extending the time-dependent Gutzwiller method to $T > 0$.

TT 41.2 Thu 14:15 HSZ 105

Exploring Local Quantum Many-Body Relaxation by Atoms in Optical Superlattices — •Andreas Flesch[1], Marcus Cramer[2], Ian P. McCulloch[3], Ulrich Schollwöck[1], and Jens Eisert[2,4] — [1]Institut für Theoretische Physik C, RWTH Aachen University, 52056 Aachen, Germany — [2]Institute for Mathematical Sci-

ences, Imperial College London, SW7 2PE London, United Kingdom — [3]School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072, Australia — [4]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

In the study of relaxation processes in coherent non-equilibrium dynamics of quenched quantum systems, ultracold atoms in optical superlattices with periodicity 2 provide a very fruitful test ground. We consider the dynamics of a particular, experimentally accessible initial state prepared in a superlattice structure evolving under a Bose-Hubbard Hamiltonian in the entire range of interaction strengths [1,2]. We investigate the relaxation dynamics of certain correlation functions analytically in the non-interacting and hard-core bosonic limits and numerically for finite interaction strengths using a time-dependent density-matrix renormalization (t-DMRG) approach. Our results show that this setup allows to experimentally probe signatures of the process of local relaxation of subsystems in non-equilibrium dynamics without the need of addressing single sites by exploiting the possibilities offered by optical superlattices.

[1] M. Cramer et al., PRL 101, 063001 (2008)
[2] A. Flesch et al., PRA 78, 033608 (2008)

TT 41.3 Thu 14:30 HSZ 105

Superfluid Boson Currents and Long Range Interactions in 1D Lattices — •Johannes Schachenmayer — Institut für Theoretische Physik, Technikerstr. 26, 6020 Innsbruck, Austria

The decay of superfluid currents for bosons moving in an optical lattice potential has attracted a lot of recent attention. In particular, experiments have shown that the decay of currents in 1D systems differs markedly from the mean-field prediction. We investigate this system here, computing the time evolution within the Bose-Hubbard model using the infinite Time Evolving Block Decimation Algorithm, and find good agreement with the experimental results. We further report on progress in extending the algorithm to allow simulation of long-range interactions.

TT 41.4 Thu 14:45 HSZ 105

Magnetism, coherent many-particle dynamics, and relaxation with ultracold bosons in optical superlattices — •Thomas Barthel[1], Christian Kasztelan[1], Ian P. McCulloch[2], and Ulrich Schollwöck[1] — [1]Institute for Theoretical Physics C, RWTH Aachen University, 52056 Aachen, Germany — [2]School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072, Australia

We study a particular setup of an ultracold two-species boson gas in an optical superlattice. This realizes in a certain parameter regime actually the physics of spin-1/2 Heisenberg magnets describing the second order hopping processes. Tuning of the superlattice allows for controlling the effect of fast first order processes versus the slower second order ones. We provide the evolution of typical experimentally available observables by means of the density-matrix renormalization-group method. The validity of the description via the Heisenberg model is studied numerically and analytically. Contrary to the case of isolated double wells which was recently realized experimentally, here, relaxation of local observables can be observed. The tunability between the Bose-Hubbard model and the Heisenberg model in this setup could be used to study experimentally the differences in equilibration processes for nonintegrable and Bethe ansatz integrable models.
Ref. arXiv:0809.5141.

TT 41.5 Thu 15:00 HSZ 105

Cold bosonic atoms in a $\pi-$flux lattice: a superfluid with orbital antiferromagnetic order — •Stephan Rachel and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe

We consider a system of neutral, bosonic atoms on a square lattice subject to an artificial magnetic field. We focus on a field strength of half a Dirac flux quantum through every plaquette, which implies two minima in the lower single particle band. For repulsive interactions, we show that the many particle ground state possesses both superfluid and orbital antiferromagnetic order. For attractive interactions, we find a fragmented Bose–Einstein condensate without net orbital currents.

TT 41.6 Thu 15:15 HSZ 105

Condensate density of interacting Bosons at finite temperature: A Functional Renormalization Group calculation — •Christopher Eichler[1], Nils Hasselmann[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue-Straße 1, 60348 Frankfurt, Germany — [2]International Center for Condensed Matter Physics, Universidade de Brasilia, Caixa Postal 04667, 70910-900 Brasilia,DF, Brazil

We use the Functional Renormalization Group to study thermodynamics of 3-dimensional interacting bosons at finite temperature. Our calculation is based on a truncated vertex expansion and a momentum independent two-body interaction including wave function renormalization. In particular, we derive the renormalization group flow of the condensate density in the symmetry broken phase and explicitly calculate the critical exponent β. Our result for β agrees quite well with the accepted numerical value for the 3-dimensional XY universality class.

15 min. break

TT 41.7 Thu 15:45 HSZ 105

Bose-Fermi Mixtures in Optical Lattices — •Irakli Titvinidze, Michiel Snoek, and Walter Hofstetter — Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt, Germany

We study a mixture of strongly interacting bosons and fermions with on-site repulsion in optical lattices. We apply the generalized dynamical mean-field theory (GDMFT), which is exact in the infinite dimensions and reliably describes the full range from weak to strong coupling. First we consider spinless fermions. We perform calculations for commensurate filling of the fermions and bosons, in particular for the case when the fermions are half-filled, whereas the filling of the bosons is 3/2. Our calculations show two different Alternating Mott insulator (AMI) phases, in which the bosons are localized, but particle density wave order occurs. These two AMI phases are separated by a supersolid phase, where bosonic superfluidity coexists with large-amplitude particle density wave order. Furthermore we consider a mixture of two-component fermions and hard-core bosons, both at half-filling. In this case in addition to the supersolid and the AMI phase, we also obtain an antiferromagnetic phase.

TT 41.8 Thu 16:00 HSZ 105

Bose-Fermi Mixtures in Disordered Optical Lattices — •Denis Semmler, Irakli Titvinidze, Ulf Bissbort, and Walter Hofstetter — Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany

We study strongly interacting bosons and fermions in an optical lattice with correlated on-site disorder. For this purpose we use a stochastic, generalized DMFT scheme, treating the fermions within the well-known dynamical mean-field theory (DMFT) and describing the bosons by the Gutzwiller mean-field theory. This scheme becomes exact in the limit of infinite dimensions. In order to investigate localization phenomena we use the geometric average of the fermionic density of states as well as the geometrically averaged bosonic superfluid order parameter. Our investigation focuses on the influence of the fermions on the bosonic phase diagram, consisting of the Bose glass phase, the Mott insulator and the superfluid. We consider the corresponding fermionic phases, Mott insulator, Anderson insulator and disordered Fermi liquid, as well. The results are related to experimental parameters.

TT 41.9 Thu 16:15 HSZ 105

Real-Space Dynamical Mean-Field Theory for Strongly Correlated Atoms — •Michiel Snoek, Irakli Titvinidze, and Walter Hofstetter — Institut für Theoretische Physik, Goethe-Universitaet Frankfurt

To describe strongly interacting atoms in an inhomogeneous optical lattice, we apply Real-Space Dynamical Mean-Field Theory (R-DMFT). R-DMFT captures the effects of strong correlations and spatial inhomogeneity in a unified, non-perturbative framework. Local correlations are taken into account exactly.

We apply this numerical scheme to antiferromagnetic states of repulsively interacting fermions with spin 1/2 in a harmonic potential. Within R-DMFT, antiferromagnetic order is found to be stable in spatial regions with total particle density close to one, but persists also in parts of the system where the local density significantly deviates from half filling. In systems with spin imbalance, we find that antiferromagnetism is gradually suppressed and phase separation emerges beyond a critical value of the spin imbalance.

We also investigate trapped Bose-Fermi mixtures in an optical lattice with R-DMFT. We look for the effect of the fermions on the bosonic visibility and analyze the stability of a supersolid in an harmonic trap.

TT 41.10 Thu 16:30 HSZ 105

Trionic liquids in exact diagonalization — •Guido Klingschat and Carsten Honerkamp — TP1, Universität Würzburg

Lattice fermions with three internal degrees of freedom ('colors') exhibit a trionic phase with conglomerates of 3 fermions on a single site if the onsite attraction between the different colors is strong enough. Using excact diagonalization we establish an effective Hamiltonian describing these fermionic quasiparticles. The effective theory is validated by a finite size scaling in the low density limit. The stability of the trion phase against breaking of the global SU(3)-symmetry is investigated for asymmetric interactions as well as for different densities per color. Furthermore we compare the trion behavior for one and two lattice dimensions.

TT 41.11 Thu 16:45 HSZ 105

Asymmetric Hubbard Model for Ultracold Fermi-Mixtures on Optical Lattices — •Tobias Gottwald and Peter van Dongen — KOMET 337, Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz

In order to understand the phases occurring in ultracold Fermi-Mixtures we perform a mean-field analysis beyond LDA of an attractive-U Hubbard model with asymmetric hopping $t_\uparrow \neq t_\downarrow$ and a superimposed parabolic trapping potential. Depending on population numbers and on the asymmetry of the hopping we expect charge-density-wave-, BCS- or FFLO-states to minimize the relevant thermodynamic potential. By tuning the asymmetry in the hopping term we can switch between standard Hubbard model physics, where only superfluidity occurs, and Falikov-Kimball model physics, where only CDW-behaviour occurs.

TT 41.12 Thu 17:00 HSZ 105

Quantum critical behavior in strongly interacting Rydberg gases — •Hendrik Weimer[1], Robert Löw[2], Tilman Pfau[2], and Hans Peter Büchler[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart — [2]5. Physikalisches Institut, Universität Stuttgart

We analyze the van der Waals blockade and the quantum evolution of an atomic gas resonantly driven by a laser into a strongly interacting Rydberg state. The main mechanism behind the van der Waals blockade is that once a Rydberg atom is excited, the van der Waals interaction shifts the surrounding atoms out of resonance with the driving laser and therefore suppresses the excitation of additional Rydberg atoms. We show that the system is close to the critical point of a second order phase transition and can be described by a universal scaling function with a critical exponent. We present an effective dynamical theory for the scaling function that provides excellent agreement with a numerical solution of the full Schrödinger equation.

[1] H. Weimer, R. Löw, T. Pfau, H. P. Büchler, Phys. Rev. Lett. **101**, 250601 (2008).

15 min. break

TT 41.13 Thu 17:30 HSZ 105

Quantum trajectories for dispersive readout in superconducting circuit QED — •Ferdinand Helmer and Florian Marquardt — Department of Physics, CeNS, and ASC, Ludwig-Maximilians-Universität, Theresienstrasse 37, D-80333 Munich, Germany

We present applications for the method of quantum trajectory simulations for the realistic simulation of single-shot readout experiments in superconducting circuit QED. Quantum trajectories generated by stochastic master equations allow to obtain a realistic measurement signal while one simultaneously gains access to the internal quantum dynamics of the system in question taking the measurement backaction into account correctly. Thus, useful insights beyond the ensemble average description of a conventional master equation can be obtained.

To illustrate the power of the method, we present two important examples: (i) How to detect single itinerant microwave photons non-destructively (ii) How to generate massively entangled N-qubit states like W- and GHZ-states by measurement. We point out the presented examples can be realized using currently available experimental setups.

TT 41.14 Thu 17:45 HSZ 105

Meissner effect in atom chips containing superconducting microstructures — •Daniel Cano, Brian Kasch, Helge Hattermann, Reinhold Kleiner, Claus Zimmermann, Dieter Koelle, and József Fortágh — Physikalisches Institut & Center for Collective Quantum Phenomena, Universität Tübingen, Germany

Superconducting microstructures for trapping and manipulating ultracold quantum gases are expected to provide intriguing physical scenarios in which atomic physics and superconductor science converge. In this study, we investigate the impact of the Meissner effect on magnetic microtraps generated by superconducting microstructures. Both numerical simulations and experiments demonstrate that the Meissner effect shortens the distance between the microtrap and the superconducting surface, reduces the radial magnetic-field gradients and lowers the trap depth. Simulations based on the London theory have been carried out to calculate the supercurrent densities in thin-film microstructures. Experiments were done in a recently-built apparatus that loads ultracold ^{87}Rb atomic clouds into a magnetic microtrap generated by a superconducting Nb wire with circular cross section. By monitoring the position of the atomic cloud, we observe how the Meissner effect changes the microtrap parameters. Measurements of the trap position reveal a complete exclusion of the magnetic field from the superconducting wire for $T < 6\,\mathrm{K}$. For higher T, the magnetic field partially penetrates the superconducting wire and the microtrap parameters become more similar to those expected for a normal-conducting wire.

[1] D. Cano *et al.*, Phys. Rev. Lett. **101**, 183006 (2008)

TT 41.15 Thu 18:00 HSZ 105

Propagation of a wave packet in the presence of random scattering and nonlinearity — •Georg Schwiete[1,2] and Alexander Finkel'stein[1,2] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, 76100, Israel — [2]Department of Physics, Texas A&M University, College Station, TX 77843-4242, US

We address the problem of propagation of an injected wave-packet in a random potential in the presence of nonlinear interactions in two spatial dimensions. This problem is relevant for studies of Anderson localization in photonic lattices or for the expansion of Bose-Einstein condensates in the presence of disorder. Our starting point is the Gross-Pitaevskii equation (nonlinear Schroedinger equation) with a disorder potential. We derive a system of coupled equations that describes the spreading of the average density.

TT 41.16 Thu 18:15 HSZ 105

Quantum Dynamics of Optomechanical Systems — •Max Ludwig, Björn Kubala, and Florian Marquardt — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München,Theresienstr 37, D-80333 München, Germany

A generic optomechanical system consists of a driven optical cavity and a movable mirror attached to a cantilever. Recently, a new kind of optomechanical system has been realized by replacing the cantilever by a cloud of cold atoms located inside a cavity.

A common feature of optomechanical systems is the instability they can exhibit towards a regime where the mechanical oscillator settles into self-sustained oscillations. We analyze the quantum dynamics of these self-sustained oscillations using a master equation approach applied to the coupled system consisting of the cavity mode and the mechanical oscillation. When a suitable "quantum parameter" is sent to zero, these results converge towards the predictions of the classical theory of the instability. By contrast, for a large value of the quantum parameter the system is strongly influenced by quantum fluctuations.

Optomechanical systems involving the motion of ultracold atoms exhibit very large values of the quantum parameter and are hence expected to show substantial quantum effects. We discuss some prospects that open up for such kind of setups.

TT 41.17 Thu 18:30 HSZ 105

Solids and Supersolids of Three-Body Interacting Polar Molecules on an Optical Lattice — Kai P. Schmidt[1], Julien Dorier[2], and •Andreas Läuchli[3] — [1]Lehrstuhl für theoretische Physik I, TU Dortmund, Dortmund, Germany — [2]CTMC, EPFL, Lausanne, Switzerland — [3]MPI für Physik komplexer Systeme, Dresden, Germany

We study the physics of cold polar molecules loaded into an optical lattice in the regime of strong three-body interactions, as put forward recently by Büchler et al. [Nature Phys. 3, 726 (2007)]. To this end, quantum Monte Carlo simulations, exact diagonalization, and a semiclassical approach are used to explore hard-core bosons on the 2D square lattice which interact solely by long-ranged three-body terms. The resulting phase diagram shows a sequence of solid and supersolid phases. Our findings are directly relevant for future experimental im-

plementations and open a new route towards the discovery of a lattice supersolid phase in experiment.

TT 41.18 Thu 18:45 HSZ 105

Phase Diagram of Polar Molecules with Three-Body Interactions — •Lars Bonnes, Stefan Wessel, and Hans-Peter Büchler — Institut für theoretische Physik III, Universität Stuttgart

Motivated by a recent proposal on using polar molecules in optical lattices driven by microwave fields to induce strong three-body interactions (H. P. Büchler et al., Nature Physics 3, 726 (2007)), we analyze the quantum phase diagram of the boson Hubbard model with dominant nearest neighbor three-body repulsions using quantum Monte Carlo simulations. In particular, we consider the case of a honeycomb-lattice in the hard-core limit. In contrast to previously studied cases of the chain and the square lattice, three-body repulsions on the honeycomb lattice exhibit clear characteristics of strongly frustrated interactions, giving rise to macroscopically degenerate classical regions and quantum state selections via order-by-disorder phenomena. We discuss the nature of the emerging insulating phases at several unconventional lattice fillings, and compare to effective low-energy descriptions, such as in terms of quantum dimer models.

TT 42: Correlated Electrons: Low-dimensional Systems - Models 2

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

TT 42.1 Thu 14:00 HSZ 301

Universal dephasing in a chiral 1D interacting Fermion system — •Clemens Neuenhahn and Florian Marquardt — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig Maximilians Universität München

We consider dephasing by interparticle interactions in a one-dimensional chiral Fermion system[1]. Such systems are realized by the edge states in the integer Quantum Hall Effect, which are used for the experimental realization of an electronic Mach-Zehnder interferometer. We calculate the spatial decay of the single particle Green's function for fixed energy, which determines the interference contrast of the interferometer. Thereby, the finite range of the interaction potential is taken into account. Drawing on both the known exact bosonization solution and a physically transparent semiclassical approach, we show that at high energies the asymptotic decay of the Green's function with increasing propagation length becomes universal: At zero temperature, for smooth interaction potentials, we obtain a power-law decay with an exponent 1, independent of the interaction strength. We comment on how the non-interacting limit is recovered and obtain the dephasing rate at finite temperature. Introducing an effective noise spectrum acting on the propagating electron, we address the physical mechanism of decoherence in the high-energy limit. [1] C. Neuenhahn and F. Marquardt, arXiv:0806.1211 (2008).

TT 42.2 Thu 14:15 HSZ 301

Even-odd Effects in Short Antiferromagnetic Heisenberg Chains — •A. Machens[1], O. Waldmann[1], I. Schneider[2], and S. Eggert[2] — [1]Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany — [2]Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

We have recently studied the magnetic properties of Cr_6 and Cr_7 molecular horseshoes by magnetometry and inelastic neutron scattering [1,2]. These molecules could be identified as chains of six or seven $s = 3/2$ spins, respectively, with antiferromagnetic nearest-neighbor Heisenberg exchange interactions. The analysis of the energy spectra has revealed a striking difference for even and odd chains: For the odd chain the energy $E(S)$ of the lowest state for each total spin S closely follows $E(S) \propto S(S+1)$, while for the even chain a strong renormalization is found at small values of S. Numerical exact diagonalization of the Heisenberg Hamiltonian for chains of different lengths N and spins s has confirmed this difference. We will present a more general understanding of this phenomenon by symmetry considerations, application of valence bond techniques and comparison with an effective Hamiltonian. This Hamiltonian will be modified depending on the couplings and symmetries of the chains.

[1] S. T. Ochsenbein *et al.*, Europhys. Lett. 79, 17003 (2007).
[2] S. T. Ochsenbein, *et al.*, Chem. Eur. J. 14, 5144 (2008).

TT 42.3 Thu 14:30 HSZ 301

First principles perspective on the microscopic model for Cs_2CuCl_4 — •Kateryna Foyevtsova, Yuzhong Zhang, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

We investigate the microscopic model for the frustrated layered antiferromagnet Cs_2CuCl_4 by performing *ab initio* density functional theory (DFT) calculations and with the help of the downfolding and tight-binding methods. The combination of these methods provide the relevant interaction paths in this material, and we estimate the corresponding exchange constants. We find for Cs_2CuCl_4 that the choice of the structural optimisation scheme within DFT is crucial for the correct evaluation of the exchange constants. We discuss the DFT-derived model by comparing our results with the exchange constants estimated from the neutron scattering data and by analyzing the ability of both theoretical and experimental models to reproduce the measured magnetic properties.

TT 42.4 Thu 14:45 HSZ 301

Effective low-energy theory for the kagomerized Kitaev model — •Michael Kamfor[1], Julien Vidal[2], Sébastien Dusuel[3], and Kai Phillip Schmidt[1] — [1]Technische Universität Dortmund Lehrstuhl für Theoretische Physik I, Germany — [2]Université Pierre et Marie Curie Paris 06, France — [3]Lycée Saint-Louis, 75006 Paris, France

The Kitaev model on the honeycomb lattice is a two-dimensional quantum spin model containing abelian and non-abelian anyonic excitations [1]. The effective low-energy theory in the abelian gapped phase is the celebrated toric code relevant for topological quantum computation [2][3]. The usually studied limit of isolated dimers leads to an effective square lattice. The ground state is in the vortex-free sector. Excitations are low-energy abelian anyons and high-energy fermions. Here we study a different limit of isolated dimers giving rise to an effective Kagome lattice. We obtain the low-energy physics of the gapped phase in terms of abelian anyons on triangle and honeycomb plaquettes of the Kagome lattice using perturbative continuous unitary transformations [3][4]. The full phase diagram is calculated exactly by Majorana fermionization. Interestingly, the spectrum is always gapped except at the isotropic point. As a consequence, the non-abelian phase present in the usual honeycomb Kitaev model is reduced to a single point.

[1] A. Kitaev, Ann. Phys. (N.Y.) 303, 2 (2003).
[2] A. Kitaev, Ann. Phys. (N.Y.) 321, 2 (2006).
[3] K. P. Schmidt, S. Dusuel, and J. Vidal, Phys. Rev. Lett. 100, 057208 (2008).
[4] J. Vidal, K. P. Schmidt, and S. Dusuel, arXiv:0809.1553, accepted for Physical Review B.

TT 42.5 Thu 15:00 HSZ 301

Effective models for Mott insulating phases in frustrated Hubbard models — •Hong-Yu Yang[1], Andreas Laeuchli[2], Frederic Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany — [2]Max Planck Institut für Physik komplexer Systeme, Nöthnitzerstr. 38, 01187 Dresden, Germany — [3]Institute for theoretical Physics, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland

We derive effective quantum spin models models for a frustrated t-t'Hubbard model on the square lattice using perturbative continuous unitary transformations. For large U the effective Hamiltonian at half filling contains only a nearest-neighbor Heisenberg interaction giving rise to long-range ordered antiferromagnetic phases. Limiting cases are the unfrustrated square lattice (t'=0) with a Neel ordered ground state and the triangular lattice (t'=t) having a 120-degree three-sublattice order. In the unfrustrated case it is known that corrections at finite U, e.g. ring-exchange couplings or Heisenberg interactions of longer range, do not destabilize the Neel-ordered ground state. Only in the limit of small U a metallic phase is stable. In this sense one has a

hard Mott insulator. In our study we investigate the question whether corrections in the frustrated case stabilize an intermediate spin liquid phase between the long-range ordered antiferromagnetic phase at large U and the metallic phase at small U. This case would be called a soft Mott insulator. We tackle this problem by solving the effective model obtained by continuous unitary transformations using exact diagonalization.

TT 42.6 Thu 15:15 HSZ 301

Momentum classification of SU(n) spin chains with arbitray representations using Young Tableaux — •Burkhard Scharfenberger and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe

Recently, Schuricht and one of us [Phys. Rev. Lett. 98, 237202(2007)] established a correspondence between the Young tableaux classifying the total spin representations of N SU(n) spins and eigenstates of the SU(n) Haldane–Shastry model for a chain of N sites. As a side product, this correspondence provides a direct link between total spin and total linear momentum content of the representations for spin chains with individual spins transforming under fundamental representations of SU(n) in general, i.e. the formalism can be used to read of directly how many of the total spin singlets have total momentum zero and so on. Here, we introduce a general tableau formalism for combining N spins transforming under an *arbitrary* representation of SU(n) into representations of total spin, with which we establish a set of rules how to obtain the linear momentum content of these representations for spin chains with N sites. The perspective goal of these studies is to set up a formalism to perform exact diagonalization studies of spin rotationally invariant models of spin chains (and eventually arbitrary lattices) in Hilbert space subspaces with both well defined total momentum (quantum numbers under lattice symmetries) and total spin.

TT 43: Correlated Electrons: Heavy Fermions 2

Time: Thursday 15:45–18:45 Location: HSZ 301

TT 43.1 Thu 15:45 HSZ 301

Cerium iron oxypnictides: from a heavy fermion system to the parent compound for high-Tc superconductivity — •Anton Jesche, Cornelius Krellner, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Within the layered FeAs systems the CeFePnO (Pn = As, P) compounds offer the unique possibility to study the interplay between strong 3d correlation effects connected with peculiar features of the FeAs layers and strong 4f correlation effects due to interaction between conduction and Ce 4f electrons. Thus we recently showed that CeFePO is a paramagnetic heavy fermion system likely close to a ferromagnetic instability [1] connected with the onset of Ce long range ordering, while Fe is non magnetic. In contrast in CeFeAsO both Fe and Ce orders antiferromagnetically around 140 K and 4 K, respectively, Ce being in a magnetic stable trivalent state due to the larger unit cell volume. In this compound F-doping lead to the suppression of Fe ferromagnetic ordering and to the formation of a superconducting state with a remarkably high Tc of 41 K [2]. We report on measurements of specific heat, electric resistance and magnetization on single crystalline CeFeAsO and CeFePO, as well as on the alloy system $CeFeAs_{1-x}P_xO$. We shall focus on the effect of P for As substitution on the magnetic ordering of Fe and Ce as well as on the superconductivity. Further on we shall address the relation between the Fe magnetic ordering and the structural distortion in pure CeFeAsO around 150 K.

[1] Phys. Rev. Lett. 101, 117206 (2008).
[2] Phys. Rev. Lett. 100, 247002 (2008).

TT 43.2 Thu 16:00 HSZ 301

Ce and T magnetism in CeTPO compounds (T = Os, Ru, Fe, Co) - Large variety of ground states. — •Cornelius Krellner, Anton Jesche, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

In the last years we have started a detailed investigation of the CeTPO compounds (T = Os, Ru, Fe, Co). These materials correspond to the family of LnTPnO systems, crystallizing in the tetragonal ZrCuSiAs structure-type, which attracts a lot of attention due the observation of high temperature superconductivity (SC) in the doped LnFeAsO compounds. Whereas the 3d-magnetism of the Fe is essentially for the occurrence of SC in LnFeAsO, the magnetism in CeTPO is dominated by the 4f-electrons of Ce^{3+}.

In this contribution, we summarize our results on the single crystal growth of the CeTPO materials together with a thorough physical characterization, including magnetization, susceptibility, resistivity, specific heat, and thermopower. These measurements reveal four different magnetic ground states: (1) CeRuPO is a rare example of a ferromagnetically ordered Kondo-lattice system with $T_C = 15\,\mathrm{K}$ and a Kondo scale of $T_K \sim 10\,\mathrm{K}$; (2) CeOsPO orders antiferromagnetically at $T_N = 4.5\,\mathrm{K}$; (3) CeFePO is a heavy-fermion system on the non-magnetic side of a ferromagnetic instability; (4) CeCoPO present ferromagnetic order of the Co-ions at $T_C = 75\,\mathrm{K}$ and Ce-moments close to magnetism. Therefore, these new materials present a nice playground to study in detail the phenomena of strongly correlated electron systems.

TT 43.3 Thu 16:15 HSZ 301

Field induced phases in the antiferromagnet UPt_2Si_2 — •Matthias Bleckmann[1], Dirk Schulze Grachtrup[1], Stefan Süllow[1], Britta Willenberg[1], Marek Bartkowiak[2], Harison Rakoto[3], and John A. Mydosh[4] — [1]Institut für Physik der Kondensierten Materie, Braunschweig, Germany — [2]Hochfeld-Magnetlabor Dresden, Germany — [3]National Pulsed Magnetic Field Laboratory , Toulouse, France — [4]Institute of Physics II, Köln, Germany

Previously, UPt_2Si_2 has been described as a moderately mass enhanced antiferromagnet with a transition temperature of $T_N = 32K$ [1]. In contrast, and more recently, it has been demonstrated that UPt_2Si_2 closely resembles the tetragonal heavy fermion superconductor/hidden order material URu_2Si_2 in various physical properties [2,3].

We present a detailed study of high field magnetization and resistivity on single crystalline UPt_2Si_2. While up to now the high field behavior of UPt_2Si_2 was discussed in terms of a crystalline electric field scheme applied to an f electron local moment system [4], we show that the high field behavior is much more complex than previously thought. In particular, the magnetic phase diagrams derived from our measurements contain various field induced phases, again analougous to URu_2Si_2. We compare the phase diagrams of both systems and discuss possible scenarios accounting for such behavior in UPt_2Si_2.

[1] R. A. Steeman, *et al.*, J. Phys.: Condens. Matter **2**, 4059 (1990).
[2] S. Süllow, *et al.*, J. Phys. Soc. Japan **77**, 024708 (2008).
[3] N. Johannsen, *et al.*, Phys. Rev. B **78**, 121103(R) (2008).
[4] G. J. Nieuwenhuys, Phys. Rev. B **35**, 5260, (1987).

TT 43.4 Thu 16:30 HSZ 301

Non-Fermi-Liquid Behaviour in $CaCu_3Ru_4O_{12}$ Studied by Nuclear Magnetic Resonance — •Wolfgang Krätschmer[1], Heiko Dekinger[1], Norbert Büttgen[1], Alois Loidl[1], Axel Günther[1], Alexander Krimmel[1], and Ernst-Wilhelm Scheidt[2] — [1]Experimentalphysik 5, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Deutschland — [2]CPM, Universität Augsburg, 86135 Augsburg, Deutschland

We present a detailed study of the electronic properties of $CaCu_3Ru_4O_{12}$ which has perovskite structure and shows strong electron correlations. Beside magnetic susceptibility, transport and specific heat data, we focus on NMR and NQR measurements at the copper and ruthenium sites in this compound [Krimmel et al., PRB 78, 165126 (2008)]. $CaCu_3Ru_4O_{12}$ is a metallic system showing non-Fermi-liquid behaviour below 2K which becomes manifest in a logarithmic increase of the specific heat $C_p/T \propto -ln(T)$ and in an NQR spin-lattice relaxation rate $1/T_1(T)$ that deviates from the Korringa law at the copper site only. Static NMR measurements were conducted to extract electric field gradients for the correction of the low-temperature specific heat data for nuclear contributions. Nuclear contributions turned out to be not sufficient to account for the Schottky-anomaly. Further investigation of the spin-lattice relaxation at the ruthenium site reveals a clearly different behaviour in comparison to the copper site and reflects the local character of the strong electron

correlations.

TT 43.5 Thu 16:45 HSZ 301

Electronic Correlations and Non-Fermi-Liquid Behaviour in $ACu_3Ru_4O_{12}$–Perovskites — •Axel Günther[1], Alexander Krimmel[1], Alois Loidl[1], Wolfgang Krätschmer[1], Heiko Dekinger[1], Norbert Büttgen[1], Ernst-Wilhelm Scheidt[2], Denis Sheptyakov[3], and Hannu Mutka[4] — [1]Experimentalphysik 5, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Deutschland — [2]CPM, Institut für Physik, Universität Augsburg, 86135 Augsburg, Deutschland — [3]Labor für Neutronenstreuung, ETHZ & PSI, 5232 Villigen PSI, Schweiz — [4]Institut Laue Langevin, 38042 Grenoble Cedex 9, France

Among the large variety of $AC_3B_4O_{12}$–type perovskites, the copper–ruthenates (C = Cu, B = Ru) form a subclass exhibiting strongly correlated electron behaviour. A special feature of these compounds is that the ideal stoichiometry and structure is preserved for a large number of different A–site cations with different valence states. We have systematically studied the electronic properties by specific heat, magnetic susceptibility, transport, NMR/NQR and neutron scattering experiments. The compound A = Ca is a correlated metal showing non–Fermi–liquid behaviour below 2K, as indicated by a logarithmic increase of the specific heat and deviations from a Korringa behaviour of the spin lattice relaxation rate. In the case of A = Pr, an anomaly in the specific heat occurs at 0.5K whose maximum shifts to higher temperatures with increasing magnetic field. Along with data acquired from inelastic neutron scattering we obtain strong indications for a pronounced crystal field splitting.

TT 43.6 Thu 17:00 HSZ 301

Exotic Ground State of $CeRu_4Sn_6$ Investigated by Means of Specific-Heat and NMR — •Eva Maria Brüning[1], Manuel Brando[1], Michael Baenitz[1], André Strydom[2], Russel E. Walstedt[3], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik Fester Stoffe, Dresden, Germany — [2]Physics Department, University of Johannesburg, South Africa — [3]Physics Department, University of Michigan, MI, USA

The tetragonal compound $CeRu_4Sn_6$ is a narrow-gap semi-metal and shows no phase transition down to 50 mK. We performed field-sweep ^{119}Sn NMR measurements at different frequencies (47, 70, 100 and 119 MHz) down to 2 K as well as specific-heat measurements in magnetic fields up to 10 T and temperatures down to 65 mK. The spin-lattice-relaxation rate $1/T_1$ in the high-T range (300 K to 20 K) is field independent and could be consistently fitted with a model for a narrow gap semi-metal ($1/T_1 \propto T\exp(-\Delta/k_BT)$) with a gap of $\Delta/k_B \simeq 30$ K. This confirms the results from resistivity and thermopower measurements. Below 10 K, $1/T_1$ becomes strongly field dependent, whereas higher fields lead to a stronger reduction of $1/T_1$. The low-T range could be fitted with an activated behavior ($1/T_1 \propto \exp(-\Delta/k_BT)$), where Δ/k_B increases with increasing field. This scenario is strongly supported by specific-heat investigations. Both results can be described consistently by assuming a double Cauchy-Lorentz function for the residual in-gap density of states $N(E)$. The ground state is governed by these correlated states which show Zeeman-type splitting in magnetic fields.

15 min. break

TT 43.7 Thu 17:30 HSZ 301

Electronic structure and thermodynamic properties of $CeRh_2Sn_4$ — •Monika Gamża[1,2], Walter Schnelle[1], Roman Gumeniuk[1], Yuri Prots[1], Andrzej Slebarski[2], Helge Rosner[1], and Yuri Grin[1] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Institute of Physics, University of Silesia, Katowice, Poland

Compounds of the system Ce–Rh–Sn have attracted a considerable attention due to a variety of strongly correlated electron phenomena, including valence fluctuations, non-Fermi liquid behavior, heavy fermion states and magnetism with reduced moments [1, 2]. Some of these systems show also evidence for spin fluctuations due to the Rh 4*d* electrons [2].

Here, we present a combined study of the electronic structure and thermodynamic properties of $CeRh_2Sn_4$. The crystal structure has been determined from single crystal diffraction experiments. The Ce core-level XPS and Ce L_{III} XAS spectra unanimously indicate a stable $4f^1$ configuration of the Ce ions. Thermodynamic measurements show a magnetic phase transition at $T_N \approx 3.16$ K. The ground state magnetic structure is of a noncollinear antiferromagnetic type. There are clear indications for spin fluctuations in the thermodynamic data. A Fermi surface analysis reveals some parallel sections of the sheets, which could generate nesting instabilities and be responsible for the spin fluctuations.

[1] Ślebarski A *et al*. Philos. Mag. B (2002) **82** 943;
[2] Gamża M *et al*. J. Phys.: Condens. Matter (2008) **20** 025201; Ślebarski A *et al*. Phys. Rev. B (2006) **73** 2051105

TT 43.8 Thu 17:45 HSZ 301

Polarization dependent Ce-M_{45} x ray absorption spectroscopy on the giant crystal-field material $CeRh_3B_2$. — •P.O. Körner[1], A. Severing[1], T. Willers[1], Z. Hu[1], N. Hollmann[1], H. Fujiwara[1], H.-J. Lin[2], C.T. Chen[2], P. Lejay[3], and L.H. Tjeng[1] — [1]Institute of Physics, II University of Cologne — [2]NSRRC, Taiwan — [3]Institut Néel, CNRS, Grenoble

The hexagonal compound $CeRh_3B_2$ exhibits exceptional magnetic properties ($T_C = 115$ K, $\mu_{ord} = 0.4\mu_B$) [1 and references therein]. The crystal-field splitting in this material is of the order of the spin orbit splitting so that the Steven's approximation is no longer valid. Neutron scattering combined with magnetization suggests a crystal-field level scheme where the intermixing of the higher lying multiplet contributes substantially to the ground state [1]. We have investigated the crystal-field splitting in $CeRh_3B_2$ with soft-x-ray absorption spectroscopy at the Ce-M_{45} edges. This technique is sensitive to the symmetry of the initial state and through the polarization dependence direct spectroscopic information about the $|J_z\rangle$ admixtures of the ground state is obtained [2]. In contrast to previous linear dichroism studies by Jo et al. we are taking the full crystal-field symmetry into account [3]. Our results for the ground state are consistent with [1], but we find a different level scheme providing better understanding of the anisotropies.

[1] F. Givord et al. J. Phys. Condens. Mater **19,** 506210 (2007).
[2] P. Hansmann et al. , Phys. Rev. Lett. **100,** 066405 (2008).
[3] T. Jo, Prog. Theor. Phys. Suppl. **101,** 303 (1990) and T. Jo and S. Imada, J. Phys. Soc. Jpn. **59,** 2312 (1990)

TT 43.9 Thu 18:00 HSZ 301

Investigation of the crystal-field ground state of $YbInNi_4$ with polarization dependent Yb-M-edge x ray absorption spectroscopy. — Peter Körner[1], •Andrea Severing[1], Thomas Willers[1], Zhiwei Hu[1], Nils Hollmann[1], Detlef Schmitz[2], Zachary Fisk[3], Andrea Bianchi[3], and Liu Hao Tjeng[1] — [1]Institute of Physics II, University of Cologne — [2]BESSY Berlin — [3]University of California, Irvine, USA

$YbInNi_4$ serves as a stable valent reference sample for $YbInCu_4$ which undergoes a first order valence transition as function of temperature. Although intensively studied in the past, the crystal-field ground state of $YbInNi_4$ remained a matter of debate [1-4]. We will present our investigations of the crystal-field ground state of $YbInNi_4$ with soft-x-ray absorption spectroscopy at the Yb-M-edge. Soft-x-ray absorption spectroscopy is sensitive to the symmetry of the initial state and through the polarization dependence direct spectroscopic information about the $|J_z\rangle$ admixtures of the ground state [5] can be obtained. However, since $YbInNi_4$ is cubic, a polarization effect can only arise when a magnetic field is applied to split up the crystal-field states. We will show that the *induced linear dichroism* allows to distinguish between the various ground state possibilities.

[1] A. Severing et al., Physica B **163,** 409 (1990).
[2] J.L. Sarrao et al., Phys. Rev. B **57,** 7785 (1998).
[3] P.G. Pagiuso et al., Phys. Rev. B **63,** 144430 (2001).
[4] T. Park et al. Phys. Rev. Lett. **96,** 046405 (2006).
[5] P. Hansmann et al. , Phys. Rev. Lett. **100,** 066405 (2008).

TT 43.10 Thu 18:15 HSZ 301

Narrow gap and electron correlation effects in $FeSb_2$ — •Peijie Sun[1], Niels Oeschler[1], Simon Johnsen[2], Bo B. Iversen[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Chemistry, University of Aarhus, Denmark

Heavy-fermion, or alternatively correlated, semiconductors are of both fundamental and practical interest due to their narrow energy gap and correlated bands at the gap edges. This talk will focus on $FeSb_2$, a new *d*-based correlated semiconductor showing thermodynamics and band structure similar to FeSi. Correlated electrons in $FeSb_2$ manifest themselves in many physical properties like specific heat, magnetic susceptibility, and optical spectra. In particular, we will show a huge thermoelectric response in $FeSb_2$ below 50 K [1] which is also

attributed to the correlated gap. Different to FeSi, a second energy gap (<100 K) was confirmed to be intrinsic to $FeSb_2$ by electrical, thermal transports and specific heat measurements. This largely contributes to the extraordinarily enhanced thermoelectricity at the same temperature range. Comparison of $FeSb_2$ to its Ru and As substituted homologues will be also presented.

[1] A. Bentien et al, Europhys. Lett. 80 (2007) 17008.

TT 43.11 Thu 18:30 HSZ 301

X-ray Absorption Spectroscopy of the Narrow Gap Semiconductor $FeSb_2$ — •N. Hollmann[1], Z. Hu[1], C. Chang[1], J. Gegner[1], S. Johnsen[2], B.B. Iversen[2], J.C. Cezar[3], N. Brookes[3], H.H. Hsieh[4], H.-J. Lin[4], C.T. Chen[4], P. Sun[5], N. Oeschler[5], F. Steglich[5], and L.H. Tjeng[1] — [1]II.Physikalisches Institut, University of Cologne — [2]Department of Chemistry, University of Aarhus, Denmark — [3]ESRF, Grenoble, France — [4]NSRRC, Hsinchu, Taiwan — [5]MPI for Chemical Physics of Solids, Dresden

$FeSb_2$ recently attracted much attention due to the observation of extremely large values of the Seebeck coefficient $S \sim -45000\mu VK^{-1}$ at 10K and the thermoelectric power $S^2\rho^{-1} = 2300\mu WK^{-2}cm^{-1}$ at 12K, the latter being a record high [1]. The material is being discussed in the framework of a Kondo insulator model with similarities to FeSi. $FeSb_2$ exhibits a diamagnetic to paramagnetic crossover at $\approx$ 100K. The ground state was proposed to have the non-magnetic d^4 configuration. Contrary to that, band structure calculations predict a d^6 configuration for the Fe. If true, this could suggest a different scenario with similarities to that of $LaCoO_3$ [2]. By now, no experimental data exists to prove the valency of the Fe ion. We have performed X-ray absorption spectroscopy on $FeSb_2$, as it is an ideal technique to study the valence and the spin state. The spectra directly show the valency for the Fe. Temperature-dependent linear dichroism and magnetic circular dichroism data will be discussed in the talk.

[1] A. Bentien *et al.*, Europhys. Lett. **80**, 17008 (2007).
[2] M.W. Haverkort *et al.*, Phys. Rev. Lett. **97**, 176405 (1996).

TT 44: Transport: Quantum Coherence and Quantum Information

Time: Thursday 14:00–19:15 Location: HSZ 304

TT 44.1 Thu 14:00 HSZ 304

Entanglement in driven spin chains — •David Zueco, Fernando Galve, Sigmund Kohler, and Peter Hänggi — Institut für Physik, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany

One-dimensional spin chains are ubiquitous in condensed matter physics and represent one of the basic models in quantum information. Therefore, insight to their behavior is rather valuable and, eventually, allows the development of methods for controlling their dynamics. Among a variety of tasks, the directed transfer of quantum entanglement through the chain presents an important challenge. In this sense we could use them as "quantum wires" pretty much like copper wires carrying electrons in the electrical circuits.

In this talk we present our recent results on the generation and control of entanglement dynamics in 1D driven spin chains. We demonstrate the feasibility of generating entanglement between the first and the last spin of a chain via applied time-dependent fields [1]. Moreover, once the entanglement has been created, the driving even allows further control of its dynamics. In particular we propose guiding entanglement into a direction of choice, which corresponds to a rectification of quantum information transfer. Finally, we will discuss how to quench the dynamics in order to preserve the entanglement during a substantial time interval.

[1] F. Galve, D. Zueco, S. Kohler, E. Lutz, and P. Hänggi arXiv:0809.3712

TT 44.2 Thu 14:15 HSZ 304

Electron and nuclear spins in double quantum dots — •Björn Erbe and John Schliemann — Institute for Theoretical Physics, University of Regensburg

Apart from fundamental interest, double quantum dots play a central role in the realization of solid state quantum computers. In the relevant set-ups, the spins of the confined electrons are controllable coupled to each other and, via hyperfine interaction, to the surrounding nuclear spins. On the one hand these can be regarded as a decohering environment for the electron system, on the other one they themselves can serve as a quantum information processing resource [1,2].

Just like the well-studied Gaudin type Hamiltonian of a single quantum dot [3], in general the Hamiltonian of a double quantum dot is very difficult to treat. We will present analytical as well as numerical results concerning simplications of the full Hamiltonian, appropriate for the different roles of the nuclear system.

[1] J.M. Taylor et al., cond-mat/0407640 (2006)
[2] D. Loss and D. DiVincenco, Phys. Rev. A 57, 120 (1998)
[3] J. Schliemann et al., J.Phys.: Condens. Matter 15 (2003) R1809-R1833

TT 44.3 Thu 14:30 HSZ 304

A quantum interface between light and nuclear spins in quantum dots — Heike Schwager, Juan Ignacio Cirac, and •Geza Giedke — Max-Planck-Institut für Quantenoptik, D-85748 Garching

We show how to exploit the hyperfine interaction of an electron in a quantum dot to realize a quantum interface between the polarized nuclear spins in a dot strongly coupled to a high-finesse optical cavity and a traveling-wave optical field. By adiabatically eliminating the electronic degree of freedom different effective couplings can be achieved that enable write-in, read-out, and the generation of entanglement between the nuclei and the output field of the cavity. Such a coherent coupling of flying photonic qubits to stationary matter-based qubits is an essential building block for quantum communication networks.

TT 44.4 Thu 14:45 HSZ 304

Quantum Simulator with Electrons Floating on a Helium Film — •sarah Mostame[1] and Ralf Schuetzhold[2] — [1]MPI-PKS, Dresden, Germany — [2]Fachbereich Physik, Universitaet Duisburg-Essen, Duisburg, Germany

We propose a physical setup that can be used to simulate the quantum dynamics of the Ising model in a transverse field. Building on currently available technology, our scheme consists of electrons which float on a superfluid helium film covering a suitable substrate and interact via Coulomb forces. At low temperatures, the system will stay near its ground state where its Hamiltonian is equivalent to the Ising model and thus shows phenomena such as quantum criticality.

TT 44.5 Thu 15:00 HSZ 304

Spin dehoherence of a heavy hole coupled to nuclear spins in a quantum dot — •Jan Fischer[1], William Anthony Coish[1,2], Denis Bulaev[1,3], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Ontario, Canada — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District, Russia

We theoretically study the interaction of a heavy hole with nuclear spins in a quasi-two-dimensional III-V semiconductor quantum dot and the resulting dephasing of heavy-hole spin states. It has frequently been stated in the literature that heavy holes have a negligible interaction with nuclear spins. We show that this is not the case. In contrast, the interaction can be rather strong and will be the dominant source of decoherence in some cases. We also show that for unstrained quantum dots the form of the interaction is Ising-like, resulting in unique and interesting decoherence properties, which might provide a crucial advantage to using dot-confined hole spins for quantum information processing, as compared to electron spins.

[1] Jan Fischer, W. A. Coish, D. V. Bulaev, and Daniel Loss, Phys. Rev. B 78, 155329 (2008)

15 min. break

TT 44.6 Thu 15:30 HSZ 304

Weak Values in solid state physics — Vadim Shpitalnik[1], Yuval Gefen[1], and •Alessandro Romito[1,2] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

The measurement of any observable in quantum mechanics is a probabilistic process described by the projection postulate. As opposed to projective (strong) measurement, weakly measuring an observable (i.e., measuring it while weakly disturbing the system), provides only partial information on the state of the system. It has been proposed that a weak measurement on pre and post-selected ensembles – i.e. a weak measurement followed by a strong one, where the outcome of the first measurement is kept provided a second post-selected outcome occurs – leads to a weak value [1]. Such a weak value may lie well beyond the range of strong values and may happen to be complex.

Here we study a weak value protocol in the context of a solid state setup, specifically, an electronic Mach-Zehnder interferometry [2] presenting the first specific proposal for full tomography of weak values. We generalization of weak values to non-pure states, and we further analyze the manifestation of many-body physics in the weak value, including finite temperature and shot-noise-like contributions.

[1] Y. Aharonov, D. Z. Albert, L. Vaidman, Phys. Rev. Lett. 60, 1351-1354 (1988).

[2] V. Shpitalnik, Y. Gefen, and A. Romito, Phys. Rev. Lett. 101, 226802 (2008).

TT 44.7 Thu 15:45 HSZ 304

Time-Resolved Measurement of a Charge Qubit — •Georg M. Reuther, David Zueco, Peter Hänggi, and Sigmund Kohler — Institut für Physik, Universität Augsburg, Universitätsstr. 1, 86159 Augsburg

We propose a scheme for monitoring coherent quantum dynamics with good time-resolution and low backaction. It relies on the response of the considered quantum system to a high-frequency ac drive. We find that the phase of the outgoing signal, which can directly be measured in an experiment with lock-in technique, is proportional to the expectation value of a particular system observable. We present explicit results for a charge qubit realized with a Cooper-pair box, where we focus on monitoring coherent oscillations and Landau-Zener transitions.

TT 44.8 Thu 16:00 HSZ 304

$Bi_2Sr_2CaCu_2O_{8+\delta}$ intrinsic SQUIDs as candidates of high-T_c phase qubits — •X. Y. Jin[1], J. Lisenfeld[1,2], Y. Koval[1], A. Lukashenko[1,2], C. Bergmann[1], A. V. Ustinov[1,2], and P. Müller[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse. 1, D-91058 Erlangen, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), Wolfgang-Gaede-Str. 1, D-76131 Karlsruhe, Germany

An intrinsic SQUID is a superconducting ring made of $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal, intercepted by two intrinsic Josephson junction stacks. When biased with dc current, the device is a typical hysteretic dc-SQUIDs with huge inductance. The inductance parameter β_L can be tuned in a wide range between 4 and 30 by changing the height and the cross-section area of the stacks. When a device was coupled with a coil and a Nb readout dc-SQUID, typical rf-SQUID behavior was observed. By applying a proper reset field, quantum escape from a single minimum has been measured on a sample of $\beta_L \sim 10$. The escape rate can be fine-tuned by applying short pulses down to 1 ns, which allows a fast readout technique. With these prerequisites, our experiments have opened the path to directly using these intrinsic SQUIDs as high-T_c phase qubits. The first attempts to measure Rabi oscillations on these devices will be discussed.

TT 44.9 Thu 16:15 HSZ 304

Relaxation of Josephson qubits due to strong coupling to two-level systems — •Clemens Müller and Alexander Shnirman — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

Naturally formed two-level systems (TLS) present in the oxide layer of nm-sized Josephson junctions pose a strong complication in the design of superconducting qubits. Recently an experiment used the coherent dynamics of a strongly coupled TLS to demonstrate its uses as a naturally formed quantum memory [1]. We calculate the effect of strongly coupled TLS on the relaxation rate Γ_1 of the qubit. In addition to providing results for single TLS we analyse the effects of an ensemble of TLS.

[1] M. Neeley at al, Nature Physics **4**, 523 (2008)

TT 44.10 Thu 16:30 HSZ 304

Renormalization of the dephasing by zero point fluctuations — •Swarnali Bandopadhyay[1] and Doron Cohen[2] — [1]Physics Department, Norwegian University of Science and Technology, NO-7491, Trondheim, Norway, — [2]Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel

One of the most fundamental properties of an quantum particle is to maintain its phase-coherence. When an quantum particle is coupled to a fluctuating environment its wave-function gets phase-randomised. During the last decade a controversy has emerged in the mesoscopic literature regarding the role of zero-point-fuctuations (ZPF) in low temperature dephasing. We propose an exactly solvable model for dephasing due to short range scattering with environmental modes in dephasing at low temperature. Unlike the Caldeira-Leggett model where the interaction is with an homogeneous fluctuating field of force, here we consider the environment consisting of infinitely many localized fluctuating modes with (say) Ohmic spectral function and the interaction is local as in "s-scattering". We find that in low temperature ZPF can enhance the inelastic cross-section. Our study shows [Phys. Rev. B 77, 155438 (2008)] we need finite temperature to see the effect. Thus indirectly ZPF might contribute to the dephasing at low temperature.

15 min. break

TT 44.11 Thu 17:00 HSZ 304

Driving-induced bistability in the Jaynes-Cummings model — •Vittorio Peano[1], Vicente Leyton Ortega[2], and Michael Thorwart[3,1] — [1]Universität Düsseldorf — [2]Universidad del Valle, Cali (Colombia) — [3]FRIAS, Universität Freiburg

As a consequence of nonlinearity and external driving, the generalized Jaynes-Cummings model exhibits a dynamical bistability. This can be conveniently investigated by introducing a quasipotential in phase space. We study the dissipative dynamics in this bistable quasipotential by means of a simple Markovian master equation and we interpret the results in terms of a quasiclassical analysis. We prove the existence of a metastable squeezed amplitude state and find resonant and antiresonant behavior of the lineshape in correspondence to multiphoton transitions. They are due to a sizeable occupation of the metastable state. We discuss similarities to the quantum Duffing oscillator [1] and also explain the lineshape of the recently observed vacuum Rabi supersplittings [2] in the superconducting transmon qubit set-up.

[1] V. Peano and M. Thorwart, New J. Phys. **8**, 21 (2006). [2] Lev S. Bishop, J. M. Chow, Jens Koch, A. A. Houck, M. H. Devoret, E. Thuneberg, S. M. Girvin, R. J. Schoelkopf, arXiv:0807.2882.

TT 44.12 Thu 17:15 HSZ 304

Cooling a Micro-Mechanical Resonator by Quantum Back-Action from a Noisy Qubit — •Yingdan Wang[1], Yong Li[1], Fei Xue[2], Kouich Semba[3], and Christoph Bruder[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Electrical Engineering, Technion, Haifa, Israel — [3]NTT Basic Research Laboratories, Atsugi, Japan

We study the different roles of qubit dephasing and relaxation in the process of cooling a mechanical resonator by quantum back-action. With a superconducting flux qubit as a specific example, we show that ground-state cooling of a mechanical resonator is possible under present experimental conditions. Our investigation suggests that the cooling limit is primarily determined by the dissipative nature of the qubit, including both relaxation and dephasing.

TT 44.13 Thu 17:30 HSZ 304

Two-Resonator Circuit QED: A Superconducting Quantum Switch — •Elisabeth Hoffmann[1,2], Matteo Mariantoni[1], Frank Deppe[1,2], Edwin P. Menzel[1], Achim Marx[1], Rudolf Gross[1,2], Frank K. Wilhelm[3], and Enrique Solano[4] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Straße 8, 85748 Garching — [2]Physics Department, TU München, 85748 Garching — [3]University Waterloo, Canada — [4]Universidad del País Vasco-Eurskal Herriko Unibertsitatea, Spain

Coupling different kind of superconducting (sc) qubits to on-chip microwave resonators has strongly advanced the field of circuit QED. Regarding the application of circuit QED systems in quantum information processing it would be highly desirable to switch on and off the interaction between two resonators. We introduce a formalism for two-resonator circuit QED where two on-chip microwave resonators are simultaneously coupled to one sc qubit. In this three-circuit network, the qubit mediates a geometric and a dynamic second-order interaction between the two resonators [1]. These two coupling strengths can be tuned to be equal by varying the qubit operation point, thus permitting

to switch on and off the interaction between the resonators. We discuss the effect of the qubit on the dynamic second-order coupling and how it can be deliberately manipulated to realize a sc quantum switch. Finally, we present a realistic design for implementing a two-resonator circuit QED setup based on a flux qubit and show preliminary experimental results. This work is supported by SFB 631 and NIM.
[1] M. Mariantoni *et al.*, Phys. Rev. B 78, 104508 (2008)

TT 44.14 Thu 17:45 HSZ 304

Mesoscopic Shelving Readout of Superconducting Qubits in Circuit QED — •Jens Siewert[1], Barbara Englert[2,3], Giuseppe Mangano[1,4], Matteo Mariantoni[3], Rudolf Gross[3], and Enrique Solano[2,5] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]LMU München, 80333 München, Germany — [3]TU München und Walther-Meißner Institut, 85748 Garching, Germany — [4]DMFCI, Università di Catania, 95125 Catania, Italy — [5]University of the Basque Country, 48080 Bilbao, Spain

We present a method for measuring the state of a superconducting qubit inside a microwave cavity, where one qubit state is associated with the generation of a mesoscopic cavity coherent field while the other remains associated with a vacuum field. By measuring the outgoing cavity field with conventional devices, an efficient detection of the qubit state can be achieved. This method uses a cyclic transition in a three-level artificial atom configuration to build the large cavity field, enabling a high-fidelity measurement in the spirit of the successful electron-shelving readout for trapped ions. We expect that the proposed technique can be adapted to different superconducting qubit designs and contribute to further improve qubit readout fidelity.

15 min. break.

TT 44.15 Thu 18:15 HSZ 304

Noise in Circuit Quantum Electrodynamics — •Michael Marthaler[1], Gerd Schön[1], and Alexander Shnirman[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

Qubits and superconducting single electron transistors (SSET) have been used to reproduce effects known from quantum optics in solid state based systems. In this type of system we have to consider noise sources which are different from known dissipation effects in quantum optics. We investigate the effect of the electromagnetic environment in circuit quantum electrodynamics (CQED) for a stripline pumped by a superconducting single electron transistor (SSET).

TT 44.16 Thu 18:30 HSZ 304

Losses in Microwave Resonators at Millikelvin Temperatures — •Pascal Macha[1], Simon H.W. van der Ploeg[1], Stefan Wünsch[2], Gregor Oelsner[1], Evgeni Il'ichev[1], Hans-Georg Meyer[1], and Michael Siegel[2] — [1]Institute of Photonic Technology, PO Box 100239, D-07702 Jena, Germany — [2]Universität Karlsruhe, Institut für Mikro– und Nanoelektronische Systeme, Hertzstraße 16, D-76187 Karlsruhe, Germany

We investigate the behaviour of a high-frequency coplanar waveguide resonator for low intensities of microwave power at low temperatures (20–700mK). In addition to the shift of the resonance frequency, we found a significant increase of losses in the resonator below 300mK. The temperature dependence correlates well with the expectation for a population of two level systems around the resonance frequency. Such two level systems have been identified as a major reason for decoherence in solid state quantum systems. We suggest that the increase of losses in our resonator is due to the coupling to such two level systems. In order to clarify the origin of the two level systems further investigations are necessary. This work is of great importance for the implementation of circuit QED and for detectors.

TT 44.17 Thu 18:45 HSZ 304

Cross-correlation heterodyne detection: Measuring the vacuum fluctuations at microwave frequencies — Matteo Mariantoni[1], Edwin P. Menzel[1], Miguel A. Araque Caballero[1], Frank Deppe[1], Elisabeth Hoffmann[1], Thomas Niemczyk[1], Achim Marx[1], •Rudolf Gross[1], and Enrique Solano[2] — [1]Walther-Meissner-Institut and TU Muenchen, Germany — [2]Departamento de Quimica Fisica, Universidad del Pais Vasco / Euskal Herriko Unibertsitatea, Spain

In order to gain a profound insight into the fundamental properties of quantum electrodynamics (QED), studying the zero-point fluctuations of microwave radiation represents an important task. Here, we present a full experimental characterization of the vacuum fluctuations by measuring the Planck distribution of its noise power at microwave frequencies and very low temperatures. We observe a cross-over from thermal noise to vacuum quantum noise and quantify the level of vacuum fluctuations for a narrow frequency band centered around 5.85 GHz. We demonstrate the change of the vacuum fluctuations level with the center frequency. Finally, we perform a new type of heterodyne detection particularly suitable for circuit QED systems. It is based on microwave beam splitters and cross-correlation measurements and allows for the reconstruction of the entire covariance matrix of the vacuum. We acknowledge support from SFB631, NIM, EuroSQUIP, and the Ikerbasque Foundation.

TT 44.18 Thu 19:00 HSZ 304

Cross-correlation heterodyne detection: Measuring microwave nontrivial propagating signals — Edwin P. Menzel[1], Matteo Mariantoni[1], Miguel Angel Araque Caballero[1], Frank Deppe[1], Elisabeth Hoffmann[1], Thomas Niemczyk[1], •Achim Marx[1], Rudolf Gross[1], and Enrique Solano[2] — [1]Walther-Meissner-Institut and TU Muenchen, Garching, Germany — [2]Departamento de Quimica Fisica, Universidad del Pais Vasco / Euskal Herriko Unibertsitatea, Bilbao, Spain

The accurate measurement of the first two moments of Gaussian states (e.g., coherent or squeezed states) allows for their complete characterization. This provides a tool to clarify the quantum nature of microwave radiation, an important issue for example in circuit quantum electrodynamics. We present a full experimental characterization of nontrivial microwave signals with an average photon number of the order of 1, whose variance exhibits an elaborate dependence on external control parameters. We experimentally access the entire covariance matrix by splitting the input signals via microwave beam splitters and performing cross-correlation measurements. In this manner, we are able to precisely resolve the first two moments, a challenging task at microwave frequencies. Furthermore, we succeeded to measure the third central moment of similar nontrivial signals. We acknowledge support from SFB631, NIM, EuroSQUIP, and the Ikerbasque Foundation.

TT 45: Superconductivity: Ferropnictides 2

Time: Friday 10:15–12:45 Location: HSZ 03

TT 45.1 Fri 10:15 HSZ 03

Proximity of LaOFeAs to a magnetic instability — •Ingo Opahle, Hem Kandpal, Yuzhong Zhang, Claudius Gros, and Roser Valenti — Institut für Theoretische Physik, Goethe Universität Frankfurt, Germany

We investigate the effect of external pressure on the Fe magnetic moment in undoped LaOFeAs within the framework of density functional theory and show that this system is close to a magnetic instability: The Fe moment is found to drop by nearly a factor of 3 within a pressure range of ± 5 GPa around the calculated equilibrium volume. While the Fe moments show an unusually strong sensitivity to the spin arrangement (type of anti-ferromagnetic structure), the low temperature structural distortion is found to have only a minor influence on them. Analysis of the Fermi surface topology and nesting features shows that these properties change very little up to pressures of at least 10 GPa. We discuss the magnetic instability in terms of the itineracy of this system.

TT 45.2 Fri 10:30 HSZ 03

Magnetic and Thermodynamic studies on iron based superconductors $RFeAsO_{1-x}F_x$ (R=La, Ce, Pr, Sm, Gd) — •Norman Leps[1], Rüdiger Klingeler[1], Christian Hess[1], Ag-

nieszka Kondrat[1], Jorge Hamann Borrero[1], Liran Wang[1], Günter Behr[1], Hans-Henning Klauss[3], Hubertus Luetkens[2], and Bernd Büchner[1] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]IFP, TU Dresden, D-01069 Dresden, Germany

We present specific heat and magnetisation data of $RFeAsO_{1-x}F_x$ with R=La, Ce, Pr, Sm, Gd in different applied magnetic fields. For the undoped compounds, i.e. $x = 0$, our data indicate only a weak dependence of both the spin-density-wave formation and the structural transition to the orthorhombic low-temperature phase on type of the R-ion. If R is magnetic, antiferromagnetic ordering of 4f-moments evolves at low temperatures which is also present at higher doping levels x for superconducting materials. The specific heat jump Δc_p at T_C is investigated and we discuss the interplay of magnetism and superconductivity based on our data.

TT 45.3 Fri 10:45 HSZ 03

Magnetic and superconducting properties of $REO_{1-x}F_xFeAs$ (RE=Ce, Sm, Pr, Gd) iron pnictide superconductors studied by muon spin relaxation — •H. Maeter[1], A. Kwadrin[1], H.-H. Klauss[1], H. Luetkens[2], R. Khasanov[2], A. Amato[2], R. Klingeler[3], C. Hess[3], J. Hamann-Borrero[3], N. Leps[3], A. Kondrat[3], G. Behr[3], J. Werner[3], and B. Büchner[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

We have investigated the superconducting properties and the interplay of iron and rare earth magnetic order in the iron-pnictide system $REO_{1-x}F_xFeAs$ with RE=Ce, Gd, Pr, Sm and $0 \leq x \leq 0.5$ by means of muon spin relaxation (μ^+SR) and compare it with $LaO_{1-x}F_xFeAs$. We find that the undoped compounds show a variety of different magnetic coupling of the rare earth ion to the antiferromagnetic iron layers ranging from independent order to strong polarization of the rare earth moments by the ordered iron. Similar to $LaO_{1-x}F_xFeAs$ the orthorhombic phase transition in $REO_{1-x}F_xFeAs$ is also intimately connected to the suppression of magnetic order and the appearance of superconductivity.

TT 45.4 Fri 11:00 HSZ 03

Thermoelectric properties of undoped iron arsenides REOFeAs (RE = La, Ce, Pr, Sm, Gd) — •Agnieszka Kondrat[1], Jorge Enrique Hamann-Borrero[1], Norman Leps[1], Liran Wang[1], Martin Kosmala[2], Olaf Schumann[2], Jochen Werner[1], Guenter Behr[1], Markus Braden[2], Ruediger Klingeler[1], Hans-Henning Klauss[3], Hubertus Luetkens[4], Christian Hess[1], and Bernd Buechner[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]II. Physikalisches Institut, Universitaet zu Koeln, Germany — [3]IFP, TU Dresden, Germany — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen, Switzerland

Polycrystalline samples from the REOFeAs system were studied by means of electrical resistivity, thermal conductivity and thermoelectric power in temperature range 5-300K. All investigated compounds undergo a magnetic and a structural phase transition around 150K, which lead to profound anomalies in electrical, thermal and thermoelectric properties. We present the influence of substituting rare earth elements for La ion on the low temperature thermopower data. We discuss also the strong impact of magnetic field (B = 14T) on thermoelectric properties.

15 min. break

TT 45.5 Fri 11:30 HSZ 03

Probing the superconductive energy gap of the iron pnictide superconductor $Ba_{1-x}K_xFe_2As_2$ by point-contact and scanning tunnelling spectroscopy — •Gernot Goll[1], Michael Marz[1], Samuel Bouvron[1], Tihomir Tomanic[1], Veronika Fritsch[1], Hilbert v. Löhneysen[1,2], and Thomas Wolf[2] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany

The size of the superconductive energy gap and its directional dependence is one of the central issues of studies on the recently discovered iron pnictide superconductors. The knowledge of both properties is essential for the characterization and a closer understanding of the mechanism of superconductivity. We report on point-contact measurements on $(Ba,K)Fe_2As_2$/Pt point contacts. $(Ba,K)Fe_2As_2$ single crystals were prepared by the flux-growth technique with Sn flux. Superconductivity was probed by resistivity and magnetization measurements. A superconducting transition temperature $T_c^{50\%} = 26.5$ K was found resistively for $x = 0.28$. Andreev reflection of charge carriers at the superconductor/normal metal interface of $Ba_{0.72}K_{0.28}Fe_2As_2$/Pt point contacts was utilized to determine the energy gap for current flow parallel and perpendicular to the FeAs planes. In first measurements, with current flow within the plane, the diffential conductance versus voltage curves reveal a multi-gap nature of the superconductive order parameter with a small gap of about 3 meV and a larger one with 7-8 meV.

TT 45.6 Fri 11:45 HSZ 03

Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors. — •Dmitri Efremov[1], Ilya Eremin[2], and Andrey Chubukov[3] — [1]TU Dresden — [2]MPIPKS Dresden — [3]Universtity of Wisconsin

We analyze antiferromagnetism and superconductivity in novel $Fe-$based superconductors within the itinerant model of small electron and hole pockets near $(0,0)$ and (π,π). We argue that the effective interactions in both channels logarithmically flow towards the same values at low energies, *i.e.*, antiferromagnetism and superconductivity must be treated on equal footings. The magnetic instability comes first for equal sizes of the two pockets, but looses to superconductivity upon doping. The superconducting gap has no nodes, but changes sign between the two Fermi surfaces (extended s-wave symmetry). We argue that the T dependencies of the spin susceptibility and NMR relaxation rate for such state are exponential only at very low T, and can be well fitted by power-laws over a wide T range below T_c.

TT 45.7 Fri 12:00 HSZ 03

Orbital and spin effects for the upper critical field in strongly disordered iron pnictide superconductors — •Guenter Fuchs[1], Stefan-Ludwig Drechsler[1], Nadezhda Kozlova[1], Konstantin Nenkov[1], Guenter Behr[1], Ernest Arushanov[1,2], Jens Freudenberger[1], Ruediger Klingeler[1], Anke Koehler[1], Bernd Buechner[1], and Ludwig Schultz[1] — [1]IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Inst. of Appl. Phys., Acad. Sci. Moldova, Chisinau, Moldova

We report upper critical field $B_{c2}(T)$ [1], resistivity, and Hall data for disordered (arsenic deficient) $LaO_{0.9}F_{0.1}FeAs_{1-\delta}$ in a wide temperature and field range up to 47 T. Due to the large linear initial slope of $B_{c2} \approx$ -5.4 to -6.6T/K near $T_c \approx 28.5$ K the T-dependence of the in-plane $B_{c2}(T)$ shows a clear flattening already near 23 K above 30 T which is intepreted as the onset of a Pauli-limited behavior with $B_{c2}(0) \approx 63$ to 68 T. Our results are discussed in terms of disorder effects within scenarios for conventional and unconventional superconductivity (SC). Proposed unconventional p- and d-wave scenarios of SC can be discarded for our samples. The enhancement of the upper critical field slope near T_c by strong disorder provides evidence for an important *attractive* intraband contribution to the pairing of Cooper pairs in the Fe pnictides. We compare our results with B_{c2}-data in the literature which show often no Pauli-limiting behavior. A novel disorder related scenario of a complex interplay of SC with two different competing magnetic instabilities is proposed.

[1] G. Fuchs, S.-L. Drechsler, N. Kozlova *et al.*, PRL **101** in press

TT 45.8 Fri 12:15 HSZ 03

Absorption spectroscopy of rare earth oxypnictides — •Friedrich Roth[1], Thomas Kroll[1], Andreas Koitzsch[1], Roberto Kraus[1], Günter Behr[1], Guoli Sun[2], Dunlu Sun[2], Chengtian Lin[2], Bernd Büchner[1], and Martin Knupfer[1] — [1]Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

A large oxypnictides family LnFeAsO (Ln= La, Ce, Pr, Nd, Sm, Gd) has been found to be superconducting with a transition temperature up to 55K and high upper critical fields. The onset of the superconducting critical temperature T_c in these compounds increases with the reduction of the rare-earth ionic size, and the highest T_c obtained so far is 55K in doped SmFeAsO. In this contribution we present results of x-ray absorption (XAS) spectroscopy measurements on the soft X-ray regime for polycrystalline LaFeAsO, CeFeAsO, SmFeAsO and GdFeAsO at various temperature as well as for $Ba_{1-x}K_xFe_2As_2$ single crystals.

TT 45.9 Fri 12:30 HSZ 03

Electronic properties of iron pnictides in the normal state probed by NMR — •Franziska Hammerath[1], Guillaume Lang[1], Hans-Joachim Grafe[1], Dalibor Paar[1,2], Katarina Manthey[1], Nicholas Curro[3], Günther Behr[1], Jochen Werner[1], and Bernd Büchner[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Dept. of Physics, Faculty of Science, Univ. of Zagreb, P. O. Box 331, HR-10002 Zagreb, Croatia — [3]Dept. of Physics, Univ. of California, Davis, CA 95616, USA

We have performed ^{75}As, ^{139}La, and ^{57}Fe Nuclear Magnetic Resonance (NMR) measurements on the new $LaO_{1-x}F_xFeAs$ superconductor. For x=0.1, NMR on all three nuclei shows that the local electronic susceptibility increases with increasing temperature in the normal state [1]. The scaling of all NMR shifts with respect to the macroscopic susceptibility indicates a single spin liquid. Relaxation measurements exhibit a similar temperature-dependence for $(T_1T)^{-1}$, and suggest that the dynamical susceptibility changes uniformly in q space with varying temperature. For x=0.05, in the underdoped regime, we find a Curie Weiss like increase of $(T_1T)^{-1}$ at low temperatures, indicating the onset of local moment fluctuations.

[1] H.-J. Grafe, G. Lang, F. Hammerath et al., arXiv:0811.4508, submitted to New Journal of Physics (invited paper, special issue on iron pnictides superconductors).

TT 46: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Friday 10:15–12:45 Location: HSZ 301

TT 46.1 Fri 10:15 HSZ 301

Spatial Variation of Fano Resonances in the STM Tunneling Density of States due to Sub-Surface Kondo Impurities — •Henning Prüser, Martin Wenderoth, Alexander Weismann, and Rainer G. Ulbrich — IV. Physikalisches Institut; Georg-August Universität Göttingen, Germany

Single magnetic atoms buried in copper have been investigated using low temperature scanning tunneling spectroscopy (STS). Cu alloys with a small amount ($\leq$ 0.02%) of iron and cobalt were epitaxially grown on a Cu(100) substrate. The embedded Fe and Co impurities were identified in STM topographies at 6K by their fourfold symmetric topography patterns. From comparison with scattering theory in anisotropic media we obtain their individual depths, ranging from 3 to 9 ML. In the STS data both Fe and Co show the expected Kondo feature: a Fano resonance centered at E_F, and a width directly related to the Kondo temperature T_K. Our T_K values for Fe and Co corroborate parameters deduced from bulk measurements. The line shape of the LDOS spectrum around E_F depends strongly on (i) the lateral distance of the tip from the impurity and (ii) the impurity depth below the surface. As a function of these two lengths the line shape shows an oscillatory behavior. The path length period equals the Friedel wave length of copper as predicted by theory [1, 2]. Work supported by DFG SFB 602 TPA3.

[1] Újsághy et al., PRL 82, 2557, 2000
[2] Plihal et al., PRB 63, 085404, 2001

TT 46.2 Fri 10:30 HSZ 301

Superperturbation solver for quantum impurity models — •Sergey Brener[1], Alexander Lichtenstein[1], Hartmut Hafermann[1], Christoph Jung[1], Kelly Patton[1], Mikhail Katsnelson[2], and Alexei Rubtsov[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Deutschland — [2]Institute for molecules and materials, Radboud University of Nijmengen, The Netherlands — [3]Department of physics, Moscow State University, Russia

We present a very efficient solver for a general Anderson impurity model. It is based on a perturbation around a solution obtained from exact diagonalization using a small number of bath sites. Satisfactory agreement is found for a single bath site over a wide range of parameters. The method proves superior to QMC for a calculation of spectral properties for real energies by analytical continuation due to the absence of statistical noise. It can also be applied to calculating of two-particle correlators, which allows to investigate, for example, transport properties of nano-systems or spin correlations which are essential for description of a Kondo cloud.

TT 46.3 Fri 10:45 HSZ 301

Kondo effect in a mesoscopic interacting electron system — •Stefan Rotter[1], Hakan Türeci[2], Yoram Alhassid[3], and Douglas Stone[3] — [1]TU–Vienna, Austria — [2]ETH–Zürich, Switzerland — [3]Yale, USA

We study the problem of a quantum dot with finite level spacing which is coupled anti-ferromagnetically to a Kondo spin ("Kondo box"). In particular, we investigate the influence of a ferromagnetic exchange interaction among the dot electrons as described by the "Universal Hamiltonian". The problem is solved numerically by diagonalizing the system Hamiltonian in a good-spin basis and analytically in the weak and strong Kondo coupling limits [1]. We provide an analytical solution for the effective strong coupling Hamiltonian which contains new interaction terms unknown from the conventional Kondo problem. The interplay between Kondo and ferromagnetic exchange correlations affects the ground-state spin of the system and can be probed with experimentally tunable parameters.

[1] S. Rotter, H. E. Türeci, Y. Alhassid, A. D. Stone, Phys. Rev. Lett. 100, 166601 (2008).

TT 46.4 Fri 11:00 HSZ 301

Kondo physics in regular and chaotic mesoscopic systems — •Rainer Bedrich[1], Sebastien Burdin[2], and Martina Hentschel[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institute of Theoretical Physics, Cologne University

We study the Kondo effect induced by a magnetic impurity interacting with a small metallic grain. Here, in contrast with the Kondo effect occurring in a bulk material, the metallic host is characterised by a finite mean level spacing. This low energy scale can generate deviations from the universal behavior which would be expected for a bulk system. The physical properties of the system are computed within a mean-field approximation for the Kondo interaction. In particular, we study the local magnetic susceptibility, the conductance, and the local density of electronic states as a function of the temperature, the mean level spacing, the Kondo coupling, and the number of electrons on the dot. As a first step, we consider a constant distribution of the non-interacting energy levels. Our results are in agreement with the results obtained from different approaches, suggesting that the mean-field approximation is valid. A more realistic situation is then considered, for which the energy levels are distributed randomly. This is realised within the random matrix theory. Finally we compare between chaotic and regular (e.g. parabolic quantum dot) systems.

15 min. break

TT 46.5 Fri 11:30 HSZ 301

Kondo decoherence: finding the right spin model for iron impurities in gold and silver — •Theodoulos Costi[1], Lars Bergqvist[1], Andreas Weichselbaum[2], Jan von Delft[2], Phivos Mavropoulos[1], Peter Dederichs[1], Tobias Micklitz[3,5], Achim Rosch[3], Francois Mallet[4], Laurent Saminadayar[4], and Christopher Bäuerle[4] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience,Ludwig-Maximilians-Universität München, 80333 München, Germany — [3]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [4]Institut Néel - CNRS and Université Joseph Fourier, 38042 Grenoble Cedex 09, France — [5]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We exploit the decoherence of electrons due to magnetic impurities, studied via weak localization, to resolve a longstanding question concerning the classic Kondo systems of Fe impurities in the noble metals gold and silver: which Kondo-type model yields a realistic description of the relevant multiple bands, spin and orbital degrees of freedom? Previous studies suggest a fully screened spin S Kondo model, but the value of S remained ambiguous. We perform density functional theory calculations that suggest $S = 3/2$. We also compare previous and new measurements of both the resistivity and decoherence rate in quasi 1-

dimensional wires to numerical renormalization group predictions for $S = 1/2, 1$ and $3/2$, finding excellent agreement for $S = 3/2$.

TT 46.6 Fri 11:45 HSZ 301

Flow Equation Analysis of a Kondo Dot in a Magnetic Field — •Peter Fritsch and Stefan Kehrein — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

Using infinitesimal unitary transformations (flow equations) [1,2] we derive a consistent perturbative scaling picture of a Kondo dot in a magnetic field for both equilibrium and non-equilibrium (dc voltage bias) situations. We work out the spin dynamics and the T-Matrix as functions of magnetic field, voltage bias and temperature. In particular, we report on the behavior of both the static spin susceptibility [3] and the magnetization including leading logarithmic corrections. This work is a generalization of the previous flow equation analysis of the non-equilibrium Kondo model in zero magnetic field [1,2,3].

[1] S. Kehrein, The Flow Equation Approach to Many-Particle Systems, Springer Tracts in Modern Physics 217

[2] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005)

[3] P. Fritsch and S. Kehrein, arxiv:0811.0759

TT 46.7 Fri 12:00 HSZ 301

Real-time renormalization group in frequency space: A complete 2-loop analysis of the nonequilibrium anisotropic Kondo model at finite magnetic field — Herbert Schoeller[1,2] and •Frank Reininghaus[1,2] — [1]Institut für Theor. Physik A, RWTH Aachen University, Germany — [2]JARA-Fundamentals of Future Information Technology

We use a recently developed real-time renormalization group method in frequency space (RTRG-FS) to describe nonequilibrium phenomena in generic fermionic quantum system coupled weakly to several reservoirs via spin and/or orbital fluctuations. Within a 2-loop analysis we derive analytic formulas for the nonlinear conductance and the kernel determining the time evolution of the reduced density matrix. We apply the general formalism to the nonequilibrium anisotropic Kondo model at finite magnetic field. Besides the nonlinear conductance and the magnetic susceptibility, we calculate for the first time the spin relaxation and dephasing rates and the renormalized g-factor beyond leading order. Furthermore, we show in all orders in the exchange coupling that the RG flow of the vertices is cut off by relaxation and dephasing rates.

TT 46.8 Fri 12:15 HSZ 301

Dynamical spin-spin correlation functions in the Kondo model out of equilibrium — •Dirk Schuricht and Herbert Schoeller — Institut fuer Theoretische Physik A, RWTH Aachen

We calculate the dynamical correlation function of a Kondo spin coupled to two noninteracting leads held at different chemical potentials. We use real-time renormalization group in frequency space up to 2-loop. The formalism includes the renormalization of the vertices and the Liouvillian determining the dynamics of the reduced density matrix of the local spin. As a result the cutoff by relaxation/dephasing rates, temperature, external frequency, Laplace variable of the time dynamics, and the voltage can be described on a microscopic level. We show show how nonequilibrium correlation function in real-frequency space can be calculated in Matsubara space without the need of any analytical continuation.

TT 46.9 Fri 12:30 HSZ 301

Using DMRG to Study Quantum Impurity Models with Time-Dependent Hamiltonians — •Cheng Guo[1], Andreas Weichselbaum[1], Stefan Kehrein[1], Tao Xiang[2], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany — [2]Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China

We use the adaptive time-dependent density matrix renormalization group method (t-DMRG) to study the nonequilibrium dynamics of a benchmark quantum impurity system which has a time-dependent Hamiltonian. This model is a resonant-level model, obtained by a mapping from a certain ohmic spin-boson model describing the dissipative Landau-Zener transition. Some techniques from the numerical renormalization group method (NRG) are borrowed to transform this model to a DMRG-friendly form. We compare t-DMRG results with exact results at zero temperature and find very good agreement. We also give a physical interpretation of the numerical results.