Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture rooms H 0104, H 2053, H3010, EB 202; Poster B)

Invited Talks

TT 3.5	Mon	10:30–11:00	H 2053	**Noise and current cross-correlations in nano-electromechanical systems** — •Christoph Bruder
TT 3.6	Mon	11:00–11:30	H 2053	**Nonlinear dynamics and cooling in optomechanical systems** — •Florian Marquardt
TT 4.1	Mon	9:30–10:00	H 3010	**Can nuclear spins reveal the nature of tunneling systems in glasses?** — •Andreas Fleischmann
TT 9.3	Mon	14:30–15:00	H 2053	**Coherent Oscillations in Josephson Phase Qubits** — •Jürgen Lisenfeld, Alexander Lukashenko, Alexey V. Ustinov
TT 11.1	Mon	15:15–15:45	H 3010	**Superconducting Quantum Interference Filters** — •Nils Schopohl
TT 17.3	Tue	14:30–15:00	H 2053	**The centennial of helium liquefaction - a century of low temperature physics** — •Dietrich Einzel
TT 20.1	Tue	14:00–14:30	EB 202	**Adiabatic pumping in nanostructures** — •Michele Governale
TT 29.8	Thu	11:30–12:00	H 3010	**Charge redistribution at YBCO-metal interfaces** — •Udo Schwingenschlögl, Cosima Schuster
TT 31.3	Thu	12:15–12:45	EB 202	**Electronic transport through nanostructures** — •Peter Schmitteckert
TT 39.1	Fri	10:15–10:45	EB 202	**EuO_{1-x} Epitaxially Integrated with Silicon** — •Andreas Schmehl, Stefan Thiel, Christoph Richter, Ross Ulbricht, Tassilo Heeg, Marco Liberati, Martin Röckerath, Sebastian Mühlbauer, Peter Böni, Yuri Barash, Jürgen Schubert, Yves Idzerda, Jochen Mannhart, Darrell G. Schlom

TT 2: Internal Symposium High Magnetic Field Phenomena in Low Dimensional Magnets

TT 2.1	Mon	9:30–10:00	H 0104	**High magnetic fields with low dimensional magnets** — •Alan Tennant
TT 2.2	Mon	10:00–10:30	H 0104	**High Field NMR in Low Dimensional Quantum Antiferromagnets** — •Claude Berthier, Hadrien Mayaffre, Martin Klanjšek, Steffen Krämer, Mladen Horvatić
TT 2.3	Mon	10:30–11:00	H 0104	**Exotic ground states in high magnetic fields** — •Andreas Läuchli
TT 2.4	Mon	11:00–11:15	H 0104	**High-field properties of a critical frustrated chain cuprate: Li_2ZrCuO_4** — •Stefan-Ludwig Drechsler, Rüdiger Klingeler, Natalia Tristan, Norman Leps, Johannes Richter, Thomas Lorenz, Olga Volkova, Alexander Vasiliev, Bernd Büchner
TT 2.5	Mon	11:30–12:00	H 0104	**Dimensional Reduction at a Quantum Critical Point** — •Cristian Batista
TT 2.6	Mon	12:00–12:15	H 0104	**Excitation hierarchy of the spin-1 large-D system $NiCl_2$-4SC$(NH_2)_2$** — •S.A. Zvyagin, J. Wosnitza, C.D. Batista, J. Krzystek, V.S. Zapf, M. Jaime, A. Paduan-Filho, M. Tsukamoto, N. Kawashima
TT 2.7	Mon	12:15–12:45	H 0104	**Exploring field-induced quantum phase transitions in molecule-based magnets** — •Michael Lang, Katarina Removic-Langer, Yeekin Tsui, Ulrich Tutsch, Bernd Wolf, Andrei Prokofiev, Wolf Assmus, Roser Valenti, Andreas Honecker, Matthias Wagner, Stefan Wessel

TT 2.8	Mon	12:45–13:00	H 0104	**Diverging low-temperature thermal expansion of the spin-ladder system $(C_5H_{12}N)_2CuBr_4$** — •Thomas Lorenz, Oliver Heyer, Markus Garst, Fabrizio Anfuso, Achim Rosch, Christian Rüegg, Karl Krämer

TT 12: Internal Symposium Cryodetectors and SQUID

TT 12.1	Tue	9:30–10:00	H 0104	**SQUID multiplexers for low-temperature detectors** — •K.D. Irwin, J.A. Beall, H.M. Cho, W.B. Doriese, W.D. Duncan, G.C. Hilton, R. Horansky, N. Jethava, J.A.B. Mates, C.D. Reintsema, D. Schmidt, J.N. Ullom, L.R. Vale, Y. Xu, K. Yoon
TT 12.2	Tue	10:00–10:30	H 0104	**Transition Edge Sensor and Kinetic Inductance Detector Developments for Astronomy Applications** — •Piet de Korte
TT 12.3	Tue	10:30–11:00	H 0104	**Metallic magnetic calorimeters for high resolution x-ray spectroscopy and particle detection** — •Loredana Fleischmann
TT 12.4	Tue	11:15–11:45	H 0104	**Methode zur berührungslosen, induktiven Messung der lokalen Übergangstemperatur supraleitender, dünner Wolframfilme** — •Karoline Schäffner, Godehard Angloher, Irina Bavykina, Antonio Bento, Dieter Hauff, Patrick Huff, Michael Kiefer, Rafael Lang, Emilija Pantic, Federica Petricca, Franz Pröbst, Jens Schmaler, Wolfgang Seidel, Hans Seitz, Leo Stodolsky
TT 12.5	Tue	11:45–12:00	H 0104	**SQUID series array current sensor for measuring dc currents** — •Jörn Beyer, Dietmar Drung
TT 12.6	Tue	12:00–12:15	H 0104	**Relaxationsmessungen mit SQUID Gradiometern** — •Frank Schmidl, Markus Büttner, Christoph Becker, Alexander Steppke, Peter Kossebau, Stefan Prass, Paul Seidel
TT 12.7	Tue	12:15–12:30	H 0104	**Scanning THz-Microscopy of microwave devices with a Josephson-Cantilever** — •Christian Brendel, Felix Stewing, Meinhard Schilling
TT 12.8	Tue	12:30–12:45	H 0104	**Highly sensitive and easy-to-use SQUID sensors** — •Frank Ruede, Cornelia Assmann, Jörn Beyer, Dietmar Drung, Alexander Kirste, Margret Peters, Thomas Schurig

TT 16: Internal Symposium Efficient Classical Simulation of Strongly Correlated Quantum Systems

TT 16.1	Tue	14:00–14:45	H 0104	**Density matrix renormalization meets quantum information** — •Ulrich Schollwöck
TT 16.2	Tue	14:45–15:15	H 0104	**Time-dependent DMRG: Applications to cold atoms in optical lattices** — •Corinna Kollath, Andreas Laeuchli, Ehud Altman
TT 16.3	Tue	15:15–15:45	H 0104	**A Renormalisation-Group Algorithm for Eigenvalue Density Functions of Interacting Quantum Systems** — •Tobias Osborne
TT 16.4	Tue	16:00–16:30	H 0104	**Projected Entangled Pair States: status and prospects** — •Frank Verstraete
TT 16.5	Tue	16:30–17:00	H 0104	**DMRG and quantum impurity models** — •Andreas Weichselbaum, Jan von Delft
TT 16.6	Tue	17:00–17:30	H 0104	**Unitary networks to describe quantum many-body systems** — •Jens Eisert, Chris Dawson, Tobias Osborne, Frank Verstraete
TT 16.7	Tue	17:30–17:45	H 0104	**Optimized ensembles in quantum Monte Carlo simulations** — •Stefan Wessel, Norbert Stoop, Emanuel Gull, Simon Trebst, Matthias Troyer

TT 27: Internal Symposium Circuit QED

TT 27.1	Thu	9:30–10:00	H 0104	**Single artificial-atom maser** — •Yasunobu Nakamura, Oleg Astafiev, Kunihiro Inomata, Antti O. Niskanen, Tsuyoshi Yamamoto, Yuri A. Pashkin, Jaw-Shen Tsai
TT 27.2	Thu	10:00–10:30	H 0104	**Sisyphus cooling and amplification by a superconducting qubit** — •Evgeni Il'ichev, M. Grajcar, S.H.W. van der Ploeg, A. Izmalkov, H.-G. Meyer, A. Fedorov, A. Shnirman, Gerd Schoen

TT 27.3	Thu	10:30–10:55	H 0104	**Quantum Computation and Quantum Optics with circuit QED** — •Jens Koch
TT 27.4	Thu	10:55–11:20	H 0104	**Engineering coherent quantum states in superconducting systems** — •Raymond W Simmonds
TT 27.5	Thu	11:35–12:00	H 0104	**Observation of Berry's Phase in a Superconducting Qubit Embedded in a Cavity** — •Peter Leek, Johannes Fink, Alexandre Blais, Romeo Bianchetti, Martin Goeppl, Jay Gambetta, David Schuster, Luigi Frunzio, Robert Schoelkopf, Andreas Wallraff
TT 27.6	Thu	12:00–12:15	H 0104	**Strong squeezing in a solid state system** — •Michael Marthaler, Alexander Shnirman, Gerd Schön
TT 27.7	Thu	12:15–12:30	H 0104	**Dissipation in circuit QED** — •Stephan André, Valentina Brosco, Gerd Schön, Alexander Shnirman
TT 27.8	Thu	12:30–12:45	H 0104	**Quantum Zeno Effect in Detection of Itinerant Microwave Photons** — •Ferdinand Helmer, Matteo Mariantoni, Enrique Solano, Florian Marquardt
TT 27.9	Thu	12:45–13:00	H 0104	**Single Photon Generation in Superconducting Microwave Cavities** — •Giuseppe Mangano, Jens Siewert, Giuseppe Falci

TT 33: Internal Symposium High-Temperature Superconductivity

TT 33.1	Thu	14:00–14:30	H 0104	**Transport Evidence for Quantum Criticality in Electron-doped Cuprates** — •Richard Greene
TT 33.2	Thu	14:30–14:45	H 0104	**Signatures of non-monotonic d-wave gap in electron-doped cuprates** — •Ilya Eremin, Evelina Tsoncheva, Andrey Chubukov
TT 33.3	Thu	14:45–15:15	H 0104	**Superconductivity in the Hubbard model and the two gap energy scales in high-temperature superconductors** — •Markus Aichhorn, Enrico Arrigoni, Michael Potthoff, Zhong Bing Huang, Werner Hanke
TT 33.4	Thu	15:30–15:55	H 0104	**Momentum-resolved electron-phonon coupling and self-energy effects in $YBa_2Cu_3O_7$: an LDA study** — •Rolf Heid, Klaus-Peter Bohnen, Roland Zeyher, Dirk Manske
TT 33.5	Thu	15:55–16:10	H 0104	**The phonon buckling mode in $YBa_2Cu_3O_{6+x}$ measured by inelastic neutron scattering** — •Markus Raichle, Dmitry Reznik, Mohammed Bakr, Vladimir Hinkov, Klaudia Hradil, Daniel Lamago, Clemens Ulrich, Markus Bröll, Philippe Bourges, Yvan Sidis, Chengtian Lin, Bernhard Keimer
TT 33.6	Thu	16:10–16:35	H 0104	**d-wave stripes in cuprates: Valence bond order coexisting with nodal quasiparticles** — •Matthias Vojta
TT 33.7	Thu	16:35–16:50	H 0104	**Charge order in $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ studied by resonant soft X-ray diffraction** — •J. Fink, E. Weschke, E. Schierle, J. Geck, H. Hawthorn, H. Widati, H.-H. Hu, H. Dürr, B. Büchner, G. A. Sawatzky
TT 33.8	Thu	16:50–17:05	H 0104	**q-dependence of the giant bond-stretching phonon anomaly in the stripe compound $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ measured by IXS** — •Daniel Lamago, Dmitry Reznik, T. Fukuda, K. Yamada, A.Q.R. Baron
TT 33.9	Thu	17:05–17:30	H 0104	**Charge ordering phenomena and superconductivity in cuprates** — •Leonardo Tassini, Bernhard Muschler, Wolfgang Prestel, Rudi Hackl, Michael Lambacher, Andreas Erb
TT 33.10	Thu	17:45–18:10	H 0104	**Electronic liquid crystal state in a strongly underdoped high-temperature superconductor** — •V. Hinkov, D. Haug, B. Fauque, Y. Sidis, P. Bourges, A. Ivanov, C. Bernhard, CT. Lin, B. Keimer
TT 33.11	Thu	18:10–18:25	H 0104	**ARPES of Bi-cuprates: Did we mix up apples and oranges?** — •Lenart Dudy, Olaf Lübben, Beate Müller, Alica Krapf, Helmut Dwelk, Christoph Janowitz, Recardo Manzke
TT 33.12	Thu	18:25–18:40	H 0104	**Effects of out-of-plane disorder on the superconductivity of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$** — •Jürgen Röhler, Christoph Trabant, Johanna Frielingsdorf, Rabia Djemour, Victor Martovitsky, Lenart Dudy, Helmut Dwelk, Alica Krapf
TT 33.13	Thu	18:40–19:10	H 0104	**Indications on fluctuation origin of the recently observed giant Nernst effect in superconductors above T_c** — •A.A. Varlamov

Sessions

TT 1.1–1.3	Sun	14:00–17:00	EW 201	**Tutorial: Quantum Shot Noise**
TT 2.1–2.8	Mon	9:30–13:00	H 0104	**Symposium: High Magnetic Field Phenomena in Low Dimensional Magnets**
TT 3.1–3.11	Mon	9:30–13:00	H 2053	**Transport: Fluctuations and Noise**
TT 4.1–4.6	Mon	9:30–11:15	H 3010	**Matter at Low Temperature: Materials**
TT 5.1–5.5	Mon	11:30–13:00	H 3010	**Superconductivity - Cryodetectors**
TT 6.1–6.12	Mon	9:30–12:45	EB 202	**Correlated Electrons: Heavy Fermions**
TT 7.1–7.23	Mon	14:00–18:00	Poster B	**Matter at Low Temperature: Poster Session**
TT 8.1–8.14	Mon	14:00–18:00	H 0104	**Correlated Electrons: Spin Systems and Itinerant Magnets 1**
TT 9.1–9.15	Mon	14:00–18:15	H 2053	**Transport: Quantum Coherence and Quantum Information Systems**
TT 10.1–10.4	Mon	14:00–15:00	H 3010	**Superconductivity: Fabrication and Characterization**
TT 11.1–11.9	Mon	15:15–18:00	H 3010	**Superconductivity: Tunneling, Josephson Junctions, SQUIDs**
TT 12.1–12.8	Tue	9:30–12:45	H 0104	**Symposium: Cryodetectors and SQUID**
TT 13.1–13.13	Tue	9:30–13:00	H 2053	**Correlated Electrons: Low-dimensional Systems - Materials 1**
TT 14.1–14.13	Tue	9:30–13:00	H 3010	**Transport: Nanoelectronics III - Molecular Electronics**
TT 15.1–15.57	Tue	14:00–18:00	Poster B	**Superconductivity: Poster Session**
TT 16.1–16.7	Tue	14:00–17:45	H 0104	**Symposium: Efficient Classical Simulation of Strongly Correlated Quantum Systems**
TT 17.1–17.3	Tue	14:00–15:00	H 2053	**Matter at Low Temperature: Measuring Devices, Cryotechnique**
TT 18.1–18.13	Tue	15:15–18:45	H 2053	**Correlated Electrons: Low-dimensional Systems - Materials 2**
TT 19.1–19.16	Tue	14:00–18:30	H 3010	**Correlated Electrons: Quantum-Critical Phenomena**
TT 20.1–20.5	Tue	14:00–15:30	EB 202	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1**
TT 21.1–21.12	Tue	15:45–19:00	EB 202	**Transport: Graphene and Carbon Nanotubes**
TT 22.1–22.63	Wed	14:00–18:00	Poster B	**Transport: Poster Session**
TT 23.1–23.17	Wed	14:00–18:45	H 0104	**Correlated Electrons: (General) Theory**
TT 24.1–24.18	Wed	14:00–19:00	H 2053	**Correlated Electrons: Low-dimensional Systems - Models**
TT 25.1–25.6	Wed	14:00–15:30	H 3010	**Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence**
TT 26.1–26.9	Wed	15:45–18:15	H 3010	**Superconductivity: Vortex Dynamics, Vortex Phases, Pinning**
TT 27.1–27.9	Thu	9:30–13:00	H 0104	**Symposium: Circuit QED**
TT 28.1–28.12	Thu	9:30–12:45	H 2053	**Correlated Electrons: Metal-Insulator Transition 1**
TT 29.1–29.12	Thu	9:30–13:00	H 3010	**Superconductivity: Mechanisms, Phase Diagram, Competing Order**
TT 30.1–30.4	Thu	10:30–11:30	EB 202	**Correlated Electrons: Spin Systems and Itinerant Magnets 2**
TT 31.1–31.4	Thu	11:45–13:00	EB 202	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2**
TT 32.1–32.88	Thu	14:00–18:00	Poster B	**Correlated Electrons: Poster Session**
TT 33.1–33.13	Thu	14:00–19:10	H 0104	**Symposium: High-Temperature Superconductivity**
TT 34.1–34.18	Thu	14:00–19:00	H 2053	**Correlated Electrons: Metal-Insulator Transition 2**
TT 35.1–35.16	Thu	14:00–18:30	H 3010	**Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3**
TT 36.1–36.10	Fri	10:15–13:00	H 0104	**Superconductivity: Properties, Electronic Structure, Order Parameter**
TT 37.1–37.10	Fri	10:15–13:00	H 2053	**Correlated Electrons: Quantum Impurities, Kondo Physics**
TT 38.1–38.10	Fri	10:15–13:00	H 3010	**Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ...**
TT 39.1–39.9	Fri	10:15–13:00	EB 202	**Transport: Nanoelectronics II - Spintronics and Magnetotransport**

The posters can be fixed to the posterboards already in the morning. The actual poster sessions will start at 14:00.

Annual General Meeting of the Low Temperature Physics Division

Donnerstag 19:30–20:30 Raum H 3010

TT 1: Tutorial: Quantum Shot Noise

Time: Sunday 14:00–17:00 Location: EW 201

Tutorial TT 1.1 Sun 14:00 EW 201

Introduction to Quantum Shot Noise — •Tobias Brandes — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, Sekr. E-W 7-1, 10623 Berlin

This tutorial introduces Quantum Shot Noise, starting from a historical perspective of photoelectron counting statistics in quantum optics where many original concepts were developed between the 1950s and the 1980s. I will therefore start with Mandel's semiclassical counting formula that promotes a simple (short time) Fermi-Golden rule calculation to a (long-time) probability distribution. The quest for a quantum version of that formula was characterised by the subtleties of theoretically describing sources, fields, and detectors in a consistent manner. It lead from rather complicated (ordered) operator expressions to the much simpler concept of counting quantum jumps directly 'at the source' in a description with modified Master equations and counting variables. In hindsight, the underlying quantum jump (quantum trajectory) approach can be regarded as a 'by-product' of counting statistics, or vice versa. In its modern version - geared towards ultrasmall, artificial structures like quantum dots - this formalism serves as a versatile tool to theoretically address various noise-related aspects of quantum transport.

Tutorial TT 1.2 Sun 15:00 EW 201

Shot noise and electron counting measurements in low dimensional electron systems — •Frank Hohls — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover

The noise is the signal! In this presentation I will first give an experimentalists introduction on what we can learn and have learned about low dimensional electron systems by measurements of the current shot noise. Noise can be used as a tool to examine fundamental aspects of a system or to characterize its parameters. In the second part I will show how even more information can be gained in quantum dot systems: we can now eavesdrop on the individual tunnelling events of electrons into and out of such small island with quantized charge. With a time resolved recording of these individual events which compose the current we can set out to characterize the detailed dynamics of the system and compile full counting statistics. I will discuss recent progress and future possibilities of this method.

Tutorial TT 1.3 Sun 16:00 EW 201

Full counting statistics - a new view on quantum transport — •Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

We introduce the concept of Full Counting Statistics (FCS) as new paradigm in the field of quantum transport of electrons. We briefly review some aspects of current fluctuations and the correspondingly investigated current-current correlations in mesoscopic physics: suppression of quantum shot noise due to Fermi statistics, universality of noise in diffusive and chaotic conductors and the influence of induced superconducting correlations. The question we try answer using FCS is, what are the underlying fundamental elementary processes leading to the observed noise properties. While this question might look trivial in simple systems (e.g. independent tunneling of single electrons), the answer in more complicated systems is much more intriguing and by no means obvious. Examples are the transport of entangled electrons, fractional charges in edge states or the transport under the influence of time-dependent fields.

TT 2: Symposium: High Magnetic Field Phenomena in Low Dimensional Magnets

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

TT 2.1 Mon 9:30 H 0104

High magnetic fields with low dimensional magnets — •Alan Tennant — Hahn Meitner Institut, Berlin, Germany

High magnetic fields provide a near perfect degree of control over the physics of low dimensional magnets. A broad array of new physical states and phase transitions are being predicted theoretically and discovered experimentally. In this talk I give an overview of some of the new magnetic states that are being discovered including quantum criticality, exotic phase transitions, and fractionalisation of quasi-particles. I shall also outline some of the challenges for the future for experiment and the developing array of tools and materials that are opening up this field of study.

Invited Talk TT 2.2 Mon 10:00 H 0104

High Field NMR in Low Dimensional Quantum Antiferromagnets — •Claude Berthier[1], Hadrien Mayaffre[2], Martin Klanjšek[1], Steffen Krämer[1], and Mladen Horvatić[1] — [1]Grenoble High Magnetic Field Laboratory (GHMFL), CNRS, BP — [2]Lab. de Spectrométrie Physique, UJF Grenoble I

We present high field NMR studies of the field induced magnetic ordering in a few quasi-1D quantum antiferromagnets. $Cu_2(C_5H_{12}N_2)_2Cl_4$ (Cu(Hp)Cl) has for long been considered as the archetype of a strong coupling spin-ladder system. We show that it can be well understood in the framework of a spin-ladder with a staggered Dzyaloshinskii-Moriya (DM) interaction on the rungs [1]. $CuBr_4(C_5H_{12}N)_2$ (BPCB) is made of regular spin-ladders (without DM interaction) weakly coupled together. Its phase diagram between the two quantum critical field H_{c1} and H_{c2} is fully dominated by the H dependence of the Luttinger liquid parameters of the ladders [2]. We also briefly report the NMR evidence for the existence of an unconventional quantum ground state in the 1/3 magnetization plateau in the frustrated diamond chain compound $Cu_3(CO_3)_2(OH)_2$ (azurite) [3].

[1] M. Clémancey *et al.*, Phys. Rev. Lett. **97**, 167204 (2006).
[2] M. Klanjšek, H. Mayaffre, *et al.*, unpublished.
[3] S. Krämer *et al.*, unpublished.

TT 2.3 Mon 10:30 H 0104

Exotic ground states in high magnetic fields — •Andreas Läuchli — IRRMA, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Over the last few years it has been discovered that quantum magnets in strong magnetic fields can host a variety of long-sought exotic phases. In this talk we review recent theoretical efforts revealing magnetization plateaux with complex structures, supersolid phases sustaining simultaneous longitudinal and transverse magnetic order, as well as spin nematic phases, which spontaneously break spin rotational symmetry in the absence of an ordered moment. We discuss the experimental signatures of these phases and point out materials which could possibly display such exciting behavior.

TT 2.4 Mon 11:00 H 0104

High-field properties of a critical frustrated chain cuprate: Li_2ZrCuO_4 — •Stefan-Ludwig Drechsler[1], Rüdiger Klingeler[1], Natalia Tristan[1], Norman Leps[1], Johannes Richter[2], Thomas Lorenz[3], Olga Volkova[4], Alexander Vasiliev[5], and Bernd Büchner[1] — [1]IFW-Dresden, P.O. Box 270116, D-01171 Dresden, — [2]Inst. f. Theoret. Physik, Universität Magdeburg — [3]II. Physikal. Inst., Universität zu Köln — [4]Inst. f. Electronics and Automatics, Moscow, Russia — [5]Lomonosov University, Moscow, Russia

We report an unusual strong field dependence of the magnetic specific heat $c_p(T,H)$, the thermal expansion $\alpha(T,H)$, and the magnetization $m(T,H)$ curve of the frustrated edge-shared chain cuprate Li_2ZrCuO_4 which is close to the quantum critical point between ferromagnetic and helical ordering [1]. The low-temperature peak of $c_p(T)$ is first down shifted for $H < 9$ T, then reaches a broad plateau before its position is up shifted at high fields $H \approx 30$ T. The thermal expansion α changes its sign at about 9 T. The magnetization $m(H)$ saturates at 15-20 T at low temperature well above the estimated saturation field $H_s \approx 4.5$ T for the 1D J_1-J_2–Heisenberg model pointing to a non-neglible influence of the interchain exchange in accord with estimates based on

the dispersion of the LDA bands perpendicular to the chain direction. Possible scenarios for the deviation of the experimental $c_p(T, H)$ data at high fields from the predictions of the isotropic 1D J_1-J_2-Heisenberg model are briefly discussed.

[1] S.-L. Drechsler *et al.*, Phys. Rev. Lett. **98**, 077202 (2007).

15 min. break

Invited Talk TT 2.5 Mon 11:30 H 0104

Dimensional Reduction at a Quantum Critical Point — •Cristian Batista — Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Competition between ground states near a quantum critical point is expected to lead to unconventional behavior in low dimensional systems. New phases of matter have been predicted, and explanations proposed for unsolved problems including non-Fermi liquid behavior and high temperature superconductivity using two-dimensional (2d) theories. In this talk, I will present a theory that describes the Bose-Einstein condensate (BEC) quantum critical point (QCP) in layered systems with a frustrated inter-layer coupling. I will demonstrate that the main effect of this geometric frustration is to reduce the dimensionality of the QCP (its critical exponents are the ones expected for a 2d system). In addition, I will present the first experimental evidence of dimensional reduction at a QCP observed in the Mott insulator $BaCuSi_2O_6$ (Han Purple).

TT 2.6 Mon 12:00 H 0104

Excitation hierarchy of the spin-1 large-D system $NiCl_2$-4SC$(NH_2)_2$ — •S.A. Zvyagin[1], J. Wosnitza[1], C.D. Batista[2], J. Krzystek[3], V.S. Zapf[4], M. Jaime[4], A. Paduan-Filho[5], M. Tsukamoto[6], and N. Kawashima[6] — [1]Hochfeld-Magnetlabor Dresden/Forschungszentrum Dresden - Rossendorf — [2]LANL, USA — [3]NHMFL, USA — [4]NHMFL/LANL, USA — [5]Sao Paulo University, Brzail — [6]ISSP, University of Tokyo, Japan

$NiCl_2$-4SC$(NH_2)_2$ (known as DTN) is an $S = 1$ chain system with the easy-plane anisotropy dominating over the exchange interaction (so-called large-D system) and a new candidate for studying the field-induced Bose-Einstein condensation of magnons. The excitation spectrum of DTN has been investigated by means of tunable-frequency ESR technique in fields up to 25 T. Based on analysis of the magnon excitation spectrum, a revised set of spin-Hamiltonian parameters was obtained. These values were used to calculate the AFM phase boundary, low-temperature magnetization and the frequency-field dependence of two-magnon bound-state excitations, predicted by theory and observed in DTN for the first time. Excellent quantitative agreement with experimental data was obtained.

[1] Phys. Rev. Lett. 98, 047205 (2007).

TT 2.7 Mon 12:15 H 0104

Exploring field-induced quantum phase transitions in molecule-based magnets — •Michael Lang[1], Katarina Removic-Langer[1], Yeekin Tsui[1], Ulrich Tutsch[1], Bernd Wolf[1], Andrei Prokofiev[1], Wolf Assmus[1], Roser Valenti[2], Andreas Honecker[3], Matthias Wagner[4], and Stefan Wessel[5] — [1]Phys. Inst. Univ. Frankfurt, SFB/TR 49 — [2]Inst. f. Theor. Physik, Univ. Frankfurt, SFB/TR 49 — [3]Inst. f. Theor. Physik, Univ. Göttingen — [4]Inst. f. Anorg. u. Analyt. Chemie, Univ. Frankfurt, SFB/TR 49 — [5]Inst. f. Theor. Physik III, Univ. Stuttgart

Molecule-based quantum magnets offer exciting new possibilities for exploring quantum many-body effects under variable and well-controlled conditions. Subjects of high current interest are the unusual magnetothermal effects close to a magnetic field-induced quantum critical point and the possibility to realize a Bose-Einstein condensation (BEC) of magnetic excitations. We focus here on Cu(II)-containing coordination polymers, which represent model systems with energy scales small enough for laboratory fields to tune the system close to their quantum critical points. We will discuss the magnetocaloric effect close to the saturation field of a uniform S = 1/2 antiferromagnetic Heisenberg chain and the field-induced BEC of magnetic excitations in a quasi-twodimensional coupled-dimer system.

TT 2.8 Mon 12:45 H 0104

Diverging low-temperature thermal expansion of the spin-ladder system $(C_5H_{12}N)_2CuBr_4$ — •Thomas Lorenz[1], Oliver Heyer[1], Markus Garst[2], Fabrizio Anfuso[2], Achim Rosch[2], Christian Rüegg[3], and Karl Krämer[4] — [1]Institue of Physics II, University of Cologne, Germany — [2]Institue of Theoretical Physics, University of Cologne, Germany — [3]Centre for Nanotechnology and Dep. of Phys. and Astronomy, University College London, UK — [4]Department of Chemistry and Biochemistry, University of Bern, Switzerland

The magnetic subsystem of piperidinium copper bromide $(C_5H_{12}N)_2CuBr_4$ represents a model system of an experimental realization of a two-leg spin-ladder Hamiltonian. Due to comparatively weak antiferromagnetic exchange couplings along the legs ($\simeq$ 12.9 K) and the rungs ($\simeq$ 3.6 K) of the ladders, two quantum phase transition are easily accessible in this compound: at $H_{c1} \simeq 6.8$ T the gap closes and at $H_{c2} \simeq 13.9$ T the field-polarized ferromagnetic state is reached. We present high-resolution measurements of the uniaxial thermal expansion and magnetostriction of $(C_5H_{12}N)_2CuBr_4$. For both quantities we observe pronounced anomalies arising from the pressure dependencies of the critical fields. The thermal expansion shows a very complex behavior with various sign changes and approaches a $1/\sqrt{T}$ divergence at the critical fields. All these low-temperature features are semi-quantitatively explained within a free fermion model; full quantitative agreement is obtained with Quantum Monte Carlo simulations.

Supported by the DFG through SFB 608.

TT 3: Transport: Fluctuations and Noise

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

TT 3.1 Mon 9:30 H 2053

Joint counting statistics of voltage and current — •Heidi Förster[1], Peter Samuelsson[2], and Markus Büttiker[1] — [1]University of Geneva, Switzerland — [2]Lund University, Sweden

Current through a conductor can be characterized by the statistics of transferred charge. Of importance are also internal properties like fluctuations of charge inside the coherent conductor, these quantities can be investigated using voltage and dephasing probes. We determine the joint distribution of charge transferred into contacts and voltage at a voltage probe and compare it with the joint distribution of transferred charge and average occupation number at a dephasing probe. Of particular interest is the manifestation of which path information in the current-voltage correlations in interferometers.

[1] H. Förster, P. Samuelsson, and M. Büttiker, New J. Phys. **9**, 117 (2007).

[2] H. Förster, P. Samuelsson, S. Pilgram, and M. Büttiker, Phys. Rev. B **75**, 035340 (2007).

[3] S. Pilgram, P. Samuelsson, H. Förster, and M. Büttiker, Phys. Rev. Lett. **97**, 066801 (2006).

TT 3.2 Mon 9:45 H 2053

Counting statistics of transport through non-Markovian systems — •Christian Flindt[1,2], Alessandro Braggio[3], Antti-Pekka Jauho[1,2], and Tomáš Novotný[4] — [1]Laboratory of Physics, Helsinki University of Technology, Finland — [2]MIC – Department of Micro and Nanotechnology, Technical University of Denmark, Denmark — [3]Dipartimento di Fisica, Università di Genova, Italy — [4]Department of Condensed Matter Physics, Charles University, Czech Republic

Current fluctuations have been promoted as a useful tool to probe the quantum dynamics of nanoscopic transport systems. In this contribution we describe a method for calculating the current cumulants of transport through systems described by non-Markovian generalized master equations. As an illustrative example, we consider transport through a Coulomb-blockade double quantum dot coupled to a dissipative heat bath [1]. We show how the cumulant generating function in the long time limit is determined by a single dominating pole of the memory kernel [2] and describe how the zero-frequency cumulants of the current can be extracted from this pole in a recursive manner. For the evaluation of the finite-frequency noise we show that not only the

full set of poles is important, but also initial system-bath correlations play a crucial role [3].

[1] R. Aguado and T. Brandes, PRL **92**, 206601 (2004)
[2] A. Braggio, J. König, and R. Fazio, PRL **96**, 026805 (2006)
[3] C. Flindt, A. Braggio, A.-P. Jauho, and T. Novotný, in preparation (2007)

TT 3.3 Mon 10:00 H 2053

Full Counting Statistics of a Quantum-Dot Aharonov-Bohm Interferometer — •Daniel Urban[1,2], Rosario Fazio[2,3], and Jürgen König[1] — [1]Ruhr-Universität Bochum — [2]Scuola Normale Superiore, Pisa — [3]International School for Advanced Studies, Trieste

The visibility of the interference signal in Aharonov-Bohm (AB) interferometers provides information about the coherence of transport channels. For instance, spin-flip processes in embedded quantum dots lead to partial destruction of the coherence [1] and thus reduction of the AB-oscillation amplitude. The occurrence of this effect depends on the dot occupation.

We perform a perturbation expansion of the Cumulant Generating Function [2] of an AB-Interferometer with embedded quantum dots in the regime of weak tunnel coupling. Different statistics are found for vanishing and infinite charging energy: Without interaction the interfering part of the statistics consists of non-resonant Poissonian processes with an even dependence on the AB-flux.

In the presence of strong interaction on the dot interaction gives rise to additional resonant processes with an odd flux dependence in non-equilibrium situations. In the regime where one dot-lead coupling is close to pinch-off, these processes consist of both single- and double-charge transfers.

[1] J. König and Y. Gefen, PRL **86**, 3855 (2001).
[2] A. Braggio, J. König, and R. Fazio, PRL **96**, 026805 (2006).

TT 3.4 Mon 10:15 H 2053

Full counting statistics of electronic transport through quantum-dot spin valves — •Stephan Lindebaum, Daniel Urban, and Jürgen König — Institut für Theoretische Physik III, Ruhr-Universität Bochum

We study the full counting statistics of electronic transport through a quantum dot weakly coupled to two ferromagnetic leads with non-collinear polarization directions. It is possible to generate a nonequilibrium spin accumulation on the dot which affects the spin valve characteristics of transport[1].
To investigate the system we perform a perturbative analysis of the transport properties to first order in the tunnel-coupling strength. A diagrammatic real-time transport theory enables us to calculate the cumulant generating function starting from a generalized master equation[2].
A comparision of the cumulants' dependence on the angle enclosed by the magnetizations reveals notable differences between the interacting and non-interacting case.

[1] M. Braun, J. König, and J. Martinek, Phys. Rev. B **70**, 195345 (2004).
[2] A. Braggio, J. König, and R. Fazio, Phys. Rev. Lett. **96**, 026805 (2006).

Invited Talk TT 3.5 Mon 10:30 H 2053

Noise and current cross-correlations in nano-electromechanical systems — •Christoph Bruder — Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel, Switzerland

After some general remarks about current cross-correlations in electronic (fermionic) three-terminal devices, I would like to focus on position measurements using the cross-correlated output of two tunnel junction position detectors. The bound on the peak-to-background ratio in a position measurement using a single detector can be overcome using detector cross-correlations. Furthermore, the double-detector setup can be exploited to drastically reduce the added displacement noise of the oscillator [C.B. Doiron, B. Trauzettel, C. Bruder, Phys. Rev. B **76**, 195312 (2007)].

I would also like to show that the momentum $\hat{p}$ of a nanomechanical oscillator can be measured [C.B. Doiron, B. Trauzettel, C. Bruder, arXiv: 0707.2709; accepted in PRL] by two tunnel junctions in an Aharonov-Bohm-type setup. The tunneling amplitude of one of the junctions depends linearly on the position $\hat{x}$ of the oscillator $t(\hat{x}) = t_0 + t_1\hat{x}$. The presence of two junctions can, under certain conditions, lead to an effective imaginary coupling $t(\hat{x}) = t_0 + it_1\hat{x}$. By calculating the equation-of-motion for the density matrix of the coupled (oscillator+tunnel junction) system, we show that in this case the finite-frequency current noise of the detector is proportional to the momentum spectrum of the oscillator.

Work done in collaboration with W. Belzig, C.B. Doiron, and B. Trauzettel.

Invited Talk TT 3.6 Mon 11:00 H 2053

Nonlinear dynamics and cooling in optomechanical systems — •Florian Marquardt — Arnold-Sommerfeld Center for Theoretical Physics, Center for NanoScience, und Department für Physik, Ludwig-Maximilians Universität München, Theresienstr. 37, 80333 München

This talk will provide an overview of ongoing developments and basic theoretical ideas concerning the manipulation of a mechanical cantilever using light-induced forces. During recent years, a series of experiments by various groups has exploited the resonant enhancement of light-induced forces in optical cavities to demonstrate both the emergence of nonlinear classical dynamics, with multiple attractors, as well as impressive progress in cooling. Ultimately, this line of research may lead to the quantum-mechanical ground state of the center-of-mass motion of objects composed of many billions of atoms. A recently developed theory of optomechanical cooling yields a quantum-limit for the reachable phonon number that can be made arbitrarily small, provided a high-finesse cavity is combined with a high-frequency cantilever. I will conclude with an outlook regarding the opportunities for quantum-coherent experiments that will open up once the ground state has been reached.

I thank J. Harris, K. Karrai, S. Girvin, A. A. Clerk, J. P. Chen, M. Ludwig, C. Neuenhahn, A. Ortlieb, C. Metzger, and I. Favero for collaboration on this topic.

15 min. break

TT 3.7 Mon 11:45 H 2053

Current correlations under AC-bias - quantum noise vs. photon-assisted transport — •Jan C. Hammer and Wolfgang Belzig — University of Konstanz, Department of Physics, Universitätsstr. 10, D-78464 Konstanz, Germany

We study coherent charge transport through a double barrier quantum dot coupled to metallic leads and driven by an AC-bias voltage. Such a voltage is produced e.g. by a laser irradiating a mesoscopic structure. For a resonant level this gives rise to photon-assisted tunneling events of electrons trough the system. The scattering formalism allows us to understand the conductance and the spectral properties of the non-symmetrized current-current correlators as an interplay between correlation induced antibunching and photon-assisted transport events. We discuss how these measurable quantities depend on the coupling to the leads, the applied bias voltage, the driving frequency and the structure of the energy levels inside the scattering region.

TT 3.8 Mon 12:00 H 2053

Noise spectra in mesoscopic transport - an exact result — •Philipp Zedler and Tobias Brandes — Sekr. EW 7-1, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The resonant level model, which is exactly solvable, provides us with the opportunity to check approaches to quantum noise in mesoscopic transport. We evaluate current cumulants using the exact Keldysh Green Functions. In this approach we can easily assume non-flat tunneling density of states and observe all quantum effects. We compare our results to those obtained with Master equations and scattering theory.

TT 3.9 Mon 12:15 H 2053

Vibrational coherences in tunneling through nanoscale oscillators — Hannes Hübener[1] and •Tobias Brandes[2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau, France — [2]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

Charging a nano-scale oscillator by single electron tunneling leads to an effective double-well potential due to image charges. We combine exact numerical diagonalizations with generalized Master equations and show [1] that the resulting quantum tunneling of the mechanical degree of freedom can be visualized in the electronic current noise spectrum.

[1] H. Hübener, T. Brandes; Phys. Rev. Lett. xxx (2007).

TT 3.10 Mon 12:30 H 2053

Decoherence by Quantum Telegraph Noise — •Benjamin Abel

and Florian Marquardt — Arnold-Sommerfeld Center for Theoretical Physics, Center for NanoScience and Department of Physics, Ludwig-Maximilians Universität München, Munich, Germany

We investigate the time-evolution of the density matrix of a charge qubit subject to quantum telegraph noise, produced by a single electronic defect level. We obtain strikingly different results for the time-evolution of the coherence from the case of Gaussian noise. Depending on the coupling strength of the qubit to the heat-bath and temperature we observe a qualitatively different behavior of the coherence. We simulated spin-echo sequences and discuss the time-evolution of the echo signal. Our analysis relies on a numerical evaluation of the exact solution for the density matrix of the qubit.

TT 3.11 Mon 12:45 H 2053

Non-Markovian dephasing in a structured environment — •Clive Emary — TU Berlin, Sekr. PN 7-1, Institut für Theoretische Physik, Hardenbergstr. 36, D-10623 BERLIN, Deutschland

We describe a theory of the non-Markovian behaviour of a quantum system coupled to an environment whose dynamics are governed by a generalised master equation. Such an environment can be, in general, far from equilibrium and exhibit strongly non-Gaussian fluctuations. We calculate the influence of such fluctuations on the system from a Dyson-like equation for the full system-environment propagator in Liouvillian space. We consider particular application to mesoscopic systems, such as a double quantum dot charge qubit, coupled to an environment of fluctuating charges. In the limit of classical environment with a "pure dephasing" coupling to a qubit, we obtain a relation between the long-time qubit dephasing rate, and a generalised full-counting statistics of the environment.

TT 4: Matter at Low Temperature: Materials

Time: Monday 9:30–11:15 Location: H 3010

Invited Talk TT 4.1 Mon 9:30 H 3010

Can nuclear spins reveal the nature of tunneling systems in glasses? — •Andreas Fleischmann — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

Most properties of amorphous materials at temperatures below 1K are caused by tunneling systems, which are assumed to be groups of atoms or molecules, cooperatively moving between two configurations of comparable energy. However, only little is known about the microscopic nature of these tunneling systems.

During the last years unexpected magnetic field effects were found in the dielectric properties of non-magnetic glasses at very low temperatures. These effects can be attributed to the tunnelling of atoms that carry nuclear quadrupole moments. As the electric quadrupole moments are interacting with the local electric field gradients, the nuclear states are coupled to the tunneling motion, resulting in energy levels and transition matrix elements that strongly depend on the atomic composition and the motion of the tunneling systems.

We present dielectric two-pulse polarization echo measurements on glasses, where the tunneling systems are coherently driven with two short microwave pulses. The observed amplitude of the spontaneous echo is strongly affected by the hyperfine structure that is introduced by the nuclear moments. The quantum beating that modulates the echo decay as well as the strong dependence of the echo amplitude on magnetic fields are found to be unique fingerprints for each glass and can be used to reveal information on the microscopic nature of the tunneling systems in these materials.

TT 4.2 Mon 10:00 H 3010

Impact of nuclear spins on two-pulse polarization echos in Glycerol. — •Masoomeh Bazrafshan, Gudrun Fickenscher, Celine Rüdiger, Marek Bartkowiak, Kathrin Reinhold, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut Für Physik,Universität Heidelberg

A few years ago surprising magnetic field effects were found in the dielectric properties of non-magnetic glasses at very low temperatures. For instance our 2-pulse polarization echo measurements on partially deuterated glycerol show strong magnetic field dependecies. It has since been established that this effect can be attributed to the tunneling motion of groups of molecules that carry nuclear quadrupole moments, between two different configurations of almost equal energy. This magnetic field effect saturates at about 60mT, when the nuclear Zeeman energy becomes larger than the quadrupole splitting. However, detailed studies have shown that one component of these magnetic effects saturates already at about 10 times smaller field. We have shown that the origin of this effect is the interaction of nuclear magnetic dipole moments of the hydrogen atoms in glycerol. Both effects are visible in the magnetic field dependence of the echo amplitude and a quantum beating at zero field which we have studied systematically on a series of glycerol samples with different degrees of deuteration. Numerical calculations were performed and compared to the experimental observations which enables us to probe the microscopic nature of tunneling systems in amorphous glycerol.

TT 4.3 Mon 10:15 H 3010

Structural phase transition in $CdCr_2O_4$ probed by far-infrared spectroscopy — •Torsten Rudolf[1], Christian Kant[1], Joachim Deisenhofer[1], Franz Mayr[1], Vladimir Tsurkan[1,2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chişinău, Republic of Moldova

Strongly frustrated single crystalline $CdCr_2O_4$ [1] was investigated by means of Fourier Transform infrared spectroscopy. The temperature dependence of the far-infrared phonon spectrum was studied from 5 to 300 K. The space group of $CdCr_2O_4$ at room temperature is $Fd\bar{3}m$ and group theory predicts four infrared active phonon modes, which is verified by experiment. The formation of a pyrochlore lattice by the chromium ions leads to a strong geometric frustration in this spinel system, represented by a high frustration parameter $f \approx 9$. It is examined whether below the Néel temperature T_N the magnetic ground state degeneracy is rather lifted by a lattice distortion or by a magnetic exchange induced symmetry breaking. However, due to a strong spin-phonon coupling each single phonon mode shows a splitting below $T_N \approx 8$ K. At 5 K the reflectivity data can be fitted with nine phonons via a generalized oscillator model using four parameters per mode. Dielectric loss data, calculated via the Kramers-Kronig transformation, even uncover a splitting into more than nine phonon modes.

[1] T. Rudolf *et al.*, New J. Phys. **9**, 76 (2007)

TT 4.4 Mon 10:30 H 3010

Spin-phonon interactions in antiferromagnetic transition metal monoxides — •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

Spin-phonon coupling in correlated matter gained a lot of attention in contemporary solid state physics. A fact which was triggered by the observation of phonon splittings in several spinel compounds [1]. Since transition metal monoxides like MnO or NiO are paramount examples for correlated electron systems and Mott-Hubbard insulators it seems to be straightforward to reinvestigate these compounds.

We performed temperature dependent measurements on MnO and NiO by means of far-infrared spectroscopy[2]. The obtained phonon spectra were analyzed in detail. Special attention is focused to the phonon splitting accompanying the transition into the magnetically ordered state.

[1] T. Rudolf *et al.*, New J. Phys. **9**, 76 (2007)
[2] T. Rudolf *et al.*, *Preprint* arXiv:0707.0820

TT 4.5 Mon 10:45 H 3010

$AECa_4(CoN_2)_2$, AE = Ca, Ba: $S = 1$ Realization of Shastry-Sutherland Model with Interlayer Interactions — •Alim Ormeci[1], Joanna Bendyna[1], Peter Höhn[1], Rüdiger Kniep[1], Johannes Richter[2], Walter Schnelle[1], and Helge Rosner[1] — [1]Max-Planck-Institut für Chem. Phys. fester Stoffe, Dresden — [2]Institut für Theoretische Physik, Universität Magdeburg, Magdeburg

Recently the tetragonal alkaline-earth nitridocobaltate compounds $BaCa_4(CoN_2)_2$ and $Ca_5(CoN_2)_2$ were synthesized [1]. The crystal

structures of these compounds have in the unit cell two Co layers separated by $c/2 \sim 6.1$ Å. Remarkably each Co layer has the lattice structure of the Cu^{2+} spins known from $SrCu_2(BO_3)_2$. The Co ions in these compounds have two missing d electrons (s^1d^8 configuration) so that they form a spin 1 system. Until now, the $S = 1/2$ system, $SrCu_2(BO_3)_2$, has been the only known realization for the Shastry-Sutherland model. The two nitridocobaltates are suggested as the first $S = 1$ realization of this model. Magnetic measurements and first-principles electronic structure calculations (based on the full-potential local orbital, FPLO, method) indicate, however, that the interlayer interactions are non-negligible. Therefore, one has to deal with a modified model of two Shastry-Sutherland layers coupled to one another. Results of first-principles and model Hamiltonian calculations will be compared with experimental data, and the implications will be discussed.

[1] J.K.Bendyna, P.Höhn, R.Kniep, Z. Kristallogr. NCS **222** (2007), CSD no. 409920 and 409921.

TT 4.6 Mon 11:00 H 3010

Effect of the Magnetic Field on the Coulomb Gap — •Barbara Sandow[1], Dirk Brossell[1], Olaf Bleibaum[2], and Walter Schirmacher[3] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg, Germany — [3]Physik-Department E13, Technische Universität München, Germany

We used break-junction tunnelling spectroscopy to investigate the Coulomb correlation in n-type Germanium. The doping concentration was smaller than the critical concentration for the metal-insulator (Anderson) transition. The tunnelling conductance, which probes the electronic density of states, was found to depend strongly on voltage, temperature and magnetic field.

At low temperatures the differential conductance shows a minimum at zero voltage, as expected for a material with a Coulomb gap near the Fermi energy. Applying a magnetic field up to B = 8 Tesla at T = 0.1 K to 1 K reduces the magnitude of the tunnelling conductance. Furthermore our data on n-type Germanium seem to indicate a strong suppression of the Coulomb gap in large fields. This could be due to the field-induced shrinking of the electron wave functions that strongly reduces the overlap between the localized electron states. Using our theory of break-junction tunnelling in the hopping regime [1] we are able to explain the disappearance of the Coulomb gap in high magnetic fields.

[1] O. Bleibaum, B. Sandow, W. Schirmacher, Phys. Rev. B 70, 045308-1 (2004)

TT 5: Superconductivity - Cryodetectors

Time: Monday 11:30–13:00 Location: H 3010

TT 5.1 Mon 11:30 H 3010

SABOCA - a multiplexed 37 channel bolometer camera for 350 micrometer wavelength — Torsten May[1], Viatcheslav Zakosarenko[1], Andre Krueger[1], Solveig Anders[1], Katja Peiselt[1], •Hans-Georg Meyer[1], Ernst Kreysa[2], Giorgio Siringo[2], and Walter Esch[2] — [1]Institute of Photonic Technology, Albert-Einstein-Str. 9, D-07745 Jena, Germany — [2]Max-Planck-Institute for radio astronomy, Auf dem Huegel 69, D-52888 Bonn, Germany

Some of the most interesting objects in the Universe are only accessible through astronomical observations in a so far only sparsely used atmospheric window at sub millimeter wavelengths. The sub millimeter emission from molecular spectral lines and from warm dust allows an almost unhindered, unique view onto ongoing star forming regions and galactic nuclei, from our own Milky Way to the most distant galaxies and quasars in the early Universe. One of the best accessible sites for submillimeter observations is the high plateau Llano de Chajnantor in Chile's Atacama desert. At 5000 meter altitude APEX (Atacama Pathfinder Experiment), a 12 meter radio telescope, has seen first light in 2005. Due to its high surface accuracy this instrument is particularly suited to utilize one of last atmospheric radio windows on earth: the 350 micron band. The Small Array BOlometer CAmera (SABOCA) is scheduled to operate at APEX in spring 2008. It is an array of 37 transition edge sensors operated at a temperature of 300 mK, provided by a 3He sorption cooler on a cryostat with liquid 4He. The instrument is read out by SQUID current sensors in a time domain multiplexing scheme. Four integrated multiplexer chips, 10 first stage SQUIDs each, are placed next to the detector chip, operating at the same temperature. Every multiplexer chip is coupled to one amplifier SQUID. The four amplifier SQUIDs are placed at the 4He stage, with a temperature of 1.5K during operation. The signals are acquired by room temperature electronics and digitized by 24bit A/D converters. The data acquisition system limits the system clock to 2 kHz, resulting in an effective data rate of 200 Hz per channel.

TT 5.2 Mon 12:00 H 3010

Numerical Optimization of the Energy Resolution of Magnetic Calorimeters — •J.-P. Porst, A. Burck, C. Domesle, C. Höhn, S. Kempf, S. Lausberg, A. Pabinger, C. Pies, S. Schäfer, R. Weldle, A. Fleischmann, L. Fleischmann, and C. Enss — Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg

We present numerical optimizations of the energy resolution of metallic magnetic calorimeters (MMC) with paramagnetic Au:Er temperature sensors. Energy deposited in such a detector leads to a change of magnetization of the paramagnetic sensor located in a weak magnetic field. SQUIDs are used to detect this change. The response of a MMC upon the deposition of energy depends on several parameters including the absorber heat capacity, the thermodynamic properties of the sensor material, and the geometry of the temperature sensor and the pickup loop. The specific heat and the magnetization of Au:Er can be calculated numerically with confidence. Furthermore, the following noise contributions are considered in these calculations: the thermodynamic fluctuations of energy, the magnetic Johnson noise, the flux noise of the SQUIDs and the 1/f-noise, so far observed in Au:Er-based MMCs. All mentioned noise contributions are parameterized. We performed a numerical optimization of the signal to noise ratio and thus the energy resolution of MMCs for different applications with absorber heat capacities ranging from 1 pJ/K to 1 nJ/K. The optimal parameters found, like shape and size of sensor and pickup coil, concentration of magnetic ions and the optimal magnetic field are presented. The contribution of each noise source to the detector performance is discussed.

TT 5.3 Mon 12:15 H 3010

SQUID based readout and characterization of superconducting single photon detectors — •Alexander Kirste[1], Dietmar Drung[1], Jörn Beyer[1], Margret Peters[1], Thomas Schurig[1], Philipp Haas[2], Alexei Semenov[2], Heinz-Wilhelm Hübers[2], Konstantin Ilin[3], Michael Siegel[3], Rudolf Herrmann[4], and Hans-Ulrich Müller[4] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]German Aerospace Center (DLR), Rutherfordstr. 2, 12489 Berlin — [3]University of Karlsruhe, Hertzstr. 16, 76187 Karlsruhe — [4]Institut für angewandte Photonik, Rudower Chaussee 29, 12489 Berlin

We report on the readout and the characterization of nanostructured superconducting single photon detectors using SQUID arrays.

As the detectors allow photon counting with a modest energy resolution, it is important to use preamplifiers of high bandwidth and low noise. For this purpose SQUID arrays are a favourable choice as they are intrinsically wide-band and offer a low noise.

For the detector readout we apply SQUID arrays containing up to 640 single SQUIDs. These arrays have a white flux noise of 0.06 $\mu\Phi_0/\mathrm{Hz}^{1/2}$ at 4.2 K and a low dynamic impedance so that they are adequate to drive a following broadband microwave amplifier. Since the relevant time constants of the detector and the resulting duration of the voltage transients are intrinsically sub-ns, the SQUID is operated in AMP mode rather than in FLL mode. Using the internal preamplifier of the SQUID electronics XXF-1 with 50 MHz bandwidth, the voltage pulses at the output have a duration of 13 ns (FWHM).

TT 5.4 Mon 12:30 H 3010

Development of a terahertz heterodyne receiver with a superconducting hot electron bolometric mixer and a quantum cascade laser — •Heiko Richter[1], Heinz-Wilhelm Hübers[1], Sergey Pavlov[1], Alexei Semenov[1], Kostea Il'in[2], Michael Siegel[2],

Lukas Mahler[3], Alessandro Tredicucci[3], Harvey Beere[4], and David Ritchie[4] — [1]DLR, Institut für Planetenforschung, Rutherfordstr. 2, 12489 Berlin — [2]Institut für Mikro- und Nanoelektronische Systeme, Hertzstr. 16, 76187 Karlsruhe — [3]NEST-INFM and Scuola Normale Superiore,Piazza dei Cavalieri 7, 56126 Pisa, Italien — [4]Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, England

We will report on the development of a terahertz (THz) heterodyne receiver with a superconducting hot electron bolometric (HEB) mixer and a quantum cascade laser as local oscillator for applications in astronomy, planetary research or security. The intermediate frequency bandwidth, noise temperature and antenna pattern of the mixer have been measured at several frequencies between 0.6 and 5 THz. Based on these results we have started the development of a cryogen-free heterodyne receiver with the QCL and the HEB mixer mounted in the same pulse tube cooler. First results obtained with this system will be reported.

TT 5.5 Mon 12:45 H 3010

Performance enhancement of a superconducting nanowire single-photon detector at low temperatures — •Alexej Semenov[1], Phillip Haas[1], Heinz-Wilhelm Huebers[1], Konstantin Il'in[2], Michael Siegel[2], and Rudolf Herrmann[3] — [1]DLR Institute of Planetary Research, 12489 Berlin, Germany — [2]Institute of Micro- and Nano-Electronic Systems, University of Karlsruhe, 76187 Karlsruhe, Germany — [3]Institute of Appplied Photonics, 12489 Berlin, Germany

We report on the low-temperature operation of superconducting nanowire single-photon detectors. The nanowires were patterned from a 5-nm thick B1 niobium nitride film to form a 100-nm wide meander-line. NbN films had a quality assuring the Ginsburg-Landau deparing current in the detector structures at all temperature below the transition temperature. At 6 K operation, a resolution of 0.55 eV was measured in the wavelength range from 1000 nm to 1500 nm along with the quantum efficiency of a few percent for ultra-violet and visible-light quanta. Decreasing operation temperature to 1.4 K with a ^{3}He sorption refrigerator combined with a mechanical pulse-tube cooler, we found a threefold increase in the quantum efficiency and an almost 50% improvement of the energy resolution. The quantum efficiency at low temperatures was limited to the absorbance of the structure. Although the energy resolution and single-photon detection ability is better explained by an unbinding of vortex-antivortex pairs, the observed temperature enhancement of the detector perfermance is most likely due to the non-homogeneity of the meander-line.

TT 6: Correlated Electrons: Heavy Fermions

Time: Monday 9:30–12:45 Location: EB 202

TT 6.1 Mon 9:30 EB 202

Crystal-field ground states of CeX_2Si_2 (X= Cu, Ru, Rh,Pd, and Au) determined by linear polarized soft x-ray absorptionat the Ce $M_{4,5}$ edges — •T. Willers[1], A. Severing[1], C.-F. Chang[1], P. Hansmann[1], M.W. Haverkort[1], N. Hollmann[1], Z. Hu[1], H.J. Lin[2], C.T. Chen[2], H. Aoki[3], E. Bauer[4], C. Geibel[5], P. Lejay[6], and L.H. Tjeng[1] — [1]Institute of Physics II, University of Cologne,Germany — [2]National Synchrotron Radiation ResearchCenter, Taiwan — [3]Center for Low TemperaturePhysics, Tohoku University, Sendai, Japan — [4]LosAlamos National Laboratory, NM, USA — [5]MPI fürChem. Physik fester Stoffe, Dresden, Germany — [6]Institut Néel, CNRS, Grenoble, France

Knowledge of the spatial distribution of the 4f wave function in rare-earth Heavy-Fermion systems forms one of the basic ingredients for the modelling of their unusual and exotic properties. In the past, neutron scattering as the standard technique to determine the crystal-field scheme has often given contradicting results Here we use an alternative method. We have recently shown that polarization dependent soft-x-ray absorption spectroscopy is a powerful tool to probe the charge distribution of the crystal-field ground state of Ce ions. Through the polarization dependence we obtain direct spectroscopic information about the various Jz admixtures of the ground state. The so-called linear dichroic signal at the Ce $M_{4,5}$ edges can be very large and is easily measured, thereby providing accurate quantitative information. A systematic investigation of the 4f ground state wave function will be presented for the CeX_2Si_2 series (X=Cu, Ru, Rh, Pd, Au).

TT 6.2 Mon 9:45 EB 202

Do magnetism and superconductivity coexist in $CeCu_2Si_2$ with 2 % and 10 % Ge doping? — •J. Arndt[1,2], O. Stockert[1], M. Deppe[1], H.S. Jeevan[1], K. Schmalzl[3], A. Schneidewind[2,4], C. Geibel[1], and F. Steglich[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]FRM-II, TU München, Germany

$CeCu_2Si_2$, the first discovered heavy-fermion superconductor, exhibits different ground states in subtle dependence on the exact stoichiometry: It shows either incommensurate magnetic order (A), superconductivity (S), or both phenomena (A/S). Ge doping decreases the hybridisation between the localised Ce 4f and the conduction electrons, and therefore allows for studying the evolution of superconductivity in the presence of a stabilised magnetic A phase. Cu-NQR measurements on polycrystals of $CeCu_2(Si_{0.98}Ge_{0.02})_2$ give indications of a coexistence of superconductivity and antiferromagnetism. We performed elastic neutron scattering on a single crystalline sample, which was mounted on a susceptibility set-up. The simultaneous recording of the susceptibility during the neutron measurement gives us the opportunity to follow the onset of superconductivity in-situ. Our results clearly indicate that, analogous to the situation in A/S $CeCu_2Si_2$, a phase separation between magnetic and superconducting volumes takes place, with a small magnetic volume fraction persisting down to low temperatures. These findings will be compared to results on 10 % Ge doped $CeCu_2Si_2$.

TT 6.3 Mon 10:00 EB 202

Investigation of the magnetic and the superconducting states of $CeCu_2(Si_{1-x}Ge_x)$ using single crystals — •Hirale S Jeevan[1], Takeshi Nakanishi[1], Julia Arndt[1], Enrico Faulhaber[2], Oliver Stockert[1], Micha Deppe[1], Tomasz Cichorek[1], Frank Steglich[1], and Christoph Geibel[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Gemany — [2]TU Dresden, IAPD, D-01062 Dresden, Germany

The discovery of superconductivity in $CeCu_2Si_2$ in 1979 opened the field of unconventional superconductivity in strongly correlated systems. Later on, another unconventional phase, the A-phase, of magnetic character was found to compete with the superconducting phase in $CeCu_2Si_2$. Recent neutron experiment confirms that the A-phase is nothing but the long range antiferromagnetic order, spin density wave type due to nesting of heavy Fermi surface. And in pure $CeCu_2Si_2$ it was shown that the long range magnetic phase and superconducting phase compete each other. Here we investigate the magnetic and the superconducting states in a series of Ge substituted single crystals $CeCu_2(Si_{1-x}Ge_x)$ with x = 0.02 and 0.1. Ge substitution has two effect, stabilises the magnetic phase due to expansion of the lattice, but it also induce disorder effect. Based on the earlier results on polycrystalline samples, we expect the possible co-existing of both long range magnetic phase and superconducting phase in some Ge concentration range. We shell analyse and discuss the single crystal growth, physical properties and neutron scattering measurements of these Ge substituted single crystals.

TT 6.4 Mon 10:15 EB 202

Magnetoresistance and anomalous Hall effect in ferromagnetic $CeSi_{1.81}$ — •Robert Ritz[1], Andreas Neubauer[1], Stefan Legl[1], Christian Pfleiderer[1], Dmitri Souptel[2], and Günter Behr[2] — [1]Physik-Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Leibniz-Institut für Festkörper-und Werkstoffforschung(IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany

As function of Si content the series $CeSi_x$ changes from an antiferromagnetic ground state for $x = 1$ to paramagnetism for $x = 2$. An abrupt magnetic to non-magnetic transition is observed just below $x = 2$, where single crystals with $x = 1.81$ exhibit an essentially ferromagnetic ground state below $T_C \approx 9.5\,\mathrm{K}$ that vanishes rapidly under

pressure [1]. We report a comparison of the low-temperature magnetoresistance and anomalous Hall effect in $CeSi_{1.81}$ with the uniform magnetization and specific heat. The longitudinal magnetoresistance suggests the additional formation of a density wave below $T_x \approx 3\,\mathrm{K}$. We also find that the spontaneous anomalous Hall effect initially tracks the ordered moment, where deviations below $\sim T_C/2$ suggests the emergence of additional magnetic modulations. Well below T_C a small hysteresis in the Hall effect exists up to $B_m \sim 4\,\mathrm{T}$, the location of an S-shaped increase in the magnetization that is naively interpreted as itinerant metamagnetism. This may hint at a novel interplay between itinerant metamagnetism and structural defects. [1] S. Drotziger, et al., Phys. Rev. B **73**, 214413 (2006).

TT 6.5 Mon 10:30 EB 202

A precursor state to unconventional superconductivity in the heavy fermion superconductor $CeIrIn_5$ — •Sunil Nair[1], S. Wirth[1], M. Nicklas[1], J. L. Sarrao[2], J. D. Thompson[2], Z. Fisk[3], and F. Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, Dresden 01187, Germany. — [2]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA. — [3]University of California, Irvine, California 92697, USA.

The $CeMIn_5$ (where M: Co, Rh or Ir) family of heavy fermion systems is currently in vogue; not only for the host of novel properties they exhibit in its normal and superconducting states, but also for the rather striking resemblance many of these properties have with the cuprate high temperature superconductors. Here, we present sensitive measurements of the Hall effect and magnetoresistance in $CeIrIn_5$, in the temperature range $0.05\,\mathrm{K} \leq T \leq 2.5\,\mathrm{K}$ and magnetic fields up to 15 T. The magnetoresistance is used to demarcate the presence of a low temperature Kondo coherent state. Furthermore, by means of Kohler's scaling plots, the crossover from a Landau-Fermi liquid to a non-Fermi liquid regime is inferred. The functional form of the Hall resistivity is observed to be in concurrence with that expected for a compensated metal. The most striking observation pertains to the presence of a precursor state to superconductivity characterized by a change in the Hall scattering rate, in similarity to the pseudogap state in the cuprates. Moreover, the critical fields of the precursor state and the superconducting one can be scaled on to each other, implying that they could arise from the same underlying physical mechanism.

TT 6.6 Mon 10:45 EB 202

Pressure and concentration tuning of $CeNi_xPt_{1-x}$ compounds — •Nadezda Bagrets[1], Veronika Fritsch[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The intermetallic alloys $CeNi_xPt_{1-x}$ are examples of heavy-fermion compounds that can be tuned to the quantum critical point (QCP) by applying hydrostatic pressure [1] or by changing the ratio between Pt and Ni constituents (chemical pressure). The pure CePt compound orders ferromagnetically (FM). With increasing Ni content, FM order is suppressed and disappears completely at x = 0.95 possibly indicating a QCP [2]. CeNi is a Pauli paramagnet. At the same time, these compounds have orthorhombic CrB type of crystal structure for all compositions. We compare the effects of hydrostatic and chemical pressure on the magnetic properties of the series $CeNi_xPt_{1-x}$ in the whole concentration range between x = 0 and 1 and, in particular, in the vicinity of the QCP. We have performed measurements of the magnetization in the temperature range 2.5 - 300 K in magnetic field up to 0.1 T under hydrostatic pressure up to 1.2 GPa for $CeNi_xPt_{1-x}$ samples with different Ni content.

[1] J. Larrea at al., Phys. Rev. B 72, 035129 (2005)
[2] J. Espeso at al., Phys. Rev. B 63, 014416 (2000)

15 min. break

TT 6.7 Mon 11:15 EB 202

Relevance of the pseudogap for the thermopower of CeNiSn — •Ulrike Köhler[1], Peijie Sun[1], Toshiro Takabatake[2], Silke Paschen[3], Niels Oeschler[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]Hiroshima University, Japan — [3]Vienna University of Technology, Austria

CeNiSn has been classified as a correlated semimetal with a low charge carrier concentration. The opening of an anisotropic pseudogap below 10 K has been confirmed from various experimental probes. The gap formation can be suppressed significantly by application of magnetic fields of 10 T along the easy a axis.

We performed thermopower and Nernst effect measurements on high-purity single crystals of CeNiSn in the temperature range between 1.5 K and 200 K and in magnetic fields up to 7 T. Special care has been taken to correct the thermopower S for contributions from transverse components in a magnetic field. Our data clearly demonstrate the relevance of the pseudogap for the low-T thermopower. $S(T)$ exhibits a large negative minimum below the temperature, at which the gap opens. Upon increasing magnetic field the minimum shifts to lower T wheras the absolute values at the minimum increase. We apply a simple model to describe this unusual field dependence of the thermopower.

TT 6.8 Mon 11:30 EB 202

The new Heavy Fermion System CeFePO: A ^{31}P NMR study — •Eva Maria Brüning, Michael Baenitz, Cornelius Krellner, Christoph Geibel, and Frank Steglich — Max-Planck-Institut für Chemische Physik fester Stoffe

Among the CeTPO system (T = Ru, Os, Co, Fe), CeFePO is particular interesting because it presents Heavy Fermion behavior. Specific heat measurements above 400 mK clearly show the absence of magnetic order and a strongly enhanced Sommerfeld ratio $\gamma = 700\,\mathrm{mJ/molK^2}$, comparable to $CeCu_2Si_2$. ^{31}P NMR field sweep measurements were performed at different fields (4.4 T and 1.5 T) and temperatures (2 K to 300 K). ^{31}P Knight shift $^{31}K(T)$ shows a field independent Curie-Weiss like behavior above 100 K consistent with $\chi(T)$ measurements, whereas towards lower temperatures a saturation occurred due to Kondo interaction. $^{31}K(T)$ vs. $\chi(T)$ gives a hyperfine coupling constant of $A_{\mathrm{hf}} = 2\,\mathrm{kOe}/\mu_B$. $^{31}(1/T_1)$ measurements were carried out at different fields (4.4 T and 1.5 T). $^{31}(1/T_1T)(T)$ is field independent and shows a strong increase towards lower temperatures and a saturation towards an enhanced Korringa value for $T \rightarrow 0$, indicating a large $N(E_F)$ value. $^{31}(1/T_1T)$ is qualitatively similar to the ^{29}Si NMR results on $CeCu_2Si_2$ (7 T). Using ^{31}P as a local probe, our ^{31}P NMR results strongly confirm the Heavy Fermion scenario for this new compound.

TT 6.9 Mon 11:45 EB 202

ESR Study on CeRuPO single crystals — •Tobias Förster, Jörg Sichelschmidt, Cornelius Krellner, and Christoph Geibel — Max Planck Institut f. Chemische Physik Fester Körper, Nöthnitzer Str. 40, 01187 Dresden, Germany

Until 2003 it was believed that the Electron Spin Resonance signal (ESR) from a Kondo ion in a dense Kondo system is not observable, because of the strong broadening due to 4f/5f- conduction electron hybridization. Hence the first observation of such a signal in $YbRh_2Si_2$ was a big surprise[1]. Very recently we found further Yb- and Ce-compounds that show well defined ESR signals [2].
In this contribution we will concentrate on single crystal data from the ferromagnetic Kondo-lattice system CeRuPO[3]. The recorded spectra show an asymmetry which is related to the local Ce^{3+}ion (Γ_6 wave function) in tetragonal point symmetry. This is surprising because to the best of our knowledge an ESR signal due to dense Ce^{3+} magnetic moments in an environment with conduction electrons has only been reported for CeP. This unexpected result is neither specific to Ce-based compounds nor to compounds with Kondo-like properties nor to the proximity of a (quantum) critical point. It turns out that strong ferromagnetic correlations in the electronic system are essential for the ESR observability of concentrated magnetic ions in intermetallic systems.[2]

[1] J. Sichelschmidt et al., Phys. Rev. Lett. 91, 156401 (2003)
[2] C. Krellner et al., submitted to Phys. Rev. Lett.
[3] C. Krellner et al., Phys. Rev. B 76,104418 (2007)

TT 6.10 Mon 12:00 EB 202

Low-temperature thermodynamic and magnetic properties of the geometrically frustrated Kondo lattice $Pr_2Ir_2O_7$ — •Jan Guido Donath[1], Philipp Gegenwart[2], Satoru Nakatsuji[3], and Yo Machida[3] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581 Japan

The ground state of f-electron Kondo-lattice systems is determined by the interplay of the Kondo- and the RKKY interaction, leading to a quantum critical point separating long-range magnetic order from paramagnetism. The interesting question arises, how this situation is modified in the presence of strong magnetic frustration. Here, we focus on the iridate $Pr_2Ir_2O_7$ which crystallizes in the highly frustrated

pyrochlore structure and has recently been proposed as a realization of a metallic spin liquid [1]. We present low-temperature thermodynamic (specific heat and thermal expansion) and magnetic properties of slightly off-stoichiometric $Pr_2Ir_2O_7$ single crystals.

[1] S. Nakatsuji *et al.*, PRL **96**, 087204 (2006)

TT 6.11 Mon 12:15 EB 202

Enhanced thermopower and related phenomena in the narrow-gap semiconductor $FeSb_2$ — •Peijie Sun[1], Niels Oeschler[1], Ulrike Köhler[1], Simon Johnsen[2], Bo Brummerstedt 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

A huge Seebeck coefficient of several tens of mV/K around 10 K was found in $FeSb_2$ [1], which shares considerable similarity with the Kondo insulator FeSi with a narrow semiconducting gap. The origin of the enhanced thermopower is yet to be understood. Strong electronic correlation producing enhanced DOS near Fermi level seems to be one possible reason.

We report new results of the Hall effect, specific heat and Nernst effect on high quality single crystals to study the effect of strong correlation. A smaller energy gap of about 50 K was detected in electrical resistivity and Hall coefficient, besides the well known gap at above 300 K. The appearance of the smaller gap accompanies a shoulder in resistivity and a huge peak in Hall coefficient, and thus could be closely related to the enhanced Seebeck coefficient that occurs in the same temperature range.

[1] A. Bentien et al., Europhys. Lett. 80 (2007) 17008.

TT 6.12 Mon 12:30 EB 202

Optical Studies on the Strongly Correlated Semiconductor $FeSb_2$ and on $RuSb_2$ — •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 Århus C, Denmark

The narrow band gap semiconductor $FeSb_2$ has similar properties to FeSi and both materials are discussed in the framework of a Kondo insulator model. We measured the optical conductivity of single crystals of $FeSb_2$ from 3 meV up to 30 eV by means of reflectivity spectroscopy. We compare the spectra of $FeSb_2$ with those of its non-magnetic homologue $RuSb_2$. In contrast to previous reports [1], our samples of $FeSb_2$ are semiconducting for all crystal axes. The far-infrared optical spectra are characterized by both phononic and electronic contributions. The phononic part displays a strong electron-phonon coupling at elevated temperatures whereas the electronic part presents an indirect gap of 30 meV which agrees well with the value inferred from transport measurements [2]. Another gap feature at 6 meV is probably related to the extraordinary large Seebeck coefficient of $FeSb_2$ [2]. We observed a temperature dependent spectral weight redistribution within a large energy range which clearly extends 1 eV indicating the presence of strong electronic correlations.

[1] A. Perucchi et al., Eur. Phys. J. B **54**, 175 (2006)
[2] A. Bentien et al., Europhys. Lett. **80**, 39901 (2007)

TT 7: Matter at Low Temperature: Poster Session

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

TT 7.1 Mon 14:00 Poster B

Combined experimental and computational study of structure and electronic properties of the chalcogenide-free phase-change material Ge_xSb_{100-x} — •Peter Zalden, Dominic Lencer, Michael Klein, Martin Salinga, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Phase Change Random Access Memory (PCRAM) has turned out to be the most promising candidate for future non-volatile memory cells. A PCRAM cell features a reversibly switchable phase change material, whose electrical resistance differs significantly between the crystalline and a melt-quenched amorphous phase. Suitable materials need to be capable of ultrafast switching between the two phases. $Ge_{15}Sb_{85}$ has been reported to be such a material, that - unlike conventional phase change materials, like $Ge_2Sb_2Te_5$ - is free of chalcogenides.

In this study, structural modifications in sputtered thin films during the phase change from the as-deposited amorphous to the crystalline phase are analysed, employing a combination of Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD). This survey includes a determination of transition temperatures, an investigation of crystallization kinetics and structural properties of polycrystalline films. Complementary, the structure of crystalline compositions of Ge_xSb_{100-x} is object of an *ab initio* study. Density Functional Theory (DFT) is employed allowing to study the variation of structural and electronic properties upon the addition of germanium. A comparison to conventional tellurium based phase change materials is presented and in conclusion the suitability for PCRAMs is evaluated.

TT 7.2 Mon 14:00 Poster B

Measurements of amorphous and nanocrystalline ferromagnetic materials at low temperatures — •René Geithner, Alexander Steppke, Ralf Neubert, Wolfgang Vodel, and Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena, Deutschland

For high-precision measurements of voltages and currents at low temperatures low-temperature superconducting DC SQUID sensors are successfully used in a wide range of applications. For an efficient coupling between the transducer and the readout DC SQUID superconducting transformers can be used. The transformer core should have a high relative permeability, even at temperatures below 4.2 K, to miniaturise the sensor. Additionally transfomers can directly be used to pickup electromagnetic fields, where the sensitivity is directly coupled to the core material. As the permeability of standard iron powder cores decreases rapidly for temperatures below 50 K we are investigating amorphous and nanocrystalline materials. We show first results of the permeability of Vitrovac, Vitroperm (VAC Hanau) and Nanoperm (Magnetec GmbH) over a wide temperature range from 300 K to 2 K. Measurements on the magnetic losses and associated noise figures are presented in respect to the permeability.

TT 7.3 Mon 14:00 Poster B

High mechanical Q-factor measurements on silicon bulk material — •Christian Schwarz[1], Ronny Nawrodt[1], Daniel Heinert[1], Anja Schroeter[1], Ralf Neubert[1], Matthias Thürk[1], Wolfgang Vodel[1], Andreas Tünnermann[2], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

The direct observation of gravitational waves is one of the biggest challenges in science. Current detectors are limited by different kinds of noise. One of the fundamental noise sources is thermal noise arising from the optical components. One of the most promising attempts to reduce the thermal noise contribution in future detectors will be the use of high Q-factor materials at cryogenic temperatures. Silicon seems to be the most interesting material due to its excellent optical and thermal properties. We present high Q-factor measurements on bulk samples of high purity silicon in a temperature range from 5 to 300 K. The sample dimensions vary between $\varnothing$ 76.2 mm × 12...75 mm. The Q-factor exceeds $4 \cdot 10^8$ at 6 K. The influence of the crystal orientation, doping and the sample preparation on the Q-factor is discussed.

This work is supported by the German science foundation under contract SFB Transregio 7.

TT 7.4 Mon 14:00 Poster B

Mechanical loss mechanisms in crystalline quartz — •Daniel Heinert[1], Anja Schroeter[1], Christian Schwarz[1], Ronny Nawrodt[1], Ralf Neubert[1], Matthias Thürk[1], Wolfgang Vodel[1], Andreas Tünnermann[2], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Crystalline quartz is an excellent material to study internal dissipation mechanisms. Low loss materials are in great demand for future

gravitational wave detectors reducing their thermal noise level within the detection band. Therefore, a deeper understanding of the loss mechanisms is necessary which depend on different parameters like the crystal orientation or the concentration of impurities. We present a detailed investigation of crystalline quartz samples ($\varnothing$ 45 mm × 50 mm) at temperatures between 5 and 300 K. Two different crystal orientations (x-cut and z-cut) are compared. The influence of the impurities on the mechanical losses is discussed.

This work is supported by the German science foundation under contract SFB Transregio 7.

TT 7.5 Mon 14:00 Poster B

Energy Fluctuations in Glasses at very low Temperatures — •Lena Maerten, Loredana Fleischmann, Andreas Fleischmann und Christian Enss — Kirchhoff-Institut für Physik Heidelberg

Coupling a system thermally to a heat reservoir, its energy content fluctuates according to statistical mechanics. In glasses these fluctuations are mainly caused by energy absorbing and releasing tunnelling systems. Measuring the energy content and investigating its variation should give information about relaxation times and whether or not the tunnelling processes are correlated. In our experiment we use a paramagnetic temperature sensor sputtered onto the quartz glass sample to be measured. The paramagnetic material changes its magnetization with temperature according to the Curie-Law. This change in magnetization is read out by a low noise double stage SQUID-magnetometer. In addition to the energy fluctuations described above, the time resolved heat release can be measured with this setup. Rapidly cooling the heat bath to a constant temperature, one can observe the energy dripping out of excited tunnelling systems while the sample gradually thermalizes. A detailed description of the experimental setup and first results will be presented.

TT 7.6 Mon 14:00 Poster B

New information on the microscopics of tunneling systems from mixtures of glycerol and deuterated glycerol. — •Celine Rüdiger, Masoomeh Bazrafshan, Gudrun Fickenscher, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut Für Physik,Universität Heidelberg

The properties of amorphous materials at temperatures below 1K are genrally described by localized groups of atoms or molecules, cooperatively moving between two configurations with comparable energy (Tunneling Systems).However, barely anything is known about the microscopic nature of these TS. Recently we have shown, that the microscopic nature of TS can be probed by the 2-pulse polarisation echo experiments, since the coupling of nuclear electric qudrupole moment to the tunneling motion leads to a quantum beating of the echo amplitude, as well as a dependence of the echo amplitude on magnetic field. Our investigations on partially deuterated amorphous glycerol revealed that the tunneling motion has a rotational component. The observed effects can e.g. be described by the rotation of one molecule by an average angle of 15°. However, also the assumption of a coherent tunneling of a large group of molecules by a fraction of this angle would explain the observed behavior. We started a series of measurements on mixtures of glycerol and partially deuterated glycerol in order to study the cooperative nature of TS and determine the average number of molecules that are involved in a TS as well as the typical angle by which they rotate. We show the first experimental results and discuss microscopic models that are able to describe the observed behavior.

TT 7.7 Mon 14:00 Poster B

Magnetic Field Dependence of Dielectric Polarization Echoes in — •Florian Klotz[1], Andreas Fleischmann[1], Manfred v. Schickfus[1], Peter Nagel[2], and Christian Enss[1] — [1]University of Heidelberg, Kirchhoff- Institute für Physik, Im Neuenheimer Feld 227, 69210 Heidelberg; Germany — [2]IFP, Forschungszentrum Karlsruhe, PO Box 3640, 76021 Karlsruhe, Germany

Since long certain point defects in alkali halides crystals have been regarded as a model system for the tunnelling of atoms in solids. In recent measurements of the dielectric properties of non-magnetic structural glasses strong magnetic field effects have been observed. These effects are caused by atoms that are involved in tunnelling processes and carry a nuclear magnetic or quadrupolar moment. We have studied the phenomenon in dielectric two pulse polarization echo experiments on KCl crystals doped with Li. In this material the fine structure of the energy levels of the tunneling systems introduced by the nuclear moments leads to a quantum beating in echo decay measurements and to a non-monotonic dependence of the echo amplitude on magnetic fields. Since the microscopic nature of Li tunnelling centres in KCl is well known, this system can be used to compare experimental results with calculations based on a detailed microscopic model. We present the experimental data and discuss the role of nuclear magnetic moments of the KCl host material in the vicinity of tunnelling Li ions on the observed magnetic field effects.

TT 7.8 Mon 14:00 Poster B

High resolution X-ray diffraction and surface/interface scattering beamline NANO coming up in 2009 at ANKA — •Thorsten Schwarz[1], Sondes Bauer[1], and Tilo Baumbach[1,2] — [1]Institut für Synchrotronstrahlung / ANKA, Forschungszentrum Karlsruhe, 76021 Karlsruhe — [2]Laboratorium für Applikationen der Synchrotronstrahlung, Universität Karlsruhe, 76128 Karlsruhe

NANO at ANKA is a future synchrotron beamline on a superconducting undulator source, specialized on high-resolution x-ray diffraction, surface and interface X-ray scattering investigations. The beamline optic has been optimized to deliver a monochromatic and highly collimated beam with sufficient flux to investigate the structure changes and the strain evolution during the growth of epitaxial films and superlattices. In order to carry out real time measurements, different types of environmental chambers, e.g., for molecular beam epitaxy, will be mounted on a heavy duty diffractometer which could support up to 500 kg. It rotates the sample and the environmental parts in all directions in space. With two different detection systems on the diffractometer, it is possible to perform two measurements simultaneously: like Grazing Incidence Small Angle X-ray Scattering (GISAXS) to determine the shape, size, position and correlation in nanostructures and Grazing Incidence Diffraction (GID) to characterize the surface-patterned structure. One of the main issues of the beamline is to study the interface properties like roughness and correlation even for less scattered materials like organic semi-conductors. For that reason, it will be possible to use a multilayer monochromator to get two orders of magnitude more flux with an energy resolution of 1

TT 7.9 Mon 14:00 Poster B

Development of a very low temperature scanning tunneling microscope — •Michael Marz[1,2], Gernot Goll[1], and Hilbert v. Löhneysen[1,2,3] — [1]Physikalisches Institut Universität Karlsruhe (TH), 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 well known techniques. STM allows to study topological surface properties of conductive materials. With STS one can measure the energy dependence of the local density of states (LDOS), as the tunneling current is a function of the LDOS and energy. In order to use the technique at very low temperatures and high magnetic fields, we installed a homebuilt scanning tunneling microscope into a dilution refrigerator, where we can reach temperatures down to 30 mK and apply magnetic fields up to 13 T. In order to improve both spatial and energy resolution, considerable efforts were taken to electrical filtering and mechanical damping of our system. First test measurements were done with a commercially available AuPd grid with a lattice constant of 160 nm. We also achieved atomic resolution on HOPG and $NbSe_2$ at room temperature and on $NbSe_2$ at 50 mK.

TT 7.10 Mon 14:00 Poster B

Design of a 300 mK UHV 9 T scanning tunnelling microscope — •Danny Baumann[1], Paul Sass[1], Torben Hänke[1], Grzegorz Urbanik[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

We present our progress in assembling an ultra high vacuum (UHV) Scanning Tunneling Microscope (STM) for operating temperatures down to 300 mK and magnetic fields up to 9 T. The microscope will be mounted in a UHV ^{3}He cryostate which is connected with a three-chamber UHV system. The system will comprise in-situ tip exchange, a coarse xy-sample positioning system and five electrical leads on the sample holder for combining STM with transport measurements. In this work we will present the characterization of the actual STM unit.

TT 7.11 Mon 14:00 Poster B

Dynamics of liquid ^{3}He-^{4}He-mixtures studied with Neutron Radiography — •Mark Faist[1], Hartmut Abele[2], Roland Gähler[3], and Andreas Van Overberghe[3] — [1]Physikalisches Institut, Universität Heidelberg — [2]E18, Technische Universität München

— [3]Institut Laue-Langevin, Grenoble

Using a Neutron Radiography setup, we visualize the dynamics in superfluid ^{3}He-^{4}He-mixtures and the process of phase separation. These measurements give a deeper insight into critical phenomena and universal scaling laws and with our method we have also direct access to transport processes in He-II driven by temperature gradients.

We perform a measurement of the mass diffusion coefficient of ^{3}He in superfluid ^{4}He for a wide temperature range of 0.5-1.3K, where only poor data exists. Using a scintillator and CCD-Camera as detector, we map the ^{3}He concentration with a spatial resolution of 0.5 mm by measuring the neutron absorption. The concentration distribution varies as a function of applied heating power and distance from the heater, so the mass diffusion coefficient can be determined directly. There is also some need for understanding these processes in a search for a permanent electric dipole moment of the neutron.

Even time-resolved measurements up to 20 fps are possible and has been be used for the observation of phase separation in ^{3}He-^{4}He mixtures with higher ^{3}He concentration. The transitions from the superfluid and the normalfluid mixtures into the phase separation zone could be observed, where inconsistent experiments and theories exist.

This work was funded by the German Federal Ministry for Research and Education under Contract No. 06HD187.

TT 7.12 Mon 14:00 Poster B

The Bose-Hubbard Model with Polaritons — •Michael Hartmann[1,2], Fernando Brandao[1,2], and Martin Plenio[1,2] — [1]Institute for Mathematical Sciences, Imperial College London, 53 Exhibition Road, London, SW7 2PG, United Kingdom — [2]QOLS, The Blackett Laboratory, Imperial College London, Prince Consort Road, London, SW7 2BW, United Kingdom

Artificial structures that can be well controlled and manipulated in the laboratory have become an important tool for the study of quantum many-particle systems.

Here we show that the Bose-Hubbard model can be generated with polaritons in arrays of coupled cavities. In particular, the scheme allows to generate a two component model in a parameter range which is not accessible with alternative approaches.

Most importantly, our scheme allows for single-site addressing.

TT 7.13 Mon 14:00 Poster B

Phase diagram for interacting Bose gases — •Michael Männel[1], Klaus Morawetz[1,2], and Michael Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

From the many-body T-matrix we obtain the condition for a medium-dependent bound state in a Bose gas with contact interaction. This condition, i.e. the phase diagram, is derived from the medium-dependent scattering length and scattering phase as well as from the pole of the T-matrix. Also the binding energy is calculated. By separating the Bose pole from the distribution function the influence of a Bose condensate is measured too.

TT 7.14 Mon 14:00 Poster B

Hardcore Bosons on a Square Lattice with Nearest- and Next Nearest Neighbour Interactions — •Ansgar Kalz, Andreas Honecker, Sebastian Fuchs, and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen

The behaviour of hardcore bosons on a square lattice with competing nearest- and next nearest neighbour interactions is an interesting subject because of the application of the model to cold atoms on an optical lattice.

In the static limit the model maps onto a classical Ising system, which has Néel- and collinear ordered phases, separated by a critical point where the competing interactions yield a degeneracy of the groundstate. We calculate structure factors, specific heat and other quantities. We use Monte-Carlo simulations with parallel tempering and line flip algorithms to avoid freezing problems near the critical point.

We present the resulting phase diagram for the classical model and give an outlook for the case with quantum mechanical hopping terms.

TT 7.15 Mon 14:00 Poster B

Bosonic Dynamical Mean-Field Theory — •Krzysztof Byczuk and Dieter Vollhardt — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

We present the first comprehensive, thermodynamically consistent theory of correlated lattice boson systems, namely a bosonic dynamical mean-field theory (B-DMFT), which is applicable for arbitrary values of the coupling parameters and temperatures [1]. B-DMFT includes all local, dynamical correlations of the many-boson system and becomes exact in the limit of infinite space dimensions in analogy with its successful fermionic counterpart. In contrast to previously formulated mean-field theories for bosons it treats normal and condensed bosons on equal footing and is thus able to describe their dynamical coupling. We discuss in detail various limits of B-DMFT where exact and well-known approximate results are recovered. In particular we elucidate the relation between B-DMFT and the static mean-field theories of Bogoliubov and that of Fisher et al. [2]. A lattice model of itinerant and localized, interacting bosons ("Bosonic Falicov-Kimball model") is solved explicitly within B-DMFT. The local correlations are found to enhance both the BEC transition temperature and the condensate fraction relative to the non-interacting system.

[1] K. Byczuk and D. Vollhardt, arXiv:0706.0839

[2] M.P. Fisher, P.B. Weichman, G.Grinstein, and D.S. Fisher, Phys. Rev. B 40, 546 (1989).

TT 7.16 Mon 14:00 Poster B

Mott transition of fermionic atoms in a three-dimensional optical trap — •Rolf Helmes[1], Theo Costi[2], and Achim Rosch[1] — [1]Institute of Theoretical Physics, University of Cologne, 50937 Cologne — [2]Institute of Solid State Research, Research Center Jülich, Germany

We study theoretically the Mott metal-insulator transition for a system of fermionic atoms confined in a three-dimensional optical lattice and a harmonic trap. We describe an inhomogeneous system of several thousand sites using an adaptation of dynamical mean field theory solved efficiently with the numerical renormalization group method. Above a critical value of the on-site interaction, a Mott-insulating phase appears in the system. We investigate signatures of the Mott phase in the density profile and in time-of-flight experiments. Moreover, the incompressible Mott phase can be detected by squeezing the trap, where we keep track of the thermodynamic quantities during this adiabatic process.

TT 7.17 Mon 14:00 Poster B

Competition between Interaction and Binary Disorder in Ultracold Fermions — •Denis Semmler[1], Krzysztof Byczuk[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany — [2]Institute of Theoretical Physics, Warsaw University, ulica Hoża 69, PL-00-681, Poland

The interplay of interaction and disorder is of key importance for the electronic properties of realistic materials. Both effects can induce metal-insulator transitions [1]. More recently, optical lattices have given access to disordered fermionic quantum systems with a high degree of control. As interaction and disorder compete in a subtle way, obtaining new insight into this interplay is of large current interest.

We investigate a single band Anderson-Hubbard model by means of dynamical mean-field theory (DMFT), extended to include localization phenomena [2]. We consider binary disorder in the onsite energies, relevant e.g. for 2-species mixtures of cold gases. As the arithmetic averaged local density of states is not critical at the Anderson localization we calculate the geometric mean [2]. Our resulting phase diagram includes a disordered Fermi liquid, a Mott insulator at general filling, and an Anderson-localized phase.

[1] K. Byczuk, W. Hofstetter, D. Vollhardt, Phys. Rev. Lett. 94, 056404 (2005)

[2] V. Dobrosavljević, A. A. Pastor, B. K. Nikolić, Europhys. Lett. 62, 76 (2003)

TT 7.18 Mon 14:00 Poster B

Collective dynamics of ultracold atoms in optical lattices — •Michiel Snoek and Walter Hofstetter — J. W. Goethe-Universität, Frankfurt am Main, Deutschland

We analyze the collective dynamics of ultracold atoms in optical lattices induced by a sudden change of the underlying harmonic trapping potential. In order to study the effect of strong interactions, dimensionality and lattice topology on dynamical properties, we consider bosonic atoms with arbitrarily strong repulsive interactions, on a two-dimensional square lattice and a hexagonal lattice. We apply dynamical Gutzwiller mean-field theory.

A shift in the center of the potential invokes dipole oscillations for small amplitudes of the shift. Changing the strenght of the harmonic confinement invokes monopole and quadrupole oscillations. We investigate the frequency of the collective modes as a function of interaction strength and study the coupling and damping of those modes.

Applying a large shift in the center of the potential brings the system far out of equilibrium. We then find insulating behavior for weakly interacting atoms on the square lattice. For strong interactions the center of mass slowly relaxes, even when a Mott plateau is present, which in one dimension blocks the dynamics. On the hexagonal lattice the center of mass relaxes to the new equilibrium position for any interaction strength.

TT 7.19 Mon 14:00 Poster B

Charge-density-waves of trions in an optical lattice — •Csaba Toke[1], Akos Rapp[2], Walter Hofstetter[1], and Gergely Zarand[2] — [1]J. W. Goethe-Universit\"at, Frankfurt am Main, Deutschland — [2]Technologische Universit\"at, Budapest, Ungarn

When fermions of three hyperfine state are loaded into an optical lattice, they provide an almost perfect implementation of the SU(3) Hubbard model. For the case of attractive interactions it was shown in previous work [Rapp et al., PRL 98, 160405 and arXiv:0707.2378] that with increasing interaction strength the color superfluid state goes over to a trionic phase in infinite dimensions. We extend this study to experimentally relevant finite dimensions, and analyze the additional structure that emerges due to the inter-trionic repulsion, which is due to suppression of quantum fluctuations for nearby trions. This interaction is derived, and the resulting density ordering instability is studied on the RPA level.

TT 7.20 Mon 14:00 Poster B

Hubbard Model for Imbalanced Fermi-Mixtures on Optical Lattices — •Tobias Gottwald and Peter G. J. van Dongen — KOMET 337, Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55099 Mainz, Germany

In order to understand the properties of imbalanced ultracold fermionic quantum gases on optical lattices, we analyze a Hubbard model with attractive interaction strength, spin-dependent hopping amplitudes and/or a Zeeman-term at low temperatures in the weak-coupling (mean-field) approximation. In experiment, interactions can be tuned via Feshbach resonances, different hopping amplitudes arise from different atomic masses or different hyperfine states, and the Zeeman-term is used to control the population imbalance. We investigate this generalized Hubbard model between two extremes, on the one hand the Falicov-Kimball model, where charge density wave phases are dominating, and on the other the standard Hubbard model with equal hopping amplitudes for each pseudo-spin species, where superfluid phases occur.

TT 7.21 Mon 14:00 Poster B

Macroscopic self-trapping regimes in Bose-Fermi mixtures with double well confinement — •Santiago Francisco Caballero Benitez[1], Miklos Gulacsi[1], Yuri S. Kivshar[2], and Elena A. Ostrovskaya[2] — [1]MPIPKS, Dresden, Germany — [2]NPC RSPhysSE ANU, Canberra, Australia

Effects of fermions in quasi one dimensional mixtures of bosons and fermions with double well confinement are discussed. It is argued that the dynamical regime where macroscopic self trapping occurs in a pure bosonic system is modified by the inclusion of fermions, leading to a change of symmetry of the wave function that evolves non-monotonically as the separation of the wells is increased. We relate our work with current experiments on ^{40}K and ^{87}Rb.

TT 7.22 Mon 14:00 Poster B

Collective quantum modes of parabolically confined mesoscopic Fermi systems — •Karsten Balzer, Christian Henning, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

For interacting few particle systems, the internal dynamics in terms of normal modes is of broad interest in many fields of research—e.g. in complex plasmas, (dilute) quantum Fermi gases/liquids or BEC-BCS systems, the normal mode spectrum is directly linked to interesting system properties and to the response to external electromagnetic fields.

Here, we go beyond linear response theory and study collective modes in the quantum regime by applying Nonequilibrium Green's function (NEGF) techniques at zero and finite temperatures [1,2]. In particular, we investigate the quantum breathing mode for fermionic 1D and 2D systems (being confined in harmonic traps) interacting via a $1/r^\alpha$ pair-potential [3]. The dependence of the breathing frequency and the time-dependent density on the relative interaction strength is discussed for a wide range of parameters including nonlinear effects [4].

[1] M. Bonitz, K. Balzer, and R. van Leeuwen, Phys. Rev. B **76**, 045341 (2007).

[2] "Nonequilibrium Green's function approach to artificial atoms", K. Balzer, Diploma thesis, Kiel University (2007).

[3] see poster "NEGF approach to correlated trapped fermions", K. Balzer, M. Bonitz, N.E. Dahlen, and R. van Leeuwen.

[4] B. Partoens, F.M. Peeters, J. Phys.: Cond. Mat. **9**, No. 25 (1997).

TT 7.23 Mon 14:00 Poster B

Nonequilibrium Green's function approach to correlated trapped fermions: Equilibrium properties and nonequilibrium behavior — •Karsten Balzer[1], Michael Bonitz[1], and Robert van Leeuwen[2] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, Leibnizstrasse 15, 24098 Kiel, Germany — [2]Department of Physics, University of Jyväskylä, 40014 Survontie 9, Jyväskylä, Finland

Using a Nonequilibrium Green's function approach, we investigate small arrangements of parabolically confined fermions interacting via a repulsive $1/r^\alpha$ pair-potential in 1D and 2D. Such reduced systems are of relevance for quantum dots and wells, metal clusters or ions in traps.

The equilibrium [1] and dynamical properties [1,2] are obtained by numerically solving the Keldysh/Kadanoff-Baym equations for the two-time Green's functions [3], where initial correlations at finite temperatures are included self-consistently starting from a correlated equilibrium Green's function. The consideration of a wide range of relative interaction strengths allows us, in particular, to observe the transition from almost ideal Fermi liquid states to Wigner crystal behavior.

[1] "Nonequilibrium Green's function approach to artificial atoms", K. Balzer, Diploma thesis, Kiel University (2007).

[2] see also poster "Collective modes of parabolically confined mesoscopic Fermi systems", K. Balzer, C. Henning, and M. Bonitz.

[3] "Introduction to Computational Methods in Many Body Physics", M. Bonitz, D. Semkat (Eds.), Rinton Press (2006).

TT 8: Correlated Electrons: Spin Systems and Itinerant Magnets 1

Time: Monday 14:00–18:00 Location: H 0104

TT 8.1 Mon 14:00 H 0104

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see SYPT 4.1

TT 8.2 Mon 14:15 H 0104

Magnetic phase diagram of MnSi revisited — •Florian Jonietz[1], Sebastian Mühlbauer[1,2], Christian Pfleiderer[1], Achim Rosch[3], Rembert Duine[4], Andreas Neubauer[1], Stefan Legl[1], Robert Georgii[1,2], 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]Institute of Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany — [4]Institute for Theoretical Physics, Department of Physics and Astronomy, Utrecht University, 3584 CE Utrecht, The Netherlands

The lack of inversion symmetry in the crystal structure of the itinerant-electron magnet MnSi results in weak Dzyaloshinsky-Moriya interactions, that stabilize a long-wavelength spin spiral ($\lambda \sim 190$ Å) in the magnetically ordered state. Motivated by recent neutron scattering

studies of the magnetic phase diagram at high pressures we have revisited the magnetic phase diagram at ambient pressure. We report the results of extensive measurements of the AC susceptibility and small angle neutron scattering of the magnetic order of MnSi as function of temperature, magnetic field and electric current. In our study we focus in particular on the stability of the A-phase, a small phase pocket, where the helical order spontaneously aligns perpendicular to the direction of an applied magnetic field.

TT 8.3 Mon 14:30 H 0104

Spherical neutron polarimetry of the magnetic structure in MnSi — •Marc Janoschek[1], Florian Bernlochner[1], Sebastian Mühlbauer[1,2], Robert Georgii[1,2], Christian Pfleiderer[1], 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

Dzyaloshinsky-Moriya interactions stabilize a long-wavelength spin spiral ($\lambda \sim 190$ Å) in the magnetically ordered state of B20 compound MnSi. Recent theoretical studies [1] suggest that the DM interactions may not only stabilize straight-forward helical order, but also additional complex magnetic textures, when the amplitude of the local magnetization is soft and supports strong longitudinal fluctuations, e.g. near critical phase transitions. Polarized neutron scattering provides a unique microscopic tool for the determination of magnetic structures. We have explored the question of the magnetic order and related magnetic textures in MnSi by means of spherical neutron polarimetry using the module MuPAD. We have focussed in particular on the nature of the magnetic state in the vicinity of the helical to paramagnetic phase boundary, where bulk properties reveal weak evidence for additional phase transitions. [1] U. K. Rößler, A. N. Bogdanov, C. Pfleiderer *Nature* **442**, 797 (2006).

TT 8.4 Mon 14:45 H 0104

Gauge theory description and possible spin charge separation in itinerant chiral magnets — •Benedikt Binz and Achim Rosch — Universitaet zu Koeln

By applying pressure to the itinerant chiral magnet MnSi, a state with non-Fermi liquid electrical transport and unusual partially ordered magnetism has been observed. These experiments quite intriguingly suggest diffuse spin correlations and slow dynamics in a pure crystalline metal.

As a possible route towards a theory of the partially ordered state, we show that electrons interacting with a fluctuating magnetic background have a natural gauge theory description. We introduce new variables, where spin and charge of the conduction electrons appear separated. In this language, the helically ordered phase appears as a Anderson-Higgs phase where the gauge field is gapped and the low-energy helimagnon spectrum is obtained. It is currently not known whether this gauge theory also has (deconfined) disordered phases, which could account for the unusual behavior of MnSi under pressure.

TT 8.5 Mon 15:00 H 0104

Search for helimagnon excitations in MnSi: an inelastic neutron scattering study — •Florian Bernlochner[1], Marc Janoschek[1], Peter Böni[1], Sarah Dunsiger[1], Bertrand Roessli[2], Peter Link[3], Christian Pfleiderer[1], and Achim Rosch[4] — [1]Physik-Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Laboratory for Neutron Scattering, ETH Zürich & Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, D-85748 Garching, Germany — [4]Institute of Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

The lack of inversion symmetry in the crystal structure of the itinerant-electron magnet MnSi results in weak Dzyaloshinsky-Moriya interactions, that stabilize a long-wavelength spin spiral ($\lambda \sim 190$ Å) in the magnetically ordered state. Recent theoretical studies [1-3] predict a rich, novel spectrum of the Goldstone modes, also referred to as helimagnons, for sufficiently small wave vectors near the helical ordering wave vector. We present the results of extensive inelastic neutron scattering studies, in which we explore the nature of the low lying excitations in MnSi in the helically ordered state.

[1] D. Belitz, T. R. Kirkpatrick *Phys. Rev. B* **72**, 180402(R) (2005)

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

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

15 min. break

TT 8.6 Mon 15:30 H 0104

Evolution of the 'Orbital Peierls State' with doping — •C. Ulrich[1], G. Khaliullin[1], M. Reehuis[1,2], K. Schmalzl[3], A. Ivanov[3], K. Hradil[4], J. Fujioka[5], Y. Tokura[5], and B. Keimer[1] — [1]MPI-FKF, Stuttgart — [2]HMI, Berlin — [3]ILL Grenoble, France — [4]FRM II, Munich — [5]University of Tokyo, Japan

Orbital degrees of freedom play an important role in the physics of strongly correlated electron systems. Our extensive investigation of insulating vanadates by neutron scattering has led to the discovery of an unusual magnetic ground state due to the interplay between spin and orbital degrees of freedom. YVO_3 exhibits two magnetic phases, a C-type phase between 116 K and 77 K and a G-type phase below 77 K. While the magnetic properties of the G-type phase are in accordance with standard theoretical descriptions, the C-type phase shows highly unusual static and dynamic spin correlations. Based on the idea of orbital fluctuations we were able to identify this phase as a theoretically predicted but hitherto unobserved 'orbital Peierls state' [1].
Our latest neutron scattering experiments show that the C-type phase in $Y_{1-x}Ca_xVO_3$, i.e., the 'orbital Peierls phase', is stabilized upon doping, while the orbitally ordered G-type phase is quite unstable and disappears at x = 2 %. Furthermore, with doping this phase also exhibits a highly unusual spin wave dispersion. This leads us to the conclusion, that the 'orbital Peierls state' becomes more robust with Ca-doping, whereas the formerly well defined G-type phase exhibits a more complex behavior, probably as a consequence of an increase in orbital fluctuations.

[1] C. Ulrich et al., PRL **91**, 257202 (2003).

TT 8.7 Mon 15:45 H 0104

Spin and Singlet Dynamics of the S=1/2 Kagome Antiferromagnet — •Andreas M. Laeuchli[1] and Claire Lhuillier[2] — [1]IRRMA, EPF Lausanne, Switzerland — [2]LPTMC, Universite P. & M. Curie, Paris, France

The kagome Heisenberg antiferromagnet with spin 1/2 has been the topic of many theoretical investigations. Most of these focused on groundstate properties or aiming at an explanation of the anomalous high density of singlet excitations. In this contribution we report on recent exact diagonalization studies concentrating on dynamical correlation functions. First the full dynamical spin structure factor S(q,omega) on 36 sites has been obtained. Then we also discuss the time dependent spin autocorrelation function as well as dynamical dimer-dimer correlation functions. All these results combined together point towards a highly fluctuating system, both in the singlet and the triplet channel. We conclude by a comparison with recent inelastic neutron scattering measurements on the Herbertsmithite compound.

TT 8.8 Mon 16:00 H 0104

High field magnetic resonance study of the spin antiferromagnet $GdNi_2B_2C$ (exchanged with TT 30.4) — •Ferenc Murányi[1], Uwe Schaufuss[1], Mathias Dörr[2], Martin Rotter[3], Vladislav Kataev[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, D-01171 Dresden, PO BOX 270116, Germany — [2]Institut for Physics of Solids, Technical University Dresden, D-01062 Dresden, Germany — [3]Institute for Physical Chemistry, University of Vienna, A-1090 Vienna, Währingerstr. 42, Austria

The Antiferromagnetic Resonance (AFMR) was measured on a thick slab of single crystal $GdNi_2B_2C$ in the antiferromagnetic state. In the paramagnetic state Electron Spin Resonance (ESR) study was done. The magnetic properties of the material were studied applying the external magnetic field parallel and perpendicular to the easy plane. The measured data revealed the anisotropy of the Korringa relaxation rate in the paramagnetic state indicating anisotropic interaction between the localized 4f moments and conduction electrons. In the antiferromagnetic state we observed a large out-of-plane anisotropy gap of ∼76 GHz which is higher than expected from the dipole-dipole interaction. Surprisingly, we also observed an in-plane gap with the same order of magnitude. In addition we found indications that the external magnetic field induces symmetry-breaking distortions in this material. The work was supported by DFG through SFB 463.

TT 8.9 Mon 16:15 H 0104

Impurity induced spin textures in quantum antiferromagnets — •Julian Engel and Stefan Wessel — Institute for Theoretical

Physics III, Stuttgart University, Germany

We present results from quantum Monte Carlo studies on the effects of a magnetic impurity on the order parameter distribution in a two-dimensional host antiferromagnet. We find that for a weak coupling to the impurity spin, the staggered magnetization is enhanced throughout the lattice, whereas increasing the coupling between the host and the impurity spin restricts this enhancement to the close vicinity of the impurity, whereas on all other sites the staggered magnetization gets suppressed compared to the clean case. Approaching the limit of an infinite coupling between host and impurity, the system hence crosses over to the case of an embedded non-magnetic impurity site. We compare our results with previous findings, based on spin-wave and perturbation theory.

TT 8.10 Mon 16:30 H 0104

Numerical investigation of the quantum dimer model on a diamond lattice — •Olga Sikora[1], Frank Pollmann[1], Nic Shannon[2], Karlo Penc[3], and Peter Fulde[1] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1 TL, UK — [3]Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.B. 49, Hungary

Quantum dimer models (QDMs) are of great interest in the study of systems with frustrated spin or charge degrees of freedom. On bipartite lattices these QDMs can be mapped onto a U(1)-gauge theory, with a liquid-like ground state and fractional excitations. However in two dimensions, these excitations are confined, except at the Rokhsar-Kivelson (RK) point, a quantum critical point occurring for one specific ratio of parameters. Recently, it has been suggested that in the QDM on a 3D diamond lattice, a U(1) liquid is not confined to a single point, but extends for a finite range of parameters bordering the RK point.

We have used Green's Function Monte Carlo (GFMC) and Variational Monte Carlo simulations to test this conjecture numerically. Our preliminary GFMC calculations suggest that the confining potential for fractional excitations vanishes in a large region of the parameter space, confirming the existence of an extended liquid phase.

15 min. break

TT 8.11 Mon 17:00 H 0104

Spectral functions of kagome lattice structures with charge degrees of freedom — •Aroon O'Brien, Frank Pollmann, and Peter Fulde — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Systems in which strong electronic interactions are frustrated can exhibit interesting physical effects. Two particularly well known frustrated lattices are the planar pyrochlore (checkerboard) lattice and the kagome lattice. For a model of spinless fermions on a checkerboard lattice, it has been demonstrated that fractional charges occur at certain filling factors [1]. A thorough study of this model has further shown that these fractional charges are linearly confined [2]. However, whether fractional charges are confined or deconfined at various fillings on the kagome lattice is not yet understood. We address this question through the numerical calculation of various properties of static and dynamic fractional charges at 1/3 and 1/6 filling, for a model of spinless fermions on the kagome lattice.

[1] P. Fulde, K.Penc, and N. Shannon, Annalen der Physik (Leipzig) **11**, 892 (2002)

[2] F. Pollmann and P. Fulde, EPL 75, 133 (2006)

TT 8.12 Mon 17:15 H 0104

Supersolid phase induced by correlated hopping in spin-1/2 frustrated quantum magnets — •Kai P. Schmidt[1], Julien Dorier[1], Andreas Laeuchli[2], and Frederic Mila[1] — [1]Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Institut Romand de Recherche Numerique en Physique des Materiaux (IRRMA), CH-1015 Lausanne, Switzerland

We show that correlated hopping of triplets, which is often the dominant source of kinetic energy in dimer-based frustrated quantum magnets, produces a remarkably strong tendency to form supersolid phases in a magnetic field. These phases are characterized by simultaneous modulation and ordering of the longitudinal and transverse magnetization respectively. Using Quantum Monte Carlo and a semiclassical approach for an effective hard-core boson model with nearest-neighbor repulsion on a square lattice, we prove in particular that a supersolid phase can exist even if the repulsion is not strong enough to stabilize an insulating phase at half-filling. Experimental implications for frustrated quantum antiferromagnets in a magnetic field at zero and finite temperature are discussed.

TT 8.13 Mon 17:30 H 0104

Spinon confinement and the Haldane gap in SU(n) spin chains: numerical studies — •Max Führinger[1], Stephan Rachel[1], Ronny Thomale[1], Peter Schmitteckert[1,2], and Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe

Recently, two of us [1] motivated a general set of rules which SU(n) spin chains exhibit spinon confinement and hence a Haldane gap in the spectrum. According to these rules, models of spin chains with SU(n) spins transforming under a representation corresponding to a Young tableau consisting of a number of boxes λ which is divisible by n, are gapped. If λ and n have no common divisor, the spin chain will support deconfined spinons and not exhibit a Haldane gap. If λ and n have a common divisor different from n, it will depend on the specifics of the model including the range of the interaction.

Here we present numerical evidence for these rules, obtained by exact diagonalization and DMRG, using the representations **3**, **6**, **8**, and **10** of SU(3) and the representations **4**, **6**, and **10** of SU(4). The numerical data obtained include the low energy spectra and results for bond and entanglement entropies. The entanglement entropy yields the central charge of the critical models as well.

[1] M. Greiter and S. Rachel, Phys. Rev. B **76**, 184441 (2007).

TT 8.14 Mon 17:45 H 0104

Field-dependent thermal transport in the Haldane chain compound NENP — •A. V. Sologubenko[1], T. Lorenz[1], J. A. Mydosh[1], and M. M. Turnbull[2] — [1]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany — [2]Carlson School of Chemistry and Department of Physics, Clark University, Worcester, MA 01610, USA

Properties of materials in the vicinity of quantum phase transitions have recently attracted considerable attention. Of particular interest are low-dimensional magnetic systems with transitions between various gapless and gapped states, induced by an external magnetic field. We present experiments on the magnetic field dependent thermal transport in the spin $S = 1$ chain material $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ [NENP]. In NENP, the Haldane energy gap in the magnon excitation spectrum can be greatly reduced by applying an external magnetic field, but it remains finite at the critical field. The thermal conductivity is strongly affected by the field-induced changes in the magnon spectrum. It is possible to clearly distinguish the magnetic and the phononic contributions to the total heat conductivity and to successfully analyze the spin contribution in terms of a quasiparticle model. The mean free path of the spin excitations, evaluated from our data, is temperature-independent and large, which has important implications for the theory of transport in quantum spin systems.

Supported by the Deutsche Forschungsgemeinschaft through SFB 608.

TT 9: Transport: Quantum Coherence and Quantum Information Systems

Time: Monday 14:00–18:15 Location: H 2053

TT 9.1 Mon 14:00 H 2053

Control of two coupled Josephson persistent current qubits at the degeneracy point — •Marcel Manheller[1,2], Pieter de Groot[1], C. J. P. M. Harmans[1], and J. E. Mooij[1] — [1]TU Delft, Netherlands — [2]IFF, FZ, Juelich, Deutschland

A Josephson persistent current qubit is created by a superconducting loop, which is interrupted by three Josephson junctions. A quantum mechanical two level system is generated, if a magnetic field close to half a flux quantum is applied at the qubit loop. Two qubits are coupled inductively, while sharing a piece of line. The two qubits are operated via two control lines, which can produce a gradient in electromagnetic field over the qubits. Thereby we are able to control a two qubit system at the degeneracy point. At this point is the theoretical lifetime of a qubit a factor of 35 higher then at the usual operation point. This promises us to apply a simple algorithm on this device.

TT 9.2 Mon 14:15 H 2053

Probing the States of a High-T_c Intrinsic Phase Qubit — •X. Y. Jin, J. Lisenfeld, Y. Koval, A. V. Ustinov, and P. Müller — Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg

We report our results on fabricating and probing high-T_c intrinsic phase qubits. An intrinsic phase qubit is a superconducting ring made of a $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal, intercepted by two intrinsic Josephson junction stacks. Macroscopic quantum tunneling was observed in these qubits, and the crossover temperature was around 600 mK. An intrinsic phase qubit is generally regarded as a multi-junction system, i.e. a system of many degrees of freedom in phase space. However, we discovered that as long as the two stacks are uniform, the intrinsic phase qubits behaves like a system with only two degrees of freedom, independent of the number of junctions in the stacks. Due to the large self-inductance, the potential of an intrinsic phase qubit has several minima in which the system can stay. In order to perform quantum operations, a technique using low-frequency microwaves is developed to assure that the system stays inside the chosen potential well.

Invited Talk TT 9.3 Mon 14:30 H 2053

Coherent Oscillations in Josephson Phase Qubits — •Jürgen Lisenfeld, Alexander Lukashenko, and Alexey V. Ustinov — Physikalisches Institut III, Universität Erlangen, D-91058 Erlangen

A phase qubit uses as its logical states discrete energy eigenstates of the Josephson phase of a current-biased tunnel junction. By embedding the junction in a superconducting loop, the qubit can be controlled by a magnetic bias flux, while its state is then read out by measuring the magnetic moment of the loop using a dc-SQUID. A maximum readout contrast is hereby achieved by strong coupling to the dc-SQUID detector, which acts as a source of decoherence.

We present a new method of data evaluation to restore the full 100 % readout contrast for a weakly coupled detector. The same technique is used to compensate for a loss of contrast induced by thermal fluctuations in the dc-SQUID. We applied this method to measure the temperature dependence of coherence times in phase qubits of different origins and featuring different materials. By observing Rabi oscillations, energy relaxation and Ramsey fringes, we find that the coherent qubit response of a sample operated in the two-level limit vanishes rapidly as soon as the thermal energy k_BT becomes larger than the energy level spacing. In contrast, a sample which was operated in the multi-level limit displayed semi-classical oscillations similar to Rabi oscillations, but showed qualitatively different temperature dependence. Our experimental data shed new light on the origin of decoherence in superconducting qubits and suggest that contemporary phase qubits can be operated at temperatures of up to several 100 mK.

TT 9.4 Mon 15:00 H 2053

Coherent oscillations in a superconducting flux qubit without microwave pulses — •Stefano Poletto[1], Jürgen Lisenfeld[1], Alexander Lukashenko[1], Maria Gabriella Castellano[2], Fabio Chiarello[2], Carlo Cosmelli[3], Pasquale Carelli[4], and Alexey V. Ustinov[1] — [1]Physikalisches Institut III, Universität Erlangen-Nürnberg, Germany — [2]Istituto di Fotonica e Nanotecnologie del CNR, Roma, Italy — [3]Dipartimento di Fisica and INFN, Universita' di Roma La Sapienza, Italy — [4]Universita' degli Studi dell'Acquila, Italy

We report on observation of coherent oscillations in a superconducting flux qubit by using no microwave excitation but only nanosecond-long dc flux pulses. The investigated circuit is a double-SQUID consisting of a superconducting loop interrupted by a small dc-SQUID, which we control via two bias fluxes ϕ_c and ϕ_x. The potential energy profile of the qubit has the shape of a double well, where the flux ϕ_c controls the height of the barrier between the two minima and the flux ϕ_x changes the potential symmetry. The two computational states of the qubit are identified with the two energy minima and physically correspond to clockwise or anticlockwise circulating currents in the double-SQUID main loop. We observed coherent oscillations, in the frequency range between 8 and 20 GHz, induced by fast pulses of the control flux ϕ_c modulating the barrier between the two potential wells. The quantum dynamics that leads to this kind of oscillations is composed of a non-adiabatic and adiabatic evolution of the two lowest energy states.

TT 9.5 Mon 15:15 H 2053

Theory of quantum non-demolition measurements of a flux qubit — •Luca Chirolli and Guido Burkard — Institute of Theoretical Physics C, RWTH Aachen University, D-52056 Aachen, Germany

Recently a new technique for a quantum non demolition measurement (QND) of the state of a flux qubit based on the coupling to a circuit oscillator has been proposed and experimentally realized (A. Lupascu *et al.*, Nature Physics **3**, 119 (2007)). In our theoretical description of the experiment, we use the positive operator value measurement (POVM) formalism to describe the qubit measurement. Two mechanisms lead to deviations from a perfect QND measurement: (i) the quantum fluctuations of the measurement oscillator, and (ii) quantum tunneling between the qubit states $|0\rangle$ and $|1\rangle$ during measurement.

TT 9.6 Mon 15:30 H 2053

2D cavity grid quantum computing — Ferdinand Helmer[1], Matteo Mariantoni[2], Austin Fowler[3], Jan von Delft[1], Enrique Solano[1], and •Florian Marquardt[1] — [1]Arnold-Sommerfeld Center for Theoretical Physics, Center for NanoScience and Department of Physics, Ludwig-Maximilians Universität München, Germany — [2]Walther-Meissner Institut, Bayerische Akademie der Wissenschaften, Garching b. München, Germany — [3]Institute for Quantum Computing, University of Waterloo, Waterloo, ON, Canada

We propose a novel scheme for scalable solid state quantum computing, where superconducting microwave transmission line resonators (cavities) are arranged in a two-dimensional grid on the surface of a chip, coupling to superconducting qubits (charge or flux) at the intersections. We analyze how tasks of quantum information processing can be implemented in such a topology, including efficient two-qubit gates between any two qubits on the grid and elements of fault-tolerant computation.

TT 9.7 Mon 15:45 H 2053

Exact Results on Dynamic Decoupling by π-Pulses in Quantum Information Processes — •Götz S. Uhrig — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund

The aim of dynamic decoupling consists in the suppression of decoherence by appropriate coherent control of a quantum register. Effectively, the interaction with the environment is reduced and hence the decoherence rate. In particular, a sequence of π-pulses is considered. Here we present exact results on the suppression of the coupling of a quantum bit to its environment by optimized sequences of π-pulses along the storage time t. The more pulses are used the higher is the order in t in which decoherence occurs [1]. To which extent the optimization pays is discussed for different high-energy cutoffs. We show that the results for a spin-boson model hold generally for any kind of bath.

[1] G.S. Uhrig, PRL 98, 100504 (2007)

15 min. break

TT 9.8 Mon 16:15 H 2053

Design of short coherent control pulses for quantum information processing — •Stefano Pasini, Tim Fischer, Peter Karbach, and Götz S. Uhrig — Technische Universität Dortmund

A systematic technique is presented to design short pulses for the coherent control of a two-level system coupled to a bath. The problem can be solved as the one for an ideal pulse, instantaneous pulse up to some order of approximation, which our π and $\frac{\pi}{2}$ optimized pulses make vanish. Their effectiveness is tested numerically on a specific spin model.

TT 9.9 Mon 16:30 H 2053

Nuclear spin dynamics in quantum dots — •Daniel Klauser, William Anthony Coish, and Daniel Loss — Departement of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The hyperfine interaction between the electron spin and the nuclear spins within a quantum dot has been established as the main source of decoherence for the electron spin. The decay of transverse and longitudinal spin components show rich dynamics including exponential, gaussian and power-law decay. Further, a universal phase-shift for driven single spin oscillations has been predicted and experimentally observed recently [1]. In this context of hyperfine induced electron spin decoherence also the dynamics of the nuclear spin system (Overhauser field dynamics) have come into focus. We discuss the dynamics of the nuclear spin system and how measurements of the Overhauser field [2] alter this dynamics.

[1] F.H.L. Koppens, D. Klauser, W.A. Coish, K.C. Nowack, L.P. Kouwenhoven, D. Loss and L.M.K. Vandersypen, Phys. Rev. Lett. 99, 106803, (2007).

[2] D. Klauser, W.A. Coish and Daniel Loss, Phys. Rev. B 73, 205302, (2006).

TT 9.10 Mon 16:45 H 2053

Exponential Decay in a Spin Bath — William Anthony Coish[1,2], •Jan Fischer[2], and Daniel Loss[2] — [1]Institute for Quantum Computing and Department of Physics and Astronomy, Waterloo, Ontario, Canada — [2]Department of Physics, University of Basel, Switzerland

We show that the coherence of an electron spin interacting with a bath of nuclear spins can exhibit a well-defined purely exponential decay for special ('narrowed') bath initial conditions in the presence of a strong applied magnetic field. This is in contrast to the typical case, where spin-bath dynamics have been investigated in the non-Markovian limit, giving super-exponential or power-law decay of correlation functions. We calculate the relevant decoherence time T_2 explicitly for free-induction decay and find a simple expression with dependence on bath polarization, magnetic field, the shape of the electron wave function, dimensionality, total nuclear spin I, and isotopic concentration for experimentally relevant heteronuclear spin systems.

TT 9.11 Mon 17:00 H 2053

Spin dynamics in InAs-nanowire quantum-dots coupled to a transmission line — •Mircea Trif[1], Vitaly N. Golovach[2], and Daniel Loss[3] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland. — [2]Department of Physics, Ludwig-Maximilians-Universität, Theresienstr. 37, D-80333 Munich, Germany. — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland.

We study theoretically electron spins in nanowire quantum dots placed inside a transmission line resonator. Because of the spin-orbit interaction, the spins couple to the electric component of the resonator electromagnetic field and enable coherent manipulation, storage, and read-out of quantum information in an all-electrical fashion. Coupling between distant quantum-dot spins, in one and the same or different nanowires, can be efficiently performed via the resonator mode either in real time or through virtual processes. For the latter case we derive an effective spin-entangling interaction and suggest means to turn it on and off. We consider both transverse and longitudinal types of nanowire quantum-dots and compare their manipulation timescales against the spin relaxation times. For this, we evaluate the rates for spin relaxation induced by the nanowire vibrations (phonons) and show that, as a result of phonon confinement in the nanowire, this rate is a strongly varying function of the spin operation frequency and thus can be drastically reduced compared to lateral quantum dots in GaAs. Our scheme is a step forward to the formation of hybrid structures where qubits of different nature can be integrated in a single device.

TT 9.12 Mon 17:15 H 2053

Cold bosonic atoms in a $\pi-$flux lattice — •Stephan Rachel and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe

We present a model where the rare phenomenon of fragmented Bose–Einstein condensation occurs: we consider a system of neutral, bosonic atoms on a square lattice subject to an effective magnetic field. We focus on a magnetic flux of half a Dirac flux quantum through every lattice cell. The effective flux yields two minima in the lower single particle band. We show that in the many particle ground state, the particles are evenly distributed over both minima. The two macroscopically occupied minima correspond to two distinct Bose condensates.

Regarding the low-energy excitations of the system, we show that Josephson tunneling is only possible for pairs of bosons, while single particle tunneling between both condensates is absent. We further find a massive mode describing fluctuations in the relative density of the two condensates.

TT 9.13 Mon 17:30 H 2053

Migration of bosonic particles across a Mott insulator to superfluid phase interface — •Michael Hartmann[1,2] and Martin Plenio[1,2] — [1]Institute for Mathematical Sciences, Imperial College London, 53 Exhibition Road, London, SW7 2PG, United Kingdom — [2]QOLS, The Blackett Laboratory, Imperial College London, Prince Consort Road, London, SW7 2BW, United Kingdom

Effective many-particle systems in artificial structures have become an important testbed for the investigation of quantum many-particle and condensed matter physics.

Very recently it has been shown, that arrays of coupled microcavities can host effective Bose-Hubbard and spin models. As a new feature, this approach offers the possibility to control and address individual lattice sites. Besides being a prerequisite for quantum information applications, this possibility opens the door to the study of many-particle systems which are inhomogeneous or out of equilibrium.

Here we discuss one such possibility, an interface between a Mott insulator and a superfluid region.

TT 9.14 Mon 17:45 H 2053

Non-Abelian Statistics in a Quantum Antiferromagnet — •Martin Greiter and Ronny Thomale — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D 76128 Karlsruhe

We propose a novel spin liquid state for a S=1 antiferromagnet in two dimensions. The ground state is a spin-singlet, fully invariant under the symmetries of the underlying lattice, and possess a threefold topological degeneracy. The spinon and holon excitations obey non-abelian statistics, with the braiding of half-quantum vortices governed by zero energy modes in the vortex cores. We present numerical evidence that the universality class of this topological liquid can be stabilized by a model Hamiltonian involving three-spin interactions. We discuss possible realizations with polar molecules in optical lattices as well as potential applications in quantum computing.

TT 9.15 Mon 18:00 H 2053

Preferred base for multiparticle states arising from subsequent two-particle scattering — •Ivo Knittel — Fachbereich Experimentalphysik, Campus, Geb. C6.3, 66041 Saarbrücken

For a quantum system coupled to its environment via a certain interaction operator, there exists a certain base, whose states exhibit minimal entanglement rate with environment states. For an interaction commuting with the position operator, this preferred base consists of highly localized states in position states.[1] This central result of decoherence theory is widely regarded as a solution of the 'preferred base' problem of the quantum theory of measurement [2]. However from decoherence theory it is not obvious how to construct the 'pointer states' for a given system. In this contribution, I investigate multiparticle states arising from a cascade of subsequent two-particle scattering events. This situation is met in a quasi-classical gas, or in the interaction of high-energy particles with a detector. A certain representation is constructed that is especially adapted to the multi-particle state arising from subsequent two-particle scattering events, and its time propagation.

[1] W. G Unruh, W. H. Zurek, Phys. Rev. D, 40, 1070 (1989) [2] M. Schlosshauer, Rev Mod. Phys. 76, 1267 (2004)

TT 10: Superconductivity: Fabrication and Characterization

Time: Monday 14:00–15:00 Location: H 3010

TT 10.1 Mon 14:00 H 3010

MOCVD and MOD process for Coated Conductors — •Oliver Stadel[1], Ruslan Muydinov[1], Jürgen Schmidt[4], Hartmut Keune[4], Georg Wahl[1], Günter Kotzyba[2], Anita Will[2], Rainer Nast[2], Alexandra Jung[2], Wilfried Goldacker[2], Sergej Samoilenkov[3], Oleg Gorbenko[3], and Andrej Kaul[3] — [1]TU Braunschweig, IOT, Bienroder Weg 53, 38108 Braunschweig — [2]Forschungszentrum Karlsruhe, ITP, Hermann von Helmholtz Platz 1, 76344 Eggenstein Leopoldshafen — [3]Mowcow State University V234, Department of Chemistry, Moscow 119 899 — [4]PerCoTech AG, Bienroder Weg 53, 38176 Braunschweig

A MOCVD and a MOD process for contiuous deposition of oxide buffer layers and YBCO at once on long metal tapes was developed. Texured Ni(W) tapes were coated with oxide buffer layers at low oxygen partial pressure without oxidation of the metal tape. YBCO films of 350-1000 nm thick were obtained using tape velocity of 4 m/h. MOCVD and MOD buffer layers, which were delivered from partners of the Virtual Institute, were covered by YBCO. Entirely obtained by MOCVD superconductive samples revealed a critical current density of 1MA/cm^2 at 77 K. The excellent in plane texture (FWHM = 5-6°) and out of plane texture (FWHM = 1.4-3°) of YBCO films may enable to increase the critical current density further. YBCO deposited on MOD obtained buffer layers reached the maximum critical current density 2MA/cm^2.

Acknowledgement - The authors thank the partners of the Virtual Institute Chemically deposited YBCO Superconductors.

TT 10.2 Mon 14:15 H 3010

Roebel Assembled Coated Conductor Cables (RACC): Ac-Losses and Application Potential — •Curt Schmidt and Wilfried Goldacker — Forschungszentrum Karlsruhe, Institut für Technische Physik

High temperature superconducting (HTS) cables for transport currents well above 1 kA, assembled from a number of tapes, are required for application in transformers, generators and for future fusion reactor coils. Coated conductor (CC) tapes are suitable candidates for an operation temperature between 50 and 77 K which is a crucial precondition for economical cooling costs. Ac-field applications require low ac-loss cables and hence transposition of the individual tapes. The in the plane inflexibility of the tapes doesn't allow classical twisting techniques. The problem can be solved using a modified Roebel technique where meander shaped tapes are assembled to a Roebel cable. The electrical connection between the tapes, necessary to allow current redistribution, and the mechanical stability is achieved by impregnation with a conductive epoxy resin. We prepared short lengths of cables with 11 and 12 structured tapes and measured ac-losses in an external ac field and coupling current time constants. In the interesting frequency range below 100 Hz the coupling losses are small compared to hysteresis losses in the tape. The possibility of hysteresis loss reduction by striating the tapes should therefore be taken into consideration. Finally we discuss the potential of this cable type with respect to ac-losses and current carrying capability as a function of operation temperature, as well as possible routes of long length cable fabrication.

TT 10.3 Mon 14:30 H 3010

Effect of rare earth and alkaline earth substitutions in the superconductor $RuA_2RECu_2O_8$ (RE=Gd, Eu, Nd, Pr; A=Ca, Sr, Ba): crystal structure and physical properties — •Eugenio Casini[1,4], Consiglia Tedesco[2], Antonio Vecchione[2], Thomas P. Papageorgiou[3], Hans F. Braun[4], Manuel Kempf[4], and Johannes Krämer[4] — [1]PANalytical, Almelo, The Netherlands — [2]Università di Salerno, Italy — [3]Forschungzentrum Dresden-Rossendorf, Germany — [4]Universität Bayreuth, Germany

For small rare earth ions (RE=Gd, Eu), single phase compounds are obtained with the typical ordered layered structure and no significant changes of physical properties. With large rare earth ions (RE=Nd, Pr), polyphase samples were obtained and the phases in equilibrium at the nominal composition $RuSr_2RECu_2O_8$ were determined. In these cases, no ordered layered structure was observed. The disorder between Ru/Cu or Sr/RE is presumably due to the similar Ru/Cu and Sr/RE ionic sizes. Magnetization studies of these compounds are discussed.

The effect of substituting Sr^{+2} with the smaller Ca^{+2} and larger Ba^{+2} is examined. The substitution with Ca^{+2} results in a complex mixture. We cannot confirm the previously reported formation of the layered $RuCa_2NdCu_2O_8$. For Ba^{+2} substitution, a binary mixture Ba_2RuNdO_6–CuO is obtained. A different number and different types of phases in equilibrium are found with different alkaline earths (A=Ca, Sr, Ba) at the nominal $RuA_2NdCu_2O_8$ composition. The variation in the mismatch of the A/Nd (A=Ca, Sr, Ba) size does not lead to the formation of an ordered layered $RuA_2NdCu_2O_8$ compound.

TT 10.4 Mon 14:45 H 3010

Growth and study of $LuNi_2B_2C$ single crystals — •Anke Köhler[1], Günter Behr[1], Beate Bergk[2], Günter Fuchs[1], Konstantin Nenkov[1], and Joachim Wosnitza[2] — [1]IFW Dresden, D-1171 Dresden — [2]Forschungszentrum Dresden-Rossendorf, D-01328 Dresden

Rare earth-nickel-borocarbides have attracted much interest in the last years because the compounds show the interplay of superconductivity and magnetic ordering. $LuNi_2B_2C$ can be considered as non-magnetic reference system of such magnetic borocarbides as $HoNi_2B_2C$ in which superconducting and antiferromagnetic ordering temperatures, T_c and T_N, are similar.

So far, $LuNi_2B_2C$ crystals were only prepared by a flux method. For growing larger crystals we used an optical floating zone (FZ) technique, which already was successful in crystal growth of other RNi_2B_2C (R = Y,Tb,Ho,Tm,Er) compounds. In the case of $LuNi_2B_2C$, the primary crystallization field is far from the stoichiometric composition, and adjacent to the properitectic LuB_2C_2 phase field an extended region of LuNiBC occurs. Systematic studies of polycrystalline samples revealed that samples with nominal compositions $LuNi_5B_{3.5}C$ and $LuNi_5B_3C_{0.5}$ are free of the properitectic LuB_2C_2 and LuNiBC phases. Thus in the FZ crystal growth experiments we used a molten zone which corresponds to these compositions.

From the grown $LuNi_2B_2C$ rods single crystalline pieces have been prepared to investigate Fermi surface peculiarities by magnetoresistance measurements and to study the electronic band structure.

TT 11: Superconductivity: Tunneling, Josephson Junctions, SQUIDs

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

Invited Talk TT 11.1 Mon 15:15 H 3010

Superconducting Quantum Interference Filters — •Nils Schopohl — Institut für Theoretische Physik der Universität Tübingen

Basic principles of Josephson junction based interferometer arrays are reviewed. Key features of parallel and also serial Superconducting Quantum Interference Filters (SQIFs) are explained in detail. It is shown that SQIF interferometers can be engineered to have a specific voltage output pattern vs. magnetic field that is well suited for applications in magnetometry and also microwave sensorics.

TT 11.2 Mon 15:45 H 3010

Tailored Josephson phase: 0, π and 0–π SIFS Josephson junctions — •Martin Weides[1], Alexey Bannykh[1], Uthayasankaran Peralagu[1], Judith Pfeiffer[2], Matthias Kemmler[2], Dieter Koelle[2], Reinhold Kleiner[2], and Edward Goldobin[2] — [1]Institute for Solid State Research, Research Centre Jülich — [2]Physikalisches Institut - Experimentalphysik II,

In superconducting/ferromagnet (S/F) systems the superconducting wave function extends into the ferromagnet with a damped oscillatory behavior. This results in novel and interesting physics, such as the possibility to realize a π Josephson junction (JJ) — a JJ with the phase drop of π in the ground state. Recently, we fabricated Nb/Al_2O_3/NiCu/Nb JJs with uniform as well as step-like ferromag-

netic layer to obtain 0, π and 0-π JJs[1,2].
Here we present our recent results on planar SIFS JJs with F-layer made of Ni, and compare them with the theory in the clean/dirty limit and with experiments by other groups. The critical current density in the π state is larger and the order parameter decay is weaker than for π JJs made using weak ferromagnetic alloys, e.g. NiCu.
The 0–π boundary in JJs with a step-like F-layer thickness may give rise to a pinned spontaneous vortex of supercurrent with magnetic flux $\leq |\Phi_0/2|$. Latest experiments on short and long stepped SIFS JJs (0–π, 0–π–0 etc.) will be discussed.

[1] M. Weides *et al.*, Phys. Rev. Lett. **97**, 247001 (2006)
[2] M. Weides *et al.*, Appl. Phys. A **89**, 613–617 (2007)

TT 11.3 Mon 16:00 H 3010

Magnetic flux dynamics in 0, π and 0-π SIFS Josephson junctions — •Judith Pfeiffer[1], Martin Weides[2], Matthias Kemmler[1], Alexey K. Feofanov[3], Jürgen Lisenfeld[3], Dieter Koelle[1], Alexey V. Ustinov[3], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Physikalisches Institut-Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, D-72076 Tübingen, Germany — [2]Center of Nanoelectronic Systems for Information Technology (CNI), Research Centre Jülich, D-52425 Jülich, Germany — [3]Physikalisches Institut III, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We present experimental and numerical studies of high quality underdamped Superconductor-Insulator-Ferromagnet-Superconductor (SIFS) Josephson junctions fabricated as $Nb/Al_2O_3/Cu_{40}Ni_{60}/Nb$ heterostructures. Varying the thickness of the ferromagnetic barrier one can fabricate 0, π and 0-π junctions. The dynamic and static properties of these junctions are studied by measuring the I-V characteristic and critical current I_c vs. magnetic field H. Using microwave spectroscopy we have investigated the eigenfrequencies of a 0, π and 0-π Josephson junction in the temperature range 4.2 K...300 mK. Harmonic, subharmonic and superharmonic pumping is observed in experiment and the experimental data are compared with numerical simulations. Perfoming thermal escape measurements at temperatures down to 300 mK we try to reach the quantum tunnelling regime.

TT 11.4 Mon 16:15 H 3010

Self resonances in Josephson π-junctions — •Georg Wild, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Due to their potential application as π-phase shift elements Josephson junctions with ferromagnetic interlayer have attracted much interest. We have developed a self-aligned multilayer process for the fabrication of superconductor/insulator/ferromagnetic metal/superconductor (SIFS) Josephson junctions (S=Nb, I=Al_2O_3, F=NiPd). Our junctions show RCSJ-like current-voltage characteristics (IVCs) and a Fraunhofer diffraction pattern for the magnetic field dependence of the critical current I_c. The dependence of the I_cR_n-product on the ferromagnet thickness shows a clear crossover between the zero- and the π-state. The π-coupled multilayers show critical current densities of about 50 A/cm^2 and I_cR_n-products of about 20 μV at $T = 1.5$ K. The IVCs of these junctions show both Fiske resonances and zero field steps. The height of the Fiske steps can be fitted by Kulik's theory. Fitting the measured height of the Fiske steps of different order we derived quality factors varying between 20 and 40.
This work was supported by the DFG via SFB 631 and the Excellence Initiative via NIM.

15 min. break

TT 11.5 Mon 16:45 H 3010

Advanced models of Josephson junction arrays (exchanged with TT 11.9) — •Carsten Hutter[1], Kai Stannigel[1,2], Eric Tholén[3], Jack Lidmar[4], and David Haviland[3] — [1]Department of Physics, Stockholm University, Sweden — [2]Institut für theoretische Festkörperphysik, Universität Karlsruhe, Germany — [3]Nanostructure Physics, Royal Institute of Technology, Stockholm, Sweden — [4]Department of Physics, Royal Institute of Technology, Stockholm, Sweden

One-dimensional Josephson junction arrays are interesting in many contexts. For instance, they can undergo quantum phase transitions [1], but they can also be used as a tunable environment in the study of other tunnel junctions or SQUIDs [2]. Here we investigate a model for the array, which besides the Josephson junction and capacitance to ground additionally includes a stray inductance for each array element. For certain parameters, the dynamics of the system change drastically: In the phase regime, the impedance becomes purely imaginary in a parameter-dependent frequency range. We further find a gap in the dispersion relation for the same frequency range. We suggest a modified array with two different junctions per array element, in which this behaviour can be observed more easily.

[1] S.L. Sondhi et al., RMP 69, 315 (1997)
[2] S. Corlevi et al., PRL 97, 096802 (2006)

TT 11.6 Mon 17:00 H 3010

Fabrication and performance of Niobium-microsquids — •Martin Batzer[1], Georg Schmidt[1], Charles Gould[1], Laurens Molenkamp[1], and Wolfgang Wernsdorfer[2] — [1]Julius-Maximilians-Universität Würzburg — [2]Institut Néel, CNRS Grenoble

Microsquids are useful instruments to detect and measure strongly localized ultrasmall magnetic moments. Here we present the fabrication and characterization of Niobium-based microsquids with diameters equal to or less than 1 μm by dry-etching. In order to avoid degradation during processing, the Nb-layer needs to be covered by a protective layer directly after the Nb-deposition. This protective layer mainly determines the further processing steps. The layers used for our experiments either consist of 15 nm of Nb covered by 2 nm of Si or of 30 nm of Nb covered by a bi-layer of 10 nm of Al and 10 nm of Ru. For the patterning process, a metal mask is patterned on top of the multilayer by electron beam lithography and lift-off. RIE-etching in a mixture of CHF_3 and O_2 is used to transfer the pattern into the niobium. For the tri-layer an additional Ar^+-etch is necessary to remove the Ru and Al layer. For both layer systems working microsquids have successfully been fabricated. The best resolution that we obtain in preliminary measurements is $\Phi_0/200$. We anticipate that additional shielding and optimization of the read out electronics will allow for a lower noise level and thus higher resolution.

TT 11.7 Mon 17:15 H 3010

Josephson spin currents in triplet superconductor junctions — •Philip Brydon and Dirk Manske — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The interplay of triplet superconductivity and magnetism leads to unconventional Josephson behaviour in junctions combining these two phases. This is shown, for example, by the dependence of the Josephson current on the alignment of the barrier magnetic moment with the bulk superconductor **d**-vectors in the triplet-superconductor–ferromagnet–triplet-superconductor (TFT) junction studied by P. M. R. Brydon *et al.* (cond-mat/0709.2918). In general, the Josephson effect between triplet superconductors allows not only for a spontaneous charge current, but also a spontaneous spin current. Using a quasiclassical Green's function theory, we investigate the spin current through the TFT junction in the ballistic regime. Results for the dependence of the spin current vs phase relations upon the orientation of the two **d**-vectors and the ferromagnetic moment are presented.

TT 11.8 Mon 17:30 H 3010

Josephson current through a single Anderson impurity coupled to BCS leads — •Christoph Karrasch[1], Akira Oguri[2], and Volker Meden[3] — [1]Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen, Germany — [2]Department of Material Science, Osaka City University, Sumiyoshi-ku, Osaka 558-8585, Japan — [3]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Germany

We investigate the Josephson current $\langle J(\phi)\rangle$ through a quantum dot embedded between two superconductors showing a phase difference ϕ. The system is modeled as a single Anderson impurity coupled to BCS leads, and the functional and the numerical renormalization group frameworks are employed to treat the local Coulomb interaction U. We reestablish the picture of a quantum phase transition occurring if the ratio between the Kondo temperature T_K and the superconducting energy gap Δ or, at appropriate T_K/Δ, the phase difference ϕ or the impurity energy is varied. We present accurate zero- as well as finite-temperature T data for the current itself, thereby settling a dispute raised about its magnitude.

TT 11.9 Mon 17:45 H 3010

Controllable manupulation and SQUID readout of two coupled semifluxons (exchanged with TT 11.5) — •Edward Goldobin, Andreas Dewes, Florian Jessen, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut–Experimentalphysik II

and Center for Collective Quantum Phenomena, University of Tübingen, Auf der Morgenstelle 14, 72076, Tübingen, Germany

Josephson vortices carrying half of the magnetic flux quantum Φ_0 naturally appear in 0-π long Josephson junctions (LJJs) that can be fabricated using various technologies[1–3]. Such semifluxons are pinned at the 0-π boundary, but may have two polarities that can be used for information processing, i.e. the state $\uparrow$, corresponding to the flux $+\Phi_0/2$, and the state $\downarrow$, corresponding to the flux $-\Phi_0/2$. The first proposed prototype of a semifluxon based qubit employs two degenerate ground states $\uparrow\downarrow$ and $\downarrow\uparrow$ of a two semifluxon molecule in 0-π-0 LJJ[4]. It was predicted that such a molecule may be switched between the states $\uparrow\downarrow$ and $\downarrow\uparrow$ by applying a small bias current[5].

Using two SQUIDs placed in front of each semifluxon to readout their magnetic flux (polarity), we experimentally demonstrate the $\uparrow\downarrow\longleftrightarrow\downarrow\uparrow$ transition controlled by uniform dc bias current. We also observe $\uparrow\uparrow$ and $\downarrow\downarrow$ states and controllably changed them to the $\uparrow\downarrow$ and $\downarrow\uparrow$ states.

[1] H. Hilgenkamp et al. Nature **422**, 50 (2003)
[2] M. Weides et al., Phys. Rev. Lett. **97**, 247001 (2006)
[3] E. Goldobin et al., Phys. Rev. B. **72**, 054527 (2005)
[4] E. Goldobin et al., Phys. Rev. B **67**, 224515 (2003)
[5] E. Goldobin et al., Phys. Rev. B.**72**, 054527 (2005).

TT 12: Symposium: Cryodetectors and SQUID

Time: Tuesday 9:30–12:45 Location: H 0104

Invited Talk TT 12.1 Tue 9:30 H 0104

SQUID multiplexers for low-temperature detectors — •K.D. Irwin, J.A. Beall, H.M. Cho, W.B. Doriese, W.D. Duncan, G.C. Hilton, R. Horansky, N. Jethava, J.A.B. Mates, C.D. Reintsema, D. Schmidt, J.N. Ullom, L.R. Vale, Y. Xu, and K. Yoon — National Institute of Standards and Technology, Boulder, Colorado 80305

The development of arrays of low-temperature detectors, including the superconducting transition-edge sensor (TES), has provided new capabilities for applications including astronomy, particle physics, and nuclear materials analysis. These applications require the implementation of large arrays of sensors. Due to constraints on cryogenic wiring heat load and complexity, it is impractical to route wires from room temperature to every pixel in a large low-temperature detector array. We have developed multiplexed readout circuits based on Superconducting Quantum Interference Devices (SQUIDs) to meet this need. We are implementing two SQUID multiplexer architectures: time-division multiplexed dc SQUID arrays operated at MHz frequencies, and frequency-division multiplexed rf SQUID arrays operated at microwave frequencies. Kilopixel TES arrays based on time-division multiplexed dc SQUIDs have reached maturity, and are being deployed in multiple instruments. Microwave frequency-division-multiplexed arrays of dissipationless rf SQUIDs coupled to superconducting microresonators have the promise of scaling to much larger array implementations in the future. The current status of these technologies, and future directions will be described.

Invited Talk TT 12.2 Tue 10:00 H 0104

Transition Edge Sensor and Kinetic Inductance Detector Developments for Astronomy Applications — •Piet de Korte — SRON Netherlands Institute for Space Research

Cryogenic radiation detectors enable significant progress in astronomy through the development of Imaging Spectrometers for X-ray astronomy based on micro-calorimeter arrays of Transition-Edge*Sensors, and through the development of highly sensitive, $< 10^{-19} W/Hz^{1/2}$, bolometer arrays for Infrared and Sub-mm astronomy. The latter application can be realized both by transion-edge-sensors as well as by kinetic inductance detectors. Both developments take place at SRON Netherlands Institute for Space Research for instruments on future missions, like XEUS (ESA) and SPICA (JAXA/ESA).

The presentation will explain the principles of both type of instruments, and show the present state of development both with regard to the sensor development as well as with regard to the read-out electronics.

TT 12.3 Tue 10:30 H 0104

Metallic magnetic calorimeters for high resolution x-ray spectroscopy and particle detection — •Loredana Fleischmann — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

An increasing number of experiments and applications employ low temperature particle detectors which are based on a calorimetric detection scheme and operated at temperatures below 100 mK. In many cases this is due to the high energy resolution achievable with these detectors. Equally important benefits are often the increased flexibility in the choice of absorber materials and the fact that the detection efficiency is independent of the ionizing character of the particles to be detected.

Metallic magnetic calorimeters (MMC) make use of a metallic paramagnetic temperature sensor, which is in tight thermal contact with an absorber for the particles of interest. The paramagnetic sensor is placed in a small magnetic field. Its magnetization is used to monitor the temperature, which in turn is related to the internal energy of the calorimeter. High energy resolution can be obtained by using a low-noise, high-bandwidth DC SQUID to measure the small change in magnetization upon the absorption of energy.

With recent x-ray detector prototypes an energy resolution of a few eV for x-ray energies up to 6 keV has been achieved. We discuss the thermodynamic properties, the energy resolution, the microfabrication and general design considerations of MMCs as well as their application in high resolution x-ray spectroscopy, beta spectroscopy and absolute activity measurements.

15 min. break

Prize Talk TT 12.4 Tue 11:15 H 0104

Methode zur berührungslosen, induktiven Messung der lokalen Übergangstemperatur supraleitender, dünner Wolframfilme — •Karoline Schäffner, Godehard Angloher, Irina Bavykina, Antonio Bento, Dieter Hauff, Patrick Huff, Michael Kiefer, Rafael Lang, Emilija Pantic, Federica Petricca, Franz Pröbst, Jens Schmaler, Wolfgang Seidel, Hans Seitz und Leo Stodolsky — Max-Planck-Institut für Physik, München — Trägerin des Georg-Simon-Ohm-Preises

Ziel des CRESST-Experimentes (Cryogenic Rare Event Search with Superconducting Thermometers) ist es, Dunkle Materie in Form von WIMPs direkt durch deren elastische Streuung an den Kernen eines Absorberkristalls nachzuweisen. Die Signalauslese der Teilchendetektoren erfolgt mit supraleitenden Phasenübergangsthermometern, welche aus dünnen Wolframfilmen bestehen.

Die supraleitende Übergangstemperatur von einkristallinem Wolfram liegt bei 15 mK. Die Übergangstemperatur dünner Wolframfilme kann jedoch durch Ausbildung einer metastabilen Beta-Phase, Filmspannungen oder Spuren von Verunreinigungen beeinflusst werden. Zur Untersuchung möglicher Inhomogenitäten dieser Filme wurde eine induktive Methode zur lokalen Messung der supraleitenden Übergangstemperatur entwickelt. Dabei wird eine Spule in geringem Abstand über einem Wolframfilm platziert. Die Änderung der Permeabilität des Wolframfilms beim Übergang in die supraleitende Phase führt zu einer Änderung der Induktivität der Spule, welche mit einem SQUID-basierten Messsystem nachgewiesen wird.

TT 12.5 Tue 11:45 H 0104

SQUID series array current sensor for measuring dc currents — •Jörn Beyer and Dietmar Drung — PTB, Berlin, Germany

Single SQUIDs are detectors of magnetic flux and show a multi-valued voltage-flux characteristics. In precision measurement systems they are used to sense changes in various physical quantities, e.g. magnetic field, electric current or mechanical displacement, which can be transformed into changes in the magnetic flux threading the SQUID loop. A dc-SQUID-based sensor able to detect a dc signal can be formed by a series array of individual dc-SQUIDs (SSA) with different loop sizes [1]. Due to the varying SQUID loop size such a SSA can per se not achieve a flux noise as low as of a same length SSA of identical SQUIDs. Here, we present a new SSA current sensor for measuring dc currents which comprises of identical individual SQUIDs. In this device, the input signal current is coupled tightly but non-uniformly

to the individual array elements. This leads to a single-valued overall voltage-flux characteristics and, therefore, allows a dc input signal to be measured. Apart form the non-uniform input signal coupling the individual SQUIDs of the SSA current sensor can be flux-biased evenly, as well. This has a significant practical advantage as flux offsets equal in all the individual SQUIDs of the array can be compensated. Such flux offsets arise for instance due to asymmetric bias current feed into the array elements which is preferential for adjusting the dynamic resistance and therefore the noise performance. We present the design, simulations and experimental results on the dc-current sensor performance.

[1] P.Carelli et.al., Europhys.Lett. 39, 569 (1997)

TT 12.6 Tue 12:00 H 0104

Relaxationsmessungen mit SQUID Gradiometern — •Frank Schmidl, Markus Büttner, Christoph Becker, Alexander Steppke, Peter Kossebau, Stefan Prass und Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

SQUID Gradiometer ermöglichen die Messung kleinster magnetischer Felder in unabgeschirmter Umgebung. Wir stellen Einsatzmöglichkeiten eines axialen SQUID Gradiometers zweiter Ordnung (Arbeitstemperatur 4,2 K) für Magnetorelaxationsmessungen an unterschiedlichen Nanopartikeln vor. Dabei kann das System zur Detektion der räumlichen Verteilung von magnetischen Nanopartikeln oder zur Untersuchung der Temperaturabhängikeit dieser Teilchensysteme genutzt werden. Letztere Untersuchungsmethode kann auf Grund des realisierten Temperaturbereichs von 4,2 K bis 320 K ein besseres Verständnis des Verhaltens dieser Materialsysteme liefern. Die aus dem experimentellen Aufbau resultierenden Möglichkeiten und Grenzen dieses Verfahrens für die Charakterisierung magnetischer Nanopartikle werden ebenso diskutiert, wie der mögliche Einsatz von Hochtemperatursupraleitern als Magnetfeldsensoren für derartige Anwendungen.

Die Arbeiten werden im Rahmen des EU-Projektes BIODIAGNOSTICS Nr.017002 gefördert.

TT 12.7 Tue 12:15 H 0104

Scanning THz-Microscopy of microwave devices with a Josephson-Cantilever — •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 $YBa_2Cu_3O_7$ on a vibrating cantilever prepared from a $SrTiO_3$-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 μm 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 768 GHz with a spatial resolution of 10 μm far below the corresponding wavelengths. For the higher frequencies we couple far-infrared laser radiation from a CO_2-laser pumped molecular laser system into the chamber. Applications of this novel instrument to microwave devices are demonstrated.

TT 12.8 Tue 12:30 H 0104

Highly sensitive and easy-to-use SQUID sensors — •Frank Ruede[1,2], Cornelia Assmann[1], Jörn Beyer[1], Dietmar Drung[1], Alexander Kirste[1], Margret Peters[1], and Thomas Schurig[1] — [1]PTB, Berlin, Germany — [2]Magnicon GbR, Hamburg, Germany

We have developed a family of low-noise superconducting quantum interference devices (SQUIDs) to cover a wide range of applications. These sensors are robust and easy to use without compromising noise performance. They are optimized for operation with the Magnicon high-speed flux-locked loop (FLL) electronics XXF-1.

This contribution focuses on SQUID current sensors with higher input inductances of up to 2μH. Typical applications for these sensors are the measurement of the magnetic field with a superconducting pickup loop connected to the input coil.

Dependent on the required noise level, single-stage and two-stage devices were realized in our latest sensor family 'C5'. The single-stage sensors achieve a coupled energy resolution around 70 times Planck's constant h at 4,2K and the two-stage sensor of 45h. They consist of a single front-end SQUID which is read out by a 16-SQUID series array. These sensors are very convenient to use as their voltage-flux characteristic is essentially single-SQUID-like. Devices optimized for low temperature operation achieve typically 4h at 300mK.

All sensor designs have an optional integrated current limiter (Q-spoiler) in series to the input coil, which can be used to reduce the current in pulsed applications like magnetorelaxometry.

TT 13: Correlated Electrons: Low-dimensional Systems - Materials 1

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

TT 13.1 Tue 9:30 H 2053

Resonant inelastic soft x-ray scattering on the spin-ladder/spin-chain system $Sr_{14}Cu_{24}O_{41}$ — •Justina Schlappa[1], T. Schmitt[1], A. Bendounan[1], X. Wang[2], A. Piazzalunga[3], V. Strocov[1], B. Delley[1], B. Thielemann[1,4], H. Ronnow[2], G. Ghiringhelli[3], M. Grioni[3], L. Braicovich[3], C. Dallera[3], J. Mesot[1,4], and L. Patthey[1] — [1]Paul Scherrer Institut, Switzerland — [2]Ecole Polytechnique Fédérale Lausanne, Switzerland — [3]Politecnico di Milano, Italy — [4]ETH Zürich, Switzerland

The layered system $(Sr,Ca)_{14}Cu_{24}O_{41}$, is a low-dimensional cuprate system that has been studied recently with large interest [1]. It is mixed-valent and built up of two different cupper-oxygen layers: 1-dim CuO_2 chains and quasi 1-dim Cu_2O_3 2-leg ladders. When cooling below 200 K a full range of interresting phenomena is observed, as structural changes, formation of charge order and formation of AF-dimers on the chains.

We investigated the electronic structure of $Sr_{14}Cu_{24}O_{41}$ by inelastic x-ray scattering (RIXS) [2] at the Cu $M_{2,3}$ edge (3p $\rightarrow$ 3d transition). The spectra show well-pronounced inelastic signal in the constant energy loss of 1.5-2.5 eV, which originates from crystal field excitations. Differences between the different crystallographic directions and between the high- and low-temperature phase are revealed.

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

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

TT 13.2 Tue 9:45 H 2053

Highly frustrated $S = 1/2$ spin chains near a quantum critical point — •R. Klingeler[1], S.-L. Drechsler[1], N. Tristan[1], V. Kataev[1], F. Kretzschmar[1], Y. Arango[1], N. Leps[1], J. Vavilova[1], A. Parameswaran[1], H.-H. Klauss[2], H. Luetkens[3], O. Volkova[4], A. Vasiliev[4], T. Lorenz[5], H. Rakoto[6], U. Zeitler[7], J. Richter[8], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden — [2]TU Dresden — [3]PSI Villingen — [4]Moscow State University — [5]University of Köln — [6]LNCMP Toulouse — [7]HMFL Nijmegen — [8]University Magdeburg

Frustrated antiferromagnetic quantum spin chains with competing nearest and next-nearest neighbor interactions exhibit a rich physics with unusual ground states. Effects of quantum fluctuations are particularly strong in the vicinity of a quantum critical point where small perturbations such as a weak external magnetic field or the inter-chain coupling strongly affect the physical properties. This situation is realized in the novel S=1/2 spin chain compound Li_2ZrCuO_4 which is close to a quantum critical point. We report on specific heat, thermal expansion and magnetisation as well as on NMR, ESR and μSR studies which confirm high frustration and strong quantum fluctuations. While inter-chain coupling yields long range antiferromagnetic order at low temperatures our data suggest short range helical/AFM correlations above T_N. Upon application of a magnetic field of 9T, however, these correlations are suppressed against ferromagnetic ones. ESR and NMR data confirm the coexistence of quasi-1D behavior and short range AFM correlations up to $80\,K \gg T_N \approx 7\,K$.

TT 13.3 Tue 10:00 H 2053

Low-dimensional spin-1/2 systems in complex vanadium phosphates — •Alexander Tsirlin[1,2], Ramesh Nath[1], Christoph Geibel[1], and Helge Rosner[1] — [1]Max-Planck Institute CPfS, Dresden, Germany — [2]Department of Chemistry, MSU, Moscow, Russia

Vanadium phosphates are known to reveal low-dimensional spin-1/2 systems and to provide unique realizations for some of the actively studied spin models like frustrated J_1-J_2 square lattice. Magnetic patterns of these compounds may be quite complicated as non-magnetic phosphate tetrahedra mediate superexchange interactions. The signs and the magnitudes of such interactions can hardly be estimated on structural basis only, therefore the choice of the appropriate spin model is sometimes very problematic. In our contribution we present the results of joint experimental (thermodynamic properties measurements) and computational studies of several complex vanadium phosphates. We employ full-potential band structure calculations in order to give reliable estimates of the exchange coupling constants. The estimates justify the choice of the particular model and help us to give reliable interpretation of the experimental data. We reach a remarkable agreement between the experimental and computational results. Our studies show that some of the vanadium phosphates are promising objects for the investigation of low-temperature quantum phenomena in low-dimensional spin-1/2 systems.
The Emmy-Noether program, GIF (I-811-257.14/03), and RFBR (07-03-00890) are acknowledged for financial support.

TT 13.4 Tue 10:15 H 2053

$KTi(SO_4)_2.H_2O$ - a possible candidate for a new spin-Peirles system — •Deepa Kasinathan[1], Goran Nilsen[2], Henrik Ronnow[2], Stefan-Ludwig Drechsler[3], and Helge Rosner[1] — [1]MPI CPfS - Dresden, Germany — [2]LQM-EPFL, Lausanne, Switzerland — [3]IFW Dresden, Germany

Recently a large number of compounds belonging to the family of J_1-J_2 chain models with competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions have been discovered. In most cases, FM-J_1 and AFM-J_2 is observed, leading to helical order with no spin gap (for frustration ratio $\alpha = \frac{J_1}{J_2} >$ -0.25). Systems with both J_1 and J_2 being AFM causing a spin gap are rather rare. The thermodynamic data of the recently prepared $KTi(SO_4)_2.H_2O$ reveal that this system is a quasi 1D spin 1/2 chain compound with both J_1 and J_2 being AFM, and a frustration ratio $\alpha \approx 0.29$. Here we report the results of electronic structure calculations within the LSDA+U method along with tight-binding models. Our calculations confirm that both J_1 and J_2 are AFM. In contrast to the experiments we obtain a larger α, slightly depending on the choice of the Coulomb repulsion U. Therefore $KTi(SO_4)_2.H_2O$ might be a new candidate for a spin-Peirles ground state. A brief comparison with other systems belonging to the class of frustrated chain materials is given with respect to their position in the general phase diagram of the 1D J_1-J_2 model.

TT 13.5 Tue 10:30 H 2053

Spin dynamics in the plateau phase of the 1D distorted diamond chain azurite, $Cu_3(CO_3)_2(OH)_2$ — Kirrily Rule[1], Anja Wolter[1], •Stefan Süllow[2], Bernd Wolf[3], Michael Lang[3], Jürgen Schreuer[4], and Alan Tennant[1] — [1]BENSC, HMI, 14109 Berlin — [2]IPKM, TU Braunschweig, 38106 Braunschweig — [3]Physikalisches Institut, J.W. Goethe-Universität Frankfurt, 60438 Frankfurt(M) — [4]Ruhr-Universität Bochum, Bochum

Recently, azurite, $Cu_3(CO_3)_2(OH)_2$, has been described as an ideal example of a frustrated one-dimensional (1D) diamond-chain antiferromagnet [1]. A 1/3 magnetisation plateau has been observed in azurite for fields between 11 and 30T applied perpendicular to both the crystallographic b axis and Cu^{2+} chain direction. Here, we present a study by means of inelastic neutron scattering, which has been performed on a large single crystal of azurite in fields up to 14T applied perpendicular to the chain direction, *viz.* in the plateau phase. Our data in the plateau phase indicate that the magnetic excitations can be described by a dimer-monomer model with two distinct energy scales. The dispersion function of the monomer chain reveals an effective spin coupling of $J_{eff} = 10.1(2)$ K, while the lowest Zeeman-split dimer branch has an effective dimer-dimer coupling of $J_{dimer} = 1.8(1)$ K. We will discuss possible values for the exchange constants J_1, J_2 and J_3 of the diamond chain model to account for these observations, based on a perturbative approach.

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

TT 13.6 Tue 10:45 H 2053

On the microscopic description of the spin-1/2 quantum magnet azurite — •Andreas Honecker[1], Johannes Richter[2], Helge Rosner[3], Oleg Janson[3], Roser Valenti[4], Hem Kandpal[4], Hena Das[5], Bernd Wolf[6], and Michael Lang[6] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [4]Institut für Theoretische Physik, J.W. Goethe-Universität Frankfurt — [5]S.N. Bose National Centre for Basic Sciences, Kolkata, India — [6]Physikalisches Institut, J.W. Goethe-Universität Frankfurt

The mineral azurite $Cu_3(CO_3)_2(OH)_2$ exhibits interesting low-temperature properties like a magnetization plateau at 1/3 of saturation [H. Kikuchi *et al.*, Phys. Rev. Lett. **94** (2005) 227201]. While the crystal structure suggests a description in terms of the spin-1/2 Heisenberg model on a distorted diamond chain, the values of the associated exchange constants have remained a matter of debate. Firstly, we present a study of the complete parameter space of the spin-1/2 Heisenberg model on the distorted diamond chain. Thermodynamic and dynamic properties are computed by exact diagonalization and compared to experimental results for azurite. In particular, we discuss the constraints obtained from recent inelastic neutron scattering results on the 1/3 plateau [K.C. Rule *et al.*, arXiv:0709.2560]. Secondly, complementary *ab-initio* computations are performed in order to obtain further information about the relevant exchange paths in azurite as well as the values of the associated magnetic exchange constants.

TT 13.7 Tue 11:00 H 2053

Molecule-based realization of an $S = 1/2$ antiferromagnetic Heisenberg chain — •K. Remović-Langer[1], Y. Tsui[1], U. Tutsch[1], B. Wolf[1], W. Assmus[1], A. Prokofiev[4], A. Honecker[2], G. Donath[3], and M. Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, Max-von-Laue-Str. 1, SFB/TR 49, D-60438 Frankfurt(M). — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen. — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden. — [4]Institut für Festkörperphysik, Technische Universität Wien, Wiedner Hauptstr. 8-10, A-1040 Wien.

Generally, fine tuning of an external control parameter is required to drive a system to a quantum critical point (QCP). This is different for the spin $S = 1/2$ antiferromagnetic Heisenberg chain (AFHC) which is inherently quantum critical. Here we present magnetic and thermodynamic measurements on single crystals of a copper coordination polymer $[Cu(\mu\text{-ox})(4\text{-apy})_2(H_2O)]_n$. Measurements of the susceptibility, magnetization and specific heat were found to be in full accordance with theoretical predictions for the uniform $S = 1/2$ AFHC with a small magnetic exchange interaction of $J/k_B \sim (3.1\pm0.1)$K. The material can be easily tuned to the saturation field $B_s \sim 4.2$ T, given by $g\mu_B B_s$=$2J$, which marks the endpoint of a quantum critical line in the $T-B$ plane.

15 min. break

TT 13.8 Tue 11:30 H 2053

Magnetic measurements on a metal-organic spin-1/2 dimer system – a possible candidate for a 2D field-induced phase transition — •Ulrich Tutsch[1], Bernd Wolf[1], Michael Lang[1], Tonia Kretz[2], Hans-Wolfram Lerner[2], Matthias Wagner[2], Stefan Wessel[3], Tanusri Saha-Dasgupta[4], Harald Jeschke[5], and Roser Valenti[5] — [1]Physikalisches Institut, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt(M), Germany — [2]Institut für Anorganische Chemie, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt(M), Germany — [3]Institut für Theoretische Physik III, Universität Stuttgart, D-70550 Stuttgart, Germany — [4]S.N. Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700098, India — [5]Institut für Theoretische Physik, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt(M), Germany

We present new data for the low-temperature (T<1K) susceptibility of $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91) as function of the magnetic field. In this material Cu^{2+} ions form spin-1/2 dimers with an intradimer exchange interaction of $J_1/k_B \approx$ 10K mediated by a hydroquinone-derived linker. Previous studies have revealed a weak interdimer coupling $J_2/k_B \sim$ 1K. Density Functional Theory calculations support these findings and furthermore indicate a quasi 2-dimensional structure of the interdimer coupling. Therefore, we compare the new susceptibility data with Quantum Monte Carlo Simulations for 2-dimensionally coupled dimers. The results indicate that this material is a candidate

for a 2D field-induced phase transition.

TT 13.9 Tue 11:45 H 2053

Magnetic properties of the spin-1/2 chain material (6MAP)$CuCl_3$ — •M. Ozerov[1], E. Čižmár[1], S. Zvyagin[1], C. Landee[2], M. Turnbull[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden - Rossendorf, Germany — [2]Clark University, Worcester, MA, USA

Recently, low-dimensional spin systems have received a considerable amount of attention due to their relevance to numerous quantum phenomena such as quantum criticality problems, spin-Peierls transitions, etc. Here we report on magnetization, electron paramagnetic resonance (EPR) and specific-heat measurements of the spin-1/2 Heisenberg antiferromagnetic chain material (6MAP)$CuCl_3$. Magnetization data measured at 0.1 T exhibit a maximum at about 70 K, indicating the low-dimensional character of the magnetic interactions. The data are in a good agreement with the temperature dependence of the resonance peak intensity measured at 73 GHz. At low temperatures (T < 25 K) the EPR linewidth drastically increases, indicating a possible enhancement of 3D short-range-order correlations. Such behavior is consistent with a broad maximum in the specific heat observed at about 1.5 K, which can be interpreted in terms of 3D magnetic ordering. In addition, we present results of room-temperature X-band EPR measurements of (6MAP)$CuCl_3$, including angular dependence of the g-factor and of the resonance linewidth.

The work was supported in part by the DFG through Grant No. ZV 6/1-1.

TT 13.10 Tue 12:00 H 2053

Magnetic properties of the Haldane-gap material NENB — •Erik Čižmár[1], Mikhaylo Ozerov[1], Oleg Ignatchik[1], Thomas P. Papageorgiou[1], J. Wosnitza[1], S. A. Zvyagin[1], Jurek Krzystek[2], Zhixian Zhou[3], Christopher P. Landee[4], Brian R. Landry[4], Mark M. Turnbull[4], and Jan L. Wikaira[5] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]National High Magnetic Field Laboratory, Tallahassee, USA — [3]Department of Physics and Astronomy, Wayne State University, Detroit, USA — [4]Department of Physics and Carlson School of Chemistry, Clark University, Worcester, USA — [5]Department of Chemistry, University of Canterbury, Christchurch, New Zealand

Results of magnetization and high-field ESR studies of the new spin-1 Haldane-chain material $[Ni(C_2H_8N_2)_2NO_2](BF_4)$ (NENB) are reported. A definite signature of the Haldane state in NENB was obtained. From the analysis of the frequency-field dependence of magnetic excitations in NENB, the spin-Hamiltonian parameters were calculated, yielding Δ/k_B = 17.4 K, $g_{\parallel}$ = 2.14, D/k_B = 7.5 K, and $|E/k_B|$ = 0.7 K for the Haldane gap, g factor. and the crystal-field anisotropy, respectively. The presence of fractional $S = 1/2$ chain-end states, revealed by ESR and magnetization measurements, is found to be responsible for spin-glass-freezing effects. In addition, extra states in the excitation spectrum of NENB have been observed in the vicinity of the Haldane gap, whose origin is discussed.

The work was supported in part by the DFG through Grant No. ZV 6/1-1.

TT 13.11 Tue 12:15 H 2053

New natural spin-1/2 kagomé systems — kapellasite $Cu_3Zn(OH)_6Cl_2$ and haydeeite $Cu_3Mg(OH)_6Cl_2$ — •Oleg Janson and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer str. 40, 01187 Dresden

New natural spin-1/2 systems with kagomé layers — kapellasite $Cu_3Zn(OH)_6Cl_2$ and haydeeite $Cu_3Mg(OH)_6Cl_2$ — are studied by full potential density functional calculations using the fplo6.00-24 code. The band structure, obtained by a paramagnetic calculation, was used to solve a tight-binding model. The transfer integrals were mapped subsequently to a Hubbard model and to a Heisenberg model, giving an estimate for the antiferromagnetic (AF) exchange. The total exchange, containing AF and ferromagnetic (FM) parts, was derived from LSDA + U supercell calculations. As the main result, we find that in both compounds only two exchange integrals are relevant: the nearest neighbour exchange J_1 and the interaction J_d along the diagonals of the Cu^{2+} hexagons. Surprisingly, the size of these integrals depends strongly on the O—H bond length which was therefor optimized with respect to the total energy, resulting in about 1 Å for both compounds. Using the optimized O—H bond length, we find $J_1 > J_d$ in kapellasite and $J_1 \sim J_d$ in haydeeite. According to our results, kapellasite can be described as a modified kagomé lattice, while interpenetrating chains should be considered for haydeeite. Our results should encourage new experimental studies of these interesting materials.

TT 13.12 Tue 12:30 H 2053

Charge excitations and local magnetism: Li_2CuO_2 — •Stefan-Ludwig Drechsler[1], Jiří Málek[1,2], Martin Knupfer[1], Ulrike Nitzsche[1], Helge Rosner[3], and Helmut Eschrig[1] — [1]IFW-Dresden, D-01171 Dresden — [2]Institute of Physics, ASCR, Prague — [3]Max-Planck-Inst. f. Chem. Phys. Fester Stoffe

Electron energy loss spectroscopy and optical conductivity data of the frustrated edge-shared chain cuprate Li_2CuO_2 are reanalyzed within exact diagonalizations of multiband Hubbard models for CuO_2 chains taking into account Cu $3d_{xy}$, $4s$ and/or $4p_{x,y}$ and O $2p_{x,y}$ orbitals. We show that Zhang-Rice (ZR) singlet charge excitations which are generic for most cuprates are strongly suppressed in favor of ZR triplets as a consequence of substantial ferromagnetic correlations at T=0. A significant suppression also at T=300 K is obtained approximately. The frequency region above 6eV is dominated by O $2p$ to Cu $4p_y$, $4s$ and $4p_x$ transitions. The cluster mapping of these multiband Hubbard models on the Heisenberg J_1-J_2 model is in accord with a total energy analysis of various magnetic structures within LSDA+U FPLO calculations. According to all these theoretical results the observed ferromagnetic ordering of Li_2CuO_2 is caused already by a strong nearest-neighbor (CuO_4 plaquette) ferromagnetic in-chain interaction $J_1 \approx$ -200 K compared with the next-nearest neighbor exchange $J_2 \approx$ 35 K and it is only a bit further stabilized by a specific frustrating weak antiferromagnetic interchain exchange in contrast with previous studies [1].

[1] Y. Mizuno *et al.*, Phys. Rev. B **57**, 5326 (1998).

TT 13.13 Tue 12:45 H 2053

Competing exchange interactions in the one-dimensional spin-1/2 system Li_2CuO_2 — •Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and Helge Rosner[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden — [2]MPI CPfS Dresden, Nöthnitzer Straße 40, D-01187 Dresden

The spin 1/2 chain-cuprate Li_2CuO_2 is the archetype for competing nearest-neighbor and next-nearest-neighbor exchange interaction J_1 and J_2 along the CuO_2 chains. The magnitude of J_1 and J_2, especially their ratio α is crucial for the understanding of the magnetic ground state and is controversially disputed since a decade. Here, we report a density functional based electronic structure study to evaluate the leading in-chain and inter-chain exchange constants. We combine an LDA+U total energy approach for different spin configurations with the results from a tight-binding fit mapped onto a Heisenberg model. Our results yield a ferromagnetic ground state with a ferromagnetic J_1 and an antiferromagnetic J_2 and an α value well inside the region of the ferromagnetically ordered phase. A brief comparison with results from literature is given.

TT 14: Transport: Nanoelectronics III - Molecular Electronics

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

TT 14.1 Tue 9:30 H 3010

Conduction Properties of Bipyridinium Functionalized Molecular Wires — •Alexei Bagrets[1,2], Andreas Arnold[2], and Ferdinand Evers[1,2] — [1]Institute of Nanotechnology, Research Center Karlsruhe, PO Box 3640, D-76021, Germany — [2]Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

For functionality of organic molecules it is of primary importance to understand how they can operate as current switches. On the way to this goal, we examine possible mechanisms of the reported experimentally "conductance switching" behavior in alkyldithiol molecular wires modified with a viologen (bipyridinium) moiety, which oxidation state

can be controlled by *electrochemical gating* [1,2]. Based on density functional theory calculations, we show that molecules under study behave as weakly coupled quantum dots, where the current is carried by a redox-active LUMO-(lowest unoccupied molecular) level [3]. We calculate how the conductance decays with increasing the wire length and thereby recover quantitatively the experimental tunneling exponent [4]. Our calculations imply, that the charging induced conformational change in the bipyridinium unit is not a main switching agent, rather than the phonon-assisted inelastic electron transport through the viologen redox-level explains the observed switching behavior [3].

[1] W. Haiss *et al.*, J. Am. Chem. Soc. **125**, 15294 (2003). [2] Zh. Li *et al.*, Nanotechnology, **18**, 044018 (2007). [3] A. Bagrets, A. Arnold, and F. Evers, arXiv:0711.XXXXv1. [4] Ch. Li, I. Pobelov, Th. Wandlowski, A. Bagrets, A. Arnold, and F. Evers, to appear in J. Am. Chem. Soc.

TT 14.2 Tue 9:45 H 3010

Effects of polaron hopping on the transport through DNA — •Benjamin B. Schmidt[1,2], Matthias H. Hettler[2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, 76021 Karlsruhe, Germany

Experiments probing the equilibrium transport in DNA [1] have led to the consensus that polaron hopping is the dominant transport mechanism of charge carriers in DNA. On the other hand in non-equilibrium experiments where short DNA molecules are connected to two biased leads various types of behaviour is seen (reaching from ballistic transport to insulating behaviour). The reason for this discrepancy is not resolved. We suggest that polaron hopping plays an important role in the non-equilibrium transport through DNA. Our theory is based on work by Böttger and Bryksin [2] on small polaron transport in bulk materials, which we extend to nanostructures where we also account for coupling of the DNA to the leads. It desribes the polaron hopping quantum mechanically by expanding the time evolution of the occupation number on the different bases along the Keldysh contour. We observe non-symmetric current-voltage characteristics which we relate to partial charge redistribution on the DNA due to the applied bias.

[1] P.Henderson et al., PNAS USA, **96**, 8353 (1999)

[2] H. Böttger and V. V. Bryksin, 'Hopping conduction in Solids', Akademie Verlag Berlin, (1985)

TT 14.3 Tue 10:00 H 3010

Dynamical effects in the conductance properties of short DNA molecular wire: a combined study using molecular dynamics and model Hamiltonians — •Rodrigo Caetano[1], Rafael Gutierrez[1], Ben Woiczikowski[2], Tomas Kubar[2], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

The potential applications of DNA either as template or as molecular wires make of crucial importance to understand the microscopic mechanism leading supporting (or hindering) charge migration through this molecule. The experimental studies give very striking results, which range from insulating up to superconducting behavior. Theoretically, it is very important to include dynamical effects, since DNA is known to be a very flexible molecule. The dynamical effects of the solvent should be taken into account. In this work, we study charge transport through short Poly(G)-Poly(C) DNA within a minimal tight binding model. The model parameters are extracted from snapshots along QM/MM trajectories via DFTB approximation and thus include internal and solvent dynamical effects. We perform a statistical analysis of the time-dependent onsite and electronic hopping and show a broad non symmetric distribution. Green function formalism is used to calculate the transport characteristics and demonstrate how the average quantities depend on the relation between system time scales.

TT 14.4 Tue 10:15 H 3010

Switching response of DNA conduction under stretching — •Bo Song[1], Marcus Elstner[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

By merging DFTB calculations and model-Hamiltonian approaches, we study the stretching-twisting process of poly(GC) DNA oligomers. A local maximum for the transfer integral t between two nearest-neighbor GC pairs is found in the stretching process, which arises from the competition between stretching and twisting. This results in a local maximum for the current in the case that the electrode-DNA coupling Γ is greater than t. Reducing Γ to the values smaller than t gives rise to plateaus in the current. The heights of such plateaus are almost equal to each other.

TT 14.5 Tue 10:30 H 3010

Modeling of tunneling through single endohedral N@C_{60} molecules — •Carsten Timm[1], Jacob E. Grose[2], Wolfgang Harneit[3], and Daniel C. Ralph[2] — [1]University of Kansas, Lawrence, USA — [2]Cornell University, Ithaca, USA — [3]Freie Universität Berlin, Germany

We report on recent experimental and theoretical results for single-molecule transistors involving endohedral N@C_{60} fullerene molecules. In this talk, we will focus on the theoretical modeling. The observed differential conductance shows strong evidence for the exchange interaction between electrons in the fullerene LUMO and the nitrogen p-electrons, favoring an antiferromagnetic interaction. In addition, soft vibrational modes are seen, which are attributed to oscillations of the molecule as a whole. We discuss a model Hamiltonian that reproduces the main features of the experimental conductance.

TT 14.6 Tue 10:45 H 3010

Silicon based nanogap devices for transport studies on molecule-nanoparticle junctions — •Sebastian Strobel[1], Rocio Murcia[1], Allan Hansen[2], and Marc Tornow[2] — [1]Walter Schottky Institut, TU München, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Germany

One possible realization of future nanoelectronics may be a hybrid combination of existing silicon circuitry with functional molecular units. Such approach requires a silicon based technology that allows for the parallel fabrication of contact structures for molecules, as well as the fundamental characterization of such hybrids.

We have fabricated arrays of individually addressable nanogap electrodes with a predefined separation down to ˜20 nm using silicon on insulator (SOI) as substrate material. The samples were processed using standard optical lithography, dry and wet chemical etching, and metal thin film deposition, only.

We realized hybrid molecular junctions using such nanogap electrode devices by self-assembling a monolayer of mercaptohexanol onto the metal contacts, and trapping 30 nm diameter Au nanoparticles between the functionalized electrodes, subsequently. Transport measurements at 4.2 K revealed pronounced Coulomb staircase behaviour, characteristic for asymmetric double-barrier tunnelling junctions. We analyse our data by means of model calculations.

TT 14.7 Tue 11:00 H 3010

Length-dependent conductance and thermopower in metal-molecule-metal junctions — •Janne Viljas[1,2], Fabian Pauly[1], and Juan Carlos Cuevas[3,1,2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Using a method based on density-functional theory, we investigate the conductance and the thermopower in metal-molecule-metal junctions made of dithiolated oligophenylenes contacted to gold electrodes [1]. We find that while the conductance decays exponentially with increasing molecular length, the thermopower increases linearly in good quantitative agreement with recent experiments [2]. We also analyze how these transport properties can be tuned with methyl side groups. The characteristic substituent effects in our ab-initio calculations are explained using a π-electron tight-binding model, which we have studied in detail.

[1] F. Pauly, J. K. Viljas, and J. C. Cuevas, arXiv:0709.3588.

[2] P. Reddy *et al.*, Science **315**, 1568 (2007).

15 min. break

TT 14.8 Tue 11:30 H 3010

Current switching in single molecule transport and con-

tact — •Velimir Meded, Alexej Bagrets, Andreas Arnold, and Ferdinand Evers — Institute of Nanotechnology, Research Centre Karlsruhe, Hermann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen, Germany

Two experiments measuring the current-voltage characteristics (IV) of the bipyridine-dinitro-dithiole-system found that the molecule can be controllably switched between two states exhibiting significantly different IV curves [1,2]. To better understand the nature of the bistable state we have performed ab initio calculations. They indicate, that molecular charging/uncharging does not lead to bistability in the presence of electrodes. By contrast, two (or more) energy minima can arise with conformational changes of the molecule alone or in the molecule-contact region (possibly combined with structural relaxations in a larger contact area). As a prototypical example of such a mechanism, we consider rotations of the molecule about the axis defined by the two anchoring Au-atoms. From an extensive analysis of possible contact structures, we conclude that bistable configurations can indeed arise for slightly disordered, i.e. realistic, contacts – though they do not appear to be generic. A scenario will be proposed, how in this light experimental findings might be understood. (We are indebted to E. Loertscher, H. Riel and M. Ruben for instructive discussions.)

[1] Z. K. Keane, J. W. Ciszek, J. M. Tour, and D. Natelson, Nano Lett., Vol. 6, No. 7, 2006. [2] E. Lörtscher, J. W. Ciszek, J. Tour, and H. Riel, Small 2, 973 (2006).

TT 14.9 Tue 11:45 H 3010

Temperature dependence of the conductance in biphenyl-dithiol single-molecule junctions — •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, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Using a density-functional-based transport method, we study the conduction properties of several biphenyl-derived dithiol (BPDDT) molecules wired to gold electrodes [1]. The BPDDT molecules differ in their side groups, which control the degree of conjugation of the π-electron system. We have analyzed the dependence of the low-bias zero-temperature conductance on the tilt angle φ between the two phenyl ring units, and find that it follows closely a $\cos^2(\varphi)$ law as observed in a recent experiment [2].

In addition, we study the temperature dependence of both the conductance and its fluctuations and find qualitative differences between the examined molecules. We illustrate that the fluctuations of the conductance due to temperature-induced changes in the geometric structure of the molecule can be reduced by an appropriate design.

[1] F. Pauly, J. K. Viljas, J. C. Cuevas, G. Schön, arXiv:0705.3285.
[2] Venkataraman *et al.*, Nature **442**, 904 (2006).

TT 14.10 Tue 12:00 H 3010

Symmetry effects in transport properties of benzene quantum dots — •Georg Begemann, Dana Darau, Andrea Donarini, and Milena Grifoni — Theoretische Physik, Universität Regensburg

We investigate electronic transport through a benzene molecule quantum dot. In particular, we investigate the influence of the contacts' position and find qualitative and quantitative differences between the para- and the meta configurations.

The Hamiltonian of the interacting isolated molecule is diagonalized and its eigenstates are classified according to their particle number, spin and symmetry representation.

Treating the coupling to the leads perturbatively, a generalized master equation for the reduced density matrix in the benzene's eigenbasis is derived, which includes coherences between degenerate eigenstates. We explicitly demonstrate that the coherences do not contribute to the linear transport, but become essential for the meta-configuration in the nonlinear regime.

Analytic expressions for the linear conductance and the current in the low bias regime agree with numeric calculations, where we are not restricted to small voltages. Interesting features appear over a wide range of gate and bias voltages, for example, due to the reduced symmetry of the problem, negative differential conductance is present in the meta-configuration, while it is absent in the para-configuration.

TT 14.11 Tue 12:15 H 3010

Vibrational Effects in Electron Transport through Molecular Junctions — •Rainer Härtle, Claudia Benesch, and Michael Thoss — Institut für Theoretische Chemie, Technische Universität München, D-85747 Garching, Germany

We investigate theoretically the role of vibrations in electron transport through single molecule junctions. The study is based on a generic model, which describes steady-state transport through a single molecule that is attached to metal leads. To address multidimensional vibrational dynamics in molecular junctions, we have extended the non-equilibrium Green function approach established by M. Galperin et al. to multiple modes. We demonstrate the effect of electronically induced coupling between different vibrational modes and study the stability of these junctions by calculating the vibrational excitations as a function of the bias voltage. In addition to a model system with two vibrational degrees of freedom, we present results for *p*-benzene-di(butanethiolate) covalently bound to gold electrodes.

TT 14.12 Tue 12:30 H 3010

Quantum fluctuations and vibration-assisted transport through single molecule transistors — •Martin Leijnse[1,2], Maarten Wegewijs[1,2], and Herbert Schoeller[1] — [1]Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany — [2]Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany

Non-equilibrium transport through a single molecule transistor is studied in the presence of strong coupling to a local vibrational mode. Employing a full fourth order perturbation expansion in the tunneling Hamiltonian, we address the experimentally relevant regime of intermediate tunneling coupling between molecule and electrodes. Using the real-time transport theory we calculate the nonlinear conductance, accounting for the so-called cotunneling contributions, as well as renormalization and broadening effects, induced by charge fluctuations. We find that broadening and in-elastic cotunneling processes are of comparable importance for the lifting of the vibration-induced Franck-Condon blockade. Strikingly, novel transport features connected to this broadening are found below the bias-voltage threshold for in-elastic cotunneling, which have gone unnoticed until now. Relaxation of the vibrational distribution, induced by coupling to an external phonon bath, leads to a uniform reduction of all higher order processes, i.e. broadening and in-elastic effects remain comparable.

TT 14.13 Tue 12:45 H 3010

Charge-memory effect in molecular junctions — •Pino D'Amico[1], Dmitry A. Ryndyk[1], Gianaurelio Cuniberti[2], and Klaus Richter[1] — [1]Institut for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Max Bergmann Centre for Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

Charge-memory effects such as bistability and switching between a charged and a neutral state, have been recently observed in an increasing number of experiments on charge transport through molecules[1,2]. We consider a charge-memory effect in the framework of a minimal polaron model. It is shown that in the case of strong electron-vibron interaction the rate of spontaneous quantum switching between two metastable states is exponentially suppressed at zero bias voltage, while remaining large enough at finite voltage. The switching between states at finite voltage and hysteretic charge-voltage curves are calculated at weak coupling to the leads by the master equation method, and at stronger coupling to the leads by the equation-of-motion method for nonequilibrium Green functions.

[1] Jascha Repp et al, Science, vol 35, 493-495 (2004)
[2] F. E. Olsson et al, PRL, vol 98, 176803 (2007)

TT 15: Superconductivity: Poster Session

Time: Tuesday 14:00–18:00 Location: Poster B

TT 15.1 Tue 14:00 Poster B

Superconducting MgB_2 films with introduced artificial pinning centers — •Anatoli Sidorenko[1,2], Vladimir Zdravkov[1], Andrei Surdu[1], Günter Obermeier[3], Christoph Frommen[4], Stefan Walheim[4], Thomas Koch[2,4], and Thomas Schimmel[2,4] — [1]Institute of Electronic Engineering and Industrial Technologies ASM, Kishinev MD2028, Moldova — [2]Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — [3]Institute of Applied Physics, University Augsburg, 86159 Augsburg, Germany — [4]Institute of Nanotechnology, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

High quality superconducting magnesium diboride films were prepared using DC-magnetron sputtering and post annealing in Mg vapor within a specially designed Nb reactor. The influence of embedded gold nano particles on resistive transition broadening in external magnetic field has been investigated. The transition broadening in strong magnetic fields could be explained by the change of the effective dimensionality of superconductivity nucleation in magnesium diboride, because of the dimensional crossover of fluctuations.

The work was supported by the BMBF project 01/007 Superconducting Magnesium Diboride Films for Techical Application, and the project Poziţionarea forţei de pinning si creşterea curentului critic in MgB_2 si applicatiile technice.

TT 15.2 Tue 14:00 Poster B

Carbon doping as an effective way of changing the superconducting properties of MgB_2 — •Marko Herrmann[1], Wolfgang Häßler[1], Margitta Schubert[1], Wolfgang Gruner[1], Manfred Ritschel[1], Bernhard Holzapfel[1,2], and Ludwig Schultz[1,2] — [1]IFW-Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany — [2]Dresden University of Technology, Department of Physics, D-01062 Dresden, Germany

Up to now, carbon doping is the only reliable way to enhance the superconducting properties of MgB_2 significantly. Precursor powders of carbon-doped and undoped MgB_2 were prepared by mechanical alloying. This very effective preparation method imparts an enormous quantity of energy to the material and produces a partially reacted, nanocrystalline powder with enhanced reactivity. The high reactivity of the milled powders promotes the formation of MgB_2 at reduced temperatures around 600°C to 650°C. Very high critical current densities of J_c = 1.1 x 10^6 A/cm^2 in self-field at 4.2 K and critical fields B_{c2} = 15.5 T at 10 K of undoped bulk samples of mechanically alloyed precursors were measured. In comparison to results of other in-situ preparation techniques this values exceed most of the superconducting properties by far and even keep up with results on optimized carbon doped samples reported so far. Starting from this high performance powders a comparison of promising carbon dopants will be presented. We show the influence of these dopants on the lattice parameter, the superconducting transition, critical field and critical current density of the bulk samples.

TT 15.3 Tue 14:00 Poster B

Film growth and anisotropic behaviour of the critical field in epitaxial $Lu_xHo_{1-x}Ni_2B_2C$ thin films — •Tim Niemeier, Ruben Hühne, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, 01171 Dresden

The research on Rare Earth Nickel Borocarbides has led to a number of new conclusions about superconductivity, particularly in regard to the interdependency with magnetic influences. Recently, it was concluded by *Wälte et al.* from specific heat measurements and thermodynamic simulations that $LuNi_2B_2C$ provides a non-magnetic corresponding partner of $HoNi_2B_2C$ [1].

Complementary to single crystal growth, we use pulsed laser deposition for the sample preparation. In the past, particularly the anisotropy of the upper critical field could be successfully measured using thin film samples [2]. We prepared epitaxial thin films of alloys of $Lu_xHo_{1-x}Ni_2B_2C$ for different x for the investigation of the transition temperature and the upper critical field. Especially we discuss the anisotropic behaviour above as well as below the magnetic ordering temperature known from $HoNi_2B_2C$ providing numerical fitting results for different simple models.

[1] Wälte, A: Doctoral thesis, TU Dresden 2007

[2] Wimbush, S. C., L. Schultz, and B. Holzapfel: Angular anisotropy of the upper critical field in YNi_2B_2C. Physica C 408-10 (2004): 83-84.

TT 15.4 Tue 14:00 Poster B

Electrical properties of thin $YBa_2Cu_3O_{7-x}$ films with embedded gold nano clusters — •Sebastian Engmann, Uwe Schinkel, Veit Grosse, Christoph Becker, Alexander Steppke, Frank Schmidl, and Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena

High temperature superconducting devices such as magnetometers or gradiometers are usually made from a single thin film, although each part of the device needs to fulfill special requirements. These are for example a low flux noise in antenna structures and a low contact resistance to the bonding pads. These requirements can be achieved by embedding gold nano clusters in thin films of $YBa_2Cu_3O_{7-x}$ (YBCO), since they can act as flux pinning centers and they increase contact area to the film.

We present studies on the formation of gold nano clusters during the pulsed laser deposition of thin YBCO films in dependence on the gold film thickness. We verified the high crystalline quality of the films by measuring Rocking curve widths. Size and distribution of the gold clusters were determined from AFM measurements. We compare the superconducting and noise properties of bridge structures and gradiometers with devices made of conventional YBCO films.

TT 15.5 Tue 14:00 Poster B

Preparation and Characterization of $YBa_2Cu_3O_7$/$PrBa_2Cu_3O_7$ Superlattices — •Ayman El Tahan, Gerhard Jakob, and Hermann Adrian — Institute of Physics, University of Mainz, 55099 Mainz

High T_c superconductor/insulator superlattices offer the possibility to create artificial superconductors with variable strength of the interlayer Josephson coupling. We want to investigate the interlayer coupling strength by measuring the transport properties perpendicular to the layers.

Our presented films are prepared from stoichiometric targets by high pressure sputter deposition in pure oxygen atmosphere. As substrates we used (100) oriented $SrTiO_3$ and $LaAlO_3$. Using x-ray diffraction we confirmed the c-axis oriented epitaxial growth of the superlattices. The superlattice quality is determined by comparison to simulated diffractograms using the program SUPREX. AC magnetic susceptibility was used for characterization of the critical temperature for our $YBa_2Cu_3O_7$ samples and $YBa_2Cu_3O_7$/$PrBa_2Cu_3O_7$ superlattices.

Financial support by the MWFZ Mainz and the government of Egypt is gratefully acknowledged.

TT 15.6 Tue 14:00 Poster B

Synthesis and characterisation of superconducting and magnetic properties of $RuSr_2Gd_{1-x}Y_xCu_2O_8$ — •Johannes Krämer, Eugenio Casini, and Hans F. Braun — Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth

It is well known that the formation of RuRE1212 (RE = rare earth) under ambient pressure is strongly affected by the size of the rare earth ion. The 1212 structure type forms just with RE = Gd, Eu and Sm. Under high pressure, the synthesis has been successful with the smaller elements Tb - Er and Y [1]. Under ambient conditions, the phase has been reported in solid solution systems $RuSr_2Gd_{1-x}RE_xCu_2O_8$ with RE = Dy - Er, Yb and Lu up to a maximum content of $x = 0.7$ [2].

In our work we investigated the partial substitution of Gd with the non-magnetic rare earth Yttrium. The samples were characterised using x-ray powder diffraction, scanning electron microscopy (SEM) and ac-susceptibility measurements. We observed a dependence of the superconducting transition temperature T_c as well as the lattice parameters on the Yttrium content. However, single-phase samples were not obtained.

[1] L.T. Yang et al., J. Solid State Chem. 177 (2004) 1072

[2] M. Abatal et al., Physica C 408-410 (2004) 185

TT 15.7 Tue 14:00 Poster B

Effect of variable Ru content on superconducting and magnetic properites of $RuSr_2GdCu_2O_8$ — •Manuel Kempf, Eugenio Casini, and Hans F. Braun — Physikalisches Institut, Universität

Bayreuth, D-95440 Bayreuth

We have investigated the effect of a variation of the Ru content in $RuSr_2GdCu_2O_8$ (RuGd1212) on sample properties as for example shifts of the superconducting and magnetic transition temperatures T_c and T_m and the presence of phases in equilibrium with RuGd1212. The procedure of sample preparation can strongly affect the magnetic and superconducting properties of RuGd1212. Due to the relatively high volatility of the Ru-oxides at temperatures around 1000°C, a Ru loss can arise during calcination of the starting materials, the preparation of the Sr_2RuGdO_6 precursor and the final sintering process of RuGd1212.

The starting composition for our RuGd1212 was a mixture of CuO and Sr_2RuGdO_6 in the stoichiometric ratio 2:1. Samples were sintered in an O_2/Ru-oxide gas flow with variable Ru content. An increase of the Ru concentration in the gas mixture leads to a decrease of T_c and an increase of T_m. In sample areas exposed to the gas flow, additional phases coexisting with RuGd1212 were observed at higher Ru-oxide partial pressure. Thus, sintering of RuGd1212 in O_2/Ru-oxide gas flow with variable partial pressure of Ru-oxide controls the loss or increase of Ru in RuGd1212. The different Ru contents in RuGd1212 result in changes of T_c and T_m. This is compatible with the results of experiments where Ru is partially substituted by Cu.

TT 15.8 Tue 14:00 Poster B

Elektromechanische und thermische Charakterisierung von Bi-2223 Hochtemperaturbandsupraleitern bei kryogenen Temperaturen — •Philipp Keller[1,2], Michael Schwarz[1], Klaus-Peter Weiss[1], Reinhard Heller[1] und Sonja Schlachter[1] — [1]Institut für Technische Physik, Forschungszentrum Karlsruhe — [2]Kirchhoff-Institut, Universität Heidelberg

Um den Energiebedarf der Menschen auch in Zukunft befriedigen zu können, sind neue Wege in der Gewinnung, der Speicherung und dem Transport nutzbarer Energien erforderlich. Hierbei spielen Supraleiter und vor allem die im Jahre 1986 entdeckten Hochtemperatursupraleiter eine zunehmend wichtige Rolle. Um diese jedoch technisch nutzen zu können, müssen die Supraleiter in einer der Anwendung angepassten Form gefertigt und physikalisch charakterisiert werden. Am Beispiel von Bi-2223 Bändern für die Anwendung in supraleitenden Stromzuführungen wurden typische Größen wie der kritische Strom Ic unter äußerer mechanischer Spannung, sowie die thermischen Eigenschaften, speziell die thermische Leitfähigkeit und die Längenausdehnung, untersucht. Somit kann der Einfluss der Leiterparameter (z.B. supraleitendes Material, Matrixmaterial, Füllfaktor) bestimmt und die gewünschten Eigenschaften des Bandsupraleiters durch den gezielten Einsatz entsprechender Materialien optimiert werden, was letztendlich die technische Anwendung ermöglicht. Ein tiefer gehendes Verständnis wird durch eine FEM-Modellierung der elektrischen, thermischen und mechanischen Eigenschaften eines Bi-2223 Bandleiters und deren Vergleich mit den durchgeführten Messungen gebildet.

TT 15.9 Tue 14:00 Poster B

In-plane anisotropy of the spin excitation spectrum in strongly underdoped $YBa_2Cu_3O_{6+x}$ — •Daniel Haug[1], Vladimir Hinkov[1], Benoît Fauqué[2], Philippe Bourges[2], Yvan Sidis[2], Alexandre Ivanov[3], Chengtian Lin[1], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Laboratoire Léon Brillouin, CEA-CNRS Saclay, France — [3]Institut Laue-Langevin, Grenoble, France

The spin excitation spectrum of the optimally doped and moderately underdoped high-temperature superconductor $YBa_2Cu_3O_{6+x}$ is dominated by the so-called resonance peak for excitation energies between 30 and 40 meV (depending on the oxygen content x) that sets in abruptly below T_c. Here we report measurements on arrays of untwinned single crystals in the strongly underdoped regime in which the situation is very different: Spectral weight is shifted towards low energies and evolves smoothly through T_c. The spectrum exhibits a peak below ∼10 meV which shows a spontaneous onset of a strong anisotropy in the a-b-plane defined by the CuO_2 layers. This phenomenon matches the symmetry properties of a nematic liquid crystal, a new symmetry-broken electronic phase that coexists with high-temperature superconductivity in strongly underdoped cuprates.

TT 15.10 Tue 14:00 Poster B

Energy gap and asymmetry of coherence peaks in 123 cuprate superconductors and their T_c dependence — •Pintu Das[1,3], Michael R. Koblischka[1], Thomas Wolf[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, University of Saarland, 66041, Saarbruecken, Germany — [2]Forschungzentrum Karlsruhe GmbH, Institute of Solid State Physics, 76021 Karlsruhe, Germany — [3]Max Planck Institute of Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The energy gap in conventional superconductors is directly proportional to the transition temperature. In high-T_c cuprate superconductors, scanning tunneling spectroscopy (STS) and angle resolved photoemission studies have often shown that the underdoped samples which have low T_c values exhibit very large energy gaps giving rise to a high value of the coupling ratio ($2\Delta/k_BT_c$). This has been mostly observed for $Bi_2Sr_2CaCu_2O_{8+\delta}$. In this work, we observe from the STS experiments on $NdBa_2Cu_3O_{7-\delta}$ single crystal samples that the average energy gap increases with the decrease of T_c. For a moderately underdoped sample the coupling ratio is found to be as high as 18. We also observed an asymmetry in coherence peaks which is minimum in the case of optimally doped (highest T_c) samples. The observed T_c dependence of the asymmetry suggests that it is related to the number of electrons and holes.

TT 15.11 Tue 14:00 Poster B

STM based inelastic electron tunneling spectroscopy on $NdBa_2Cu_3O_{7-\delta}$ — •Pintu Das[1,2], Michael R. Koblischka[1], Helge Rosner[2], Thomas Wolf[3], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, University of Saarland, 66041, Saarbruecken, Germany — [2]Max Planck Institute of Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]Forschungzentrum Karlsruhe GmbH, Institute of Solid State Physics, 76021 Karlsruhe, Germany

Inelastic electron tunneling spectroscopy (IETS) is a very powerful tool to detect collective excitations in conducting materials. Due to inelastic excitation by tunneling electrons, a very weak kink is usually observed in dI/dV curves at the bias voltage corresponding to the excitation energy. In IETS on s wave superconductors, phonon modes (ω_{ph}) were observed at energies given by $E = \Delta + \hbar\omega_{ph}$, where Δ is the energy gap. Recently IETS using scanning tunneling spectroscopy (STS) has been used to detect a bosonic mode in $Bi_2Sr_2CaCu_2O_{8+\delta}$ [1]. In the STS data obtained on $NdBa_2Cu_3O_{7-\delta}$ single crystals, we observed peaks in d^2I/dV^2 curves beyond the coherence peaks from which collective excitation energies of ∼ 23 meV and ∼ 34 meV have been found for the samples with T_c of 93.5 K and 95.5 K respectively. Band structure calculation shows that there is no structure in the density of state at the observed energies which thus supports the presumption that the observed kinks in dI/dV curves are due to inelastic scattering of electrons.

[1] Lee et al., Nature **442**, 546 (2006).

TT 15.12 Tue 14:00 Poster B

Magic doping fractions in Bi2201 — •Lenart Dudy, Alica Krapf, Beate Müller, Olaf Lübben, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr.15, D-12489 Berlin, Germany

One interesting feature in the hole doped cuprates is the depression of the superconducting transition temperature at certain hole doping fractions. The 1/8 depression in $La_{2-x}Sr_xCuO_4$(LSCO) [1] is widely accepted, and can be interpreted in terms of static stripes [2] - but also by a structural tetragonal-orthorhombic (LTT-LTO) phase transition [3]. In our view the structural interpretation can be ruled out, as additional to 1/8 other fractional depressions were deduced for LSCO (i.e. at 1/16; 3/32; 1/8; 3/16) [4]. But these fractions may also violate the stripe picture, as they can not be interpreted by a static one-dimensional arrangement of holes in the CuO_2-plane but by a two-dimensional one. Despite one controversial report [5] in the Bismuth cuprates the knowledge of the existence or non existence of such fractions is very poor. We will show that also in the one-layer Bismuth cuprate the depressions at certain hole doping fractions exist which are equal to the fractions found by [4]. This may point to a generality of magic doping fractions in the cuprates.

[1] A. R. Moodenbaugh et al., Phys. Rev. B 38, 4596 (1988)
[2] D.L. Feng et al., Journ. of Phys. and Chem. of Solids 67, 198 (2006)
[3] J. Zhao et al., Supercond. Sci. Technol. 18, 966 (2005)
[4] S. Komiya et al., Phys. Rev. Lett. 94, 207004 (2005)
[5] W.L. Yang et al., Phys. Rev. B 62, 1361 (2000) 1

TT 15.13 Tue 14:00 Poster B

STM investigated characteristics of Pb-Bi2201 in dependence of the lead content — •Olaf Lübben, Lenart Dudy, Alica Krapf,

Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Institut f. Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

The single layered superconductor $Bi_{2-y}Pb_ySr_{2-x}La_xCuO_{6+\delta}$ ($x = 0.4$) around optimal doping has been investigated by scanning tunneling microscopy (STM). Continuously changing the amount of lead showed a fascinating structural development and revealed new modulations in the BiO layer.

Special attention has been given to the "inhomogeneous" background modulation. It is suggested, like in [1], that this background is not just caused by electronic reasons, but has structural origin. Because of the short range of this modulation it could influence the electronic structure of the CuO_2 plane and the charge transfer between this plane and the carrier reservoir (BiO-SrO). In this context the question arises if a "good" and a "bad" background with respect to superconductivity exists.

[1] H. Mashima et al., Phys. Rev. B **73**, 060502 (2006).

TT 15.14 Tue 14:00 Poster B

Possibility of hole density modulation in highly overdoped Bi(Pb)-2201 single crystals: XAS measurements — •Ariffin Ahmad Kamal, Beate Müller, Rüdiger Mitdank, Lenart Dudy, Helmut Dwelk, Alica Krapf, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

The polarization i.e. angular dependence of the relative intensity of the satellite peak and the main peak of the CuL_3 edge of highly overdoped Bi(Pb)-2201 single crystals was studied by XAS. The spectrum near the CuL_3 edge displays the interaction of the Cu atom with the oxygen localized holes. The relative intensity of the satellite peak and the main peak, which gives the value and distribution of the hole content, has been measured by varying the angle of the electrical field vector E of the synchrotron light within the ab-plane. We have found that the relative intensity of the satellite peak and the white line of highly overdoped Bi(Pb)-2201 single crystals is polarization dependent. The modulation shows that the maximum occurs at nearly 60^0 intervals. This suggests the hole density being distributed with some form of periodicity.

TT 15.15 Tue 14:00 Poster B

The nature of the sharp peak — •Beate Müller, Lenart Dudy, Helmut Dwelk, Alica Krapf, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

In the high-T_c cuprates the excitations investigated by photoemission in the antinodal direction are incoherent. Only at low temperatures a quasiparticle like excitation, the so-called sharp or superconducting peak, emerges. Mainly the sharp peak is interpreted as a coherent excitation marking e.g. a dimensional crossover [1] but it was also seen as the signature of superfluid density [2,3] or the consequence of the coupling to the magnetic resonance mode [4]. The distinction between the different approaches is the definition of the sharp peak as a consequence of a change in lineshape of the band theory derived excitations or as an additional excitation. In our opinion ARPES measurements at different photon energies point towards the sharp peak being an additional excitation. From this point of view it is possible to reevaluate the various models.

[1] T. Valla, P. Johnson, Z. Yusof, B. Wells, Q. Li, S. Loureiro, R. Cava, M. Mikami, Y. Mori, M. Yoshimura, Nature 417, 627 (2002)

[2] R. H. He, D. L. Feng, H. Eisaki, J.-I. Shimoyama, K. Kishio, and G. D. Gu, Phys. Rev. B 69, 220502 (2004)

[3] D. Feng, D. Lu, K. Shen, C. Kim, H. Eisaki, A. Damascelli, R. Yoshizaki, J.-i. Shimoyama, K. Kishio, G. Gu, Science 289, 277 (2000)

[4] M. Eschrig and M. R. Norman, Phys. Rev. Lett. 89, 277005 (2002)

TT 15.16 Tue 14:00 Poster B

Probing the superconducting state via Andreev bound states in $(La,Ce)_2CuO_4$ — Michael Wagenknecht[1], •Sebastian Scharinger[1], Dieter Koelle[1], Reinhold Kleiner[1], Siegfried Graser[2], Nils Schopohl[2], Boris Chesca[3], Aiko Tsukada[4], Sebastian T. B. Goennenwein[5], and Rudolf Gross[5] — [1]Physikalisches Institut – Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]Institut für Theoretische Physik, Universität Tübingen, Germany — [3]Department of Physics, Loughborough University, United Kingdom — [4]NTT Basic Research Laboratories, Atsugi-shi, Japan — [5]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

We present quasiparticle tunneling data of $(La,Ce)_2CuO_4$ thin film bicrystal junctions. The differential conductance in the superconducting state shows a pronounced zero bias conductance peak (ZBCP). This peak is attributed to zero energy surface Andreev bound states due to the d-wave symmetry of the order parameter in this electron doped cuprate. Such bound states are closely related to the macroscopic phase coherence of the superconducting state. Hence the ZBCP due to these bound states must disappear at or below the upper critical field $B_{c2}(T)$. By following the disappearance of the ZBCP in the $B-T-$phase diagram we find a lower bound for $B_{c2}(0) \approx 25\,\mathrm{T}$ which is higher than values reported previously for any electron doped cuprate. Following this observation we suggest a modified $B-T-$phase diagram with a larger region of superconductivity, leaving less room for a possible pseudogap phase.

TT 15.17 Tue 14:00 Poster B

Dynamical spin susceptibility in different phases of the electron-doped cuprate superconductors — •Jan-Peter Ismer[1], Ilya Eremin[1], Enrico Rossi[2], and Dirk Morr[3] — [1]MPI für Physik komplexer Systeme, Dresden — [2]University of Maryland, College Park, USA — [3]University of Illinois at Chicago, USA

We present a study of the dynamical spin susceptibility in the electron-doped cuprate superconductors. We show that the resonance peak observed recently in $Pr_{0.88}LaCe_{0.12}CuO_{4-\delta}$ represents rather an effect of the magnetic coherence than a bound state seen in the hole-doped counterparts. We further analyze some aspects of the peculiar behavior of the spin excitations in the presence of the spin density wave (SDW) instability in $d_{x^2-y^2}$-wave superconducting state ($T_N \ll T_C$). We find that the spin resonance will show a remarkable temperature dependence in contrast to the hole-doped cuprates.

TT 15.18 Tue 14:00 Poster B

Raman spectroscopy study of the pyrochlore superconductors KOs_2O_6 and $RbOs_2O_6$ — •Ana Maria Racu[1], Joachim Schoenes[1], Zbigniev Bukowski[2], and Janusz Karpinski[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

The discovery of superconductivity in the pyrochlore oxides KOs_2O_6, $RbOs_2O_6$ and $CsOs_2O_6$ has attracted much interest due to their unusual properties. Crystallographic studies proposed two different structures whithin the centrosymmetric $Fd\bar{3}m$ and the non-centrosymmetric $Fd\bar{4}3m$ [1] space groups. Both reveal a very special feature: the alkali atom is situated in an oversized Os-O cage. It is believed that the anharmonic rattling of the alkali atom in the cage strongly influences the electronic structure and the superconductivity [2]. We performed Raman measurements on single crystals of KOs_2O_6 and $RbOs_2O_6$. The experimental results are compared with a factor group analysis for the two proposed crystal structures. The number and the symmetry of the observed modes is compatible with the centrosymmetric space group. In the low energy range we observe a mode which is strongly dependent on the alkali atom. Its energy corresponds to one of the fine structures observed in KOs_2O_6[3] in the photoemission spectra. We attribute this low energy mode to the Raman active rattling vibration of the K and Rb atoms.

[1] Schuck et al., PRB 73, 144506 (2006)
[2] Hiroi et al., J. Phys. Soc Jpn. 74, 3400 (2005)
[3] Shimojima et al., PRL 99, 117003 (2007)

TT 15.19 Tue 14:00 Poster B

Superconductivity on the Border of Weak Itinerant Ferromagnetism in UCoGe — N. T. Huy[1], A. Gasparini[1], D. E. de Nijs[1], Y. Huang[1], J. C. P. Klaasse[1], T. Gortenmulder[1], A. de Visser[1], •A. Hamann[2], T. Görlach[2], and H. v. Löhneysen[2,3] — [1]Van der Waals-Zeeman Institute, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

We report the coexistence of ferromagnetic order and superconductivity in UCoGe at ambient pressure [1]. Magnetization measurements show that UCoGe is a weak ferromagnet with a Curie temperature $T_C \approx 3\,\mathrm{K}$ and a small ordered moment $m_0 \approx 0.03\,\mu_B$. Superconductivity is observed with a resistive transition temperature $T_s \approx 0.8\,\mathrm{K}$ for the best sample. Thermal-expansion and specific-heat measurements provide solid evidence for bulk magnetism and superconductivity. The

proximity to a ferromagnetic instability, the defect sensitivity of T_s, and the absence of Pauli limiting, suggest triplet superconductivity mediated by critical ferromagnetic fluctuations.

[1] N. T. Huy et al., PRL 99, 067006 (2007)

TT 15.20 Tue 14:00 Poster B

Electronic and structural properties of two novel Palladium-based Heusler superconductors. — •Jürgen Winterlik, Gerhard H. Fecher, and Claudia Felser — Institut für Anorganische und Analytische Chemie, Johannes Gutenberg - Universität, 55099 Mainz, Germany

This work reports the two novel superconducting Heusler compounds Pd_2ZrAl and Pd_2HfAl. Magnetization and resistance measurements were carried out to verify their transitions to the superconducting states. The compounds exhibit transition temperatures of 3.2 K for Pd_2ZrAl and 3.4 K for Pd_2HfAl. From their behavior in external magnetic fields, it was determined that both compounds are type II superconductors. Similar to the half-metallic ferromagnets, the superconducting Heusler compounds follow an electron counting scheme based on theoretical considerations, the van Hove scenario. As found from *ab initio* calculations, the superconductivity can be explained by a valence instability at the L-point, that has been used as design criterion.

TT 15.21 Tue 14:00 Poster B

Superconductivity, magnetic order and intermediate valence in the new platinum germanium skutterudites $M\mathbf{Pt_4Ge_{12}}$ (M = Sr, Ba, La, Ce, Nd, Pr, Eu) — •Roman Gumeniuk, Michael Nicklas, Helge Rosner, Walter Schnelle, Ulrich Burkhardt, Andreas Leithe-Jasper, and Yuri Grin — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

In the new germanium-platinum compounds with the filled-skutterudite crystal structure $M\mathrm{Pt_4Ge_{12}}$ superconductivity was observed for the non-magnetic cations $M = Sr^{2+}$, Ba^{2+}, La^{3+} and for Pr^{3+} which has a singlet crystal field ground state [1,2]. The isostructural compound with cerium shows no superconductivity above 0.45 K but displays intermediate valence. With the cations Nd^{3+} and Eu^{2+} magnetic order is found at temperatures below 1.8 K. Interestingly, from Curie-Weiss fits to magnetic susceptibility data much stronger antiferromagnetic interactions could be inferred.

[1] R. Gumeniuk *et al.* Phys. Rev. Lett. submitted. ArXiV 0710.1413v1.
[2] W. Schnelle *et al.* Talk, this conference.

TT 15.22 Tue 14:00 Poster B

Unusual Property of Spin Dynamical Susceptibility and its Effect on Superconductivity in Non-centrosymmetric Systems — •Tetsuya Takimoto and Peter Thalmeier — max planck institute for chemical physics of solids, dresden

Recently, non-centrosymmetric superconductors like $CePt_3Si$ attract much attention. For centrosymmetric system, Hubbard model consisting of hopping term and on-site interaction term will be a minimal model. In addition to these terms, the model hamiltonian of non-centrosymmetric system involves Rashba-field term, by which inversion symmetry is broken. In order to study effect of the Rashba-field on relation between spin fluctuation and superconductivity, we calculate spin dynamical susceptibility in the system. It is shown that unlike centrosymmetric system, spin dynamical susceptibilities show unusual momentum dependences, which is induced by Rashba-field. In order to explain these unusual features, group theoretical consideration is carried out. We will discuss its effect on superconductivity.

TT 15.23 Tue 14:00 Poster B

Theory for cooper pairing in non-centrosymmetric superconductors — •Ludwig Klam and Dirk Manske — Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

With the discovery of superconductivity in the non-centrosymmetric heavy Fermion compound $CePt_3Si$ by E. Bauer *et al.* a new field of research has developed. Since in this compound the order parameter is – due to a large antisymmetric spin-orbit coupling – a superposition of a spin singlet and spin triplet state, many new interesting properties have been observed. The pairing interaction giving rise to this mixed parity order parameter can be parameterized, and depending on the strength of the different interaction contributions we explore the phase diagram and the nodal structure.

We use a Green's function approach in order to calculate response and transport functions such as the Knight shift and the spin susceptibility. Furthermore we investigate the role of the band-structure obtained from LDA calculations and use a parametrization for the so-called β-band of $CePt_3Si$ in order to compare our numerical results to the experiments.

TT 15.24 Tue 14:00 Poster B

Contribution of the surface dipole to deformation of superconductors — Pavel Lipavsky[1,2], •Klaus Morawetz[3,4], Jan Kolacek[4], Ernst Helmut Brandt[5], and Michael Schreiber[3] — [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]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [5]Max Planck Institute for Metals Research, 70506 Stuttgart, Germany

The interaction of the ionic lattice with the superconducting condensate is treated in terms of the electrostatic force in superconductors. It is shown that the surface dipole supplies the force responsible for the volume difference of the normal and superconducting states. Assuming this mechanism we argue that the usual parametrization of the theory of deformable superconductors should be revisited.
arXiv:0708.3760

TT 15.25 Tue 14:00 Poster B

The nonadiabatic regime in optically excited BCS superconductors — •Thomas Papenkort[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

We have calculated the coherent dynamics of a BCS superconductor excited by short laser pulses using the density matrix formalism in mean field approximation. For very short pulses a nonadiabatic regime emerges in which the superconductor is put into a state with nonvanishing quasiparticle coherences. For such states the modulus of the BCS order parameter performs a damped oscillation in time. It turns out that this oscillation cannot be measured by means of pump-probe spectroscopy as only its temporal mean is reflected in the spectra. However we will show that this drawback can be overcome by using two coherent pump pulses.

TT 15.26 Tue 14:00 Poster B

Pump-probe spectra and nonlinear dynamics of BCS superconductors — Thomas Papenkort[1], •Norina Richter[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

We present numerical calculations of the reaction of a BCS superconductor to short laser pulses. Starting from the BCS ground state, a laser pulse decreases the modulus of the order parameter, $|\Delta|$. The intensity dependence of this shift depends strongly on the temporal width of the laser pulse. It may be measured using pump-probe spectroscopy: $|\Delta|$ ist directly linked to the energy gap of the superconductor which in turn is clearly visible in the absorption spectra. If the probe pulse precedes the pump pulse, an oscillation is superimposed on the spectrum and both the gap before and after the pump pulse can be seen. After very short pump pulses $|\Delta|$ does not remain constant but instead oscillates. The time dependence of this oscillation is in very good agreement with exact results obtained for the dynamics of a BCS system without external driving following a sudden change into a nonequilibrium state.

TT 15.27 Tue 14:00 Poster B

Microwave conductivity of superconducting aluminum films — •Katrin Steinberg and Martin Dressel — 1.Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

BCS-Superconductors show a coherence peak in real part of the conductivity below the energy gap. We investigated the development of the coherence peak in thin aluminum films with different mean free path. Microwave measurements of the complex conductivity were done in a range from 45 MHz to 40 GHz down to 1.2 K. The temperature and frequency dependence of the coherence peak gives information about

the quasiparticle scattering and coherence effects in a superconductor.

TT 15.28 Tue 14:00 Poster B

Investigation of proximity systems with very low temperature STS — •Wolz Michael, Debuschewitz Christian, Kunej Vojko, and Scheer Elke — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

We have investigated the superconducting proximity effect of double layer superconductor (S)- normal metal (N) systems with a very low temperature STM with high energy resolution. We used the BCS-superconductor Al. We have measured the density of states (DOS) for different thicknesses of the N-layer and for different N-materials (Au, Ag and Pd). The DOS of the Pd samples show a strong suppression of the superconuctivity in comparison to the Au and Ag samples. A possible explanation for that could be the strong electron-spin fluctuation coupling in Pd [2]. Our experimental data were fitted with a theoretical model of Belzig et al. [1] to check the dependence of the DOS on the interface quality and on the coherence lengths in N and S.

[1] W. Belzig, C. Bruder and G. Schön, Phys. Rev. B 54, 9443 (1996)

[2] T. Konzos et al., Phys. Rev. Lett. 93, 137001 (2004)

TT 15.29 Tue 14:00 Poster B

Geometrical Confinement in Superconducting/Ferromagnetic Heterostructures — •Silvia Haindl[1], Tanya Shapoval[1], Thomas Thersleff[1], Jens Ingolf Mönch[2], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]Institute for Metallic Materials, IFW Dresden, PF 270116, 01171 Dresden, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, PF 270116, 01171 Dresden, Germany

In superconducting thin films, geometrical confinement and thus microstructuring has a strong influence on the nucleation of superconductivity. Additionally, in superconducting/ferromagnetic thin films an influence on the superconducting properties is exerted by the magnetic stray field of the ferromagnet. Superconducting/ferromagnetic heterostructures were prepared by UHV pulsed laser deposition (PLD). Ferromagnetic dots with and without microstructuring were covered by a superconducting thin Nb film. In order to demonstrate the direct influence of the geometrical confinement, a recently developed polishing technique was employed to reduce the thickness of the superconducting layer.

TT 15.30 Tue 14:00 Poster B

Ferromagnet/superconductor heterostructures with different magnetic anisotropies — Niraj Joshi[1,2], Ajay Singh[3], •Christoph Sürgers[1,2], and Hilbert v. Löhneysen[1,2,4] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe, Germany — [3]Bhabha Atomic Research Centre, Mumbai 400 085, India — [4]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

In order to explore the interplay between magnetism and superconductivity in ferromagnet (F) / superconductor (S) heterostructures we have investigated various systems with different magnetic anisotropies by measurements of the transition temperature T_c, upper critical field B_{c2}, critical current I_c, and anomalous Hall effect. In the case where F is a Co/Pt multilayer with strong magnetic out-of-plane anisotropy, the superconducting properties of FSF triple layers depend on the relative orientation of the two F layer magnetizations. In a second approach we have modified the magnetic properties of ferrimagnetic $Fe_{1-x}Gd_x$ films in FS bilayers and FSF triple layers by small variations of the concentration x around $x = 0.25$ where the individual magnetizations of the Fe and Gd sublattices are nearly compensated. Finally, we present first magnetization measurements of epitaxially grown Co/Cu multilayers on Nb(110) single crystals in the superconducting and normal state.

TT 15.31 Tue 14:00 Poster B

Andreev reflection measurements using amorphous WC superconducting contact — •Jose Barzola-Quiquia, Michael Ziese, and Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, Leipzig, Germany

In this contribution we present point-contact Andreev reflection measurements of Co/ and Cu/tungsten-carbide (WC) contacts. The patterning of the metallic thin films samples was done using e-beam lithography. The tungsten carbide (WC) superconductor tip was grown directly on the investigated sample by decomposition of a metallo-organic vapor (tungsten hexacarbonil) under a focused Ga ion beam (FIB). Measurements were performed in standard four-point configuration with and without applied magnetic field. The experimental conductance-voltage curves were analyzed with the Blonder-Tinkham-Klapwijk theory [Phys. Rev. B 25, 4515 (1982)]. The results highlight the possibilities and advantages of using amorphous WC tips for point-contact spectroscopy of mesoscopic metallic samples.

TT 15.32 Tue 14:00 Poster B

Tunneling transport properties in $(La,Sr)_2CuO_4$ grain boundary Josephson junctions — •Andreas Stöhr[1], Michael Wagenknecht[1], Dieter Koelle[1], Reinhold Kleiner[1], Gennady Logvenov[2], and Ivan Bozovic[2] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Brookhaven National Laboratory, Upton, NY, U.S.A.

We investigate tunneling transport properties in thin film grain boundary Josephson junctions (GBJ's) of epitaxially grown $(La,Sr)_2CuO_4$ (LSCO) on bicrystal substrates. These optimally doped LSCO films were made by molecular beam epitaxy producing a very smooth film at the grain boundary. Measurements of the critical current I_c at low magnetic fields B (mT range) are used to characterize the quality of the junctions. Deviations from the ideal $I_c(B)$ pattern enable us to indicate the homogeneity of the GBJ. Measurements of the differential conductance in high magnetic fields (T range) are used to investigate quasiparticle tunneling across the grain boundary. Results are compared to theoretical predictions.

TT 15.33 Tue 14:00 Poster B

Development of Josephson junctions with ferromagnetic barrier — •Dirk Sprungmann, Kurt Westerholt, and Hartmut Zabel — Ruhr-Universität Bochum Experimentalphysik IV, 44780 Bochum, Germany

π-coupled Josephson junctions with ferromagnetic interlayers enjoy an increasing interest in the spin electronic community since they are considered as candidates to be used for quantum bits. In order to investigate π-coupled Josephson junctions it is initially necessary to find a sample design which allows to produce reproducibly high quality Josephson junctions with a low or negligible sub-gap leakage. On our poster we present a sample design with a minimized number of process steps, which allows us to produce a complete sample within six hours. We describe the optimization of the different process steps in the preparation of the SIFS-type junctions, where I and F denote an Al_2O_3 and a ferromagnetic layer respectively.

We acknowledge financial support through SFB 491

TT 15.34 Tue 14:00 Poster B

Fraunhofer pattern of a S-F-S Josephson junction as a function of the magnetization orientation — •Franz Czeschka[1], Sebastian T.B. Goennenwein[1], Rudolf Gross[1], Ruurd S. Keizer[2], Teun M. Klapwijk[2], and Arunava Gupta[3] — [1]Walther-Meissner-Insitut, Garching, Germany — [2]Kavli Institute of NanoScience, Delft, The Netherlands — [3]MINT Center, Tuscaloosa, Alabama

In the last decade the interest in superconductor-ferromagnet hybrid structures has substantially increased due to their potential application in spintronics and quantum computation. Moreover the competing ordering phenomena in superconductors (S) and ferromagnets (F) lead to interesting physical effects.

We have fabricated S-F-S Josephson junctions made of the superconductor NbTiN and the ferromagnet CrO_2. With its high spin polarization and large ferromagnetic domains, CrO_2 is ideally suited for the investigation of magnetization orientation dependent effects in S-F-S Josephson junctions. We have investigated the dependence of the critical current on the magnitude and the orientation of the external magnetic field of $NbTiN/CrO_2/NbTiN$ lateral Josephson junctions, fabricated by e-beam lithography, sputtering and lift-off. We find a strongly hysteretic Fraunhofer pattern with an oscillation period which characteristically changes with the magnetization orientation. We interpret these results in terms of the total magnetic flux $B = \mu_0(H+M)$ in the structure.

Financial support of the German Excellence Initiative via the "Nanosystems Initiative Munich (NIM)" is gratefully acknowledged.

TT 15.35 Tue 14:00 Poster B

Critical current of Nb-$(Nb/Pd_{0.95}Fe_{0.05})$-Nb Josephson junctions — •O. Vávra, W. Meindl, and C. Strunk — Institut für

experimentelle und angewandte

The antagonism of superconductivity and magnetism is investigated by fabricating Nb based Josephson Junction with lateral weak links consisting of Nb-$Pd_{0.95}Fe_{0.05}$ bi-layers with lengths between 200 and 500 nm. The critical current (I_C) of the Nb-$Pd_{0.95}Fe_{0.05}$ bi-layer is found to be significantly reduced by the weak ferromagnetism in the $Pd_{0.95}eFe_{0.05}$ alloy. We have studied the temperature and magnetic field (B) dependencies of the critical current. In magnetic field an irregular supercurrent interference pattern $I_C(B)$ is observed. The shape of the $I_C(B)$ oscillations is similar to that observed for grain boundary junctions between cuprate superconductors. We also investigate the dependence of $I_C(B)$ oscillations on the orientation of the magnetic field.

TT 15.36 Tue 14:00 Poster B

Multi-terminal Josephson Junctions with Ferromagnetic Elements — •Martin Leib and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

The interplay between magnetism and superconductivity in heterostructures has attracted considerable interest since the discovery of the 0-π transition in superconductor-ferromagnet (SF) contacts. Here we investigate the supercurrent in systems of multiple tunnel junctions in the framework of the quantum circuit theory. The considered network consists of two superconducting and two ferromagnetic reservoirs with non-collinear magnetization direction connected by tunnel contacts to a normal metal. We find and interesting interplay between the superconducting phase difference and the relative magnetization angle, which manifests itself in the current phase relation and the critical current.

TT 15.37 Tue 14:00 Poster B

SQUID readout of the magnetic flux states of fractional Josephson vortices. — •Andreas Dewes, Dieter Kölle, Reinhold Kleiner, and Edward Goldobin — Physikalisches Institut-Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen

We present an experimental study of a direct SQUID readout of the various states of a fractional vortex molecule in a long 0-κ-0 or 0-κ-2κ Josephson junction[1]. The fractional vortices appear at the discontinuities of the Josephson phase that are created by using tiny pairs of current injectors[2,3]. The magnetic field of each vortex is coupled to an integrated DC SQUID placed in front of it. In experiment, we measure the magnetic flux Φ in the SQUID loop as a function of the bias current of the junction I, of the injector current $I_{\rm inj}$ and of the magnetic field H. By changing the bias current of the junction or by modifying the discontinuity $\kappa \propto I_{\rm inj}$ we can induce and observe transitions between all four states of the fractional vortex molecule ($\uparrow\uparrow$, $\downarrow\uparrow$, $\uparrow\downarrow$ and $\downarrow\downarrow$). The readout system is intended to be part of a prospective fractional vortex qubit[4].

[1] E. Goldobin et. al., *Phys. Rev. B* **70**, 174519 (2004).
[2] B. A. Malomed et. al., *Phys. Rev. B* **69**, 064502 (2004).
[3] E. Goldobin et. al., *Phys. Rev. Lett.* **92**, 057005 (2004).
[4] E. Golodbin et. al., *Phys. Rev. B* **72**, 054527 (2005).

TT 15.38 Tue 14:00 Poster B

Spectroscopy of the eigenfrequencies of a fractional Josephson vortex molecule — •Uta Kienzle[1], Tobias Gaber[1], Kai Buckenmaier[1], Konstantin Ilin[2], Michael Siegel[2], Dieter Koelle[1], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen — [2]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH)

Using a pair of tiny current injectors one can create an arbitrary κ discontinuity of the phase in a long Josephson junction (LJJ) [1]. To compensate this discontinuity a κ vortex spontaneously appears [2]. This vortex carries an arbitrary fraction $\propto\kappa$ of the magnetic flux quantum Φ_0 and is a generalization of a semifluxon observed in 0-π LJJs [3]. Such a vortex is pinned at the discontinuity point, but in an underdamped system it is able to oscillate around its equilibrium position with an eigenfrequency [4,5]. In annular LJJs with two injector pairs two coupled κ vortices, forming a molecule, can be studied.

The dependence of the eigenfrequency on temperature and κ of one and two coupled vortices was measured in the range from 300 mK up to 4.2 K. We discuss the results and compare them with simulations based on the perturbed sine-Gordon equation.

[1] E. Goldobin *et al.*, Phys. Rev. Lett. **92**, 57005 (2004)
[2] E. Goldobin *et al.*, Phys. Rev. B **70**, 174519 (2004)
[3] H. Hilgenkamp *et al.*, Nature **422**, 50 (2003)
[4] E. Goldobin *et al.*, Phys. Rev. B **71**, 104518 (2005)
[5] K. Buckenmaier *et al.*, Phys. Rev. Lett. **98**, 117006 (2007)

TT 15.39 Tue 14:00 Poster B

Two dimensional planar superconducting quantum interference device gradiometer on a $SrTiO_3$ bicrystal — •Uwe Schinkel, Christoph Becker, Veit Grosse, Alexander Steppke, Frank Schmidl, and Paul Seidel — Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Germany

Superconducting sensors are state of the art for the measurement of small magnetic signals. Gradiometers with DC SQUID sensors can be used in magnetically unshielded areas, due to the high surpression of homogeneous magnetic fields. 2nd order gradiometers achieve an even higher reduction of external noise.

We show a new gradiometer layout based on YBCO thin films to detect the second order field gradient. In a planar configuration four galvanically coupled antenna structures are read out by a symmetric DC SQUID with four Josephson junctions on $SrTiO_3$ bicrystals. Simulations, the preparation process and first electric measurements are presented.

TT 15.40 Tue 14:00 Poster B

Planar flip-chip HTSC DC-SQUID gradiometers for non-destructive evaluations — •Christoph Becker[1], Alexander Steppke[1], Uwe Schinkel[1], Markus Buettner[1], Veit Grosse[1], Hendrik Schneidewind[2], Frank Schmidl[1], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Institut für Photonische Technologien e.V., Jena, Germany

For the detection of small magnetic signals, for example in applications like non-destructive evaluation DC-SQUID gradiometers are successfully used today. The low noise level of our sensors and the possibility of working in unshielded environments cannot be achieved with convential methods. The sensors made out of high-temperature superconducting thin film gradiometers are inductively coupled to a flux-transformer in a flip-chip configuration.

The field gradient resolution of the complete system is below $1\,\mathrm{pT}/(\sqrt{\mathrm{Hz}}\,\mathrm{cm})$. In our investigations we focused on the spatial resolution of the sensors. Different approaches to characterize the resolution and methods to improve the signal to noise ratio for small magnetic sources are shown.

TT 15.41 Tue 14:00 Poster B

Different transport mechanisms across semiconductor junctions — •Barbara Sandow[1], Dirk Brossell[1], and Walter Schirmacher[2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Physik-Department E13, Technische Universität München, Germany

We used break-junction tunnelling spectroscopy to investigate the Coulomb correlation in n-type Germanium. The Charge transport across break-junctions of n-type Germanium has been investigated. The low-T spectra of our Ge break junctions vary systematically with contact size. However, it is not always clear what kind of processes dominate the spectra of those contacts. We show how to identify and separate the different transport mechanisms across the junctions, necessary to derive the Density of states.

TT 15.42 Tue 14:00 Poster B

Fine structure in the tunneling characteristic of MgB_2 thin films — •Rudolf Schneider[1], Jochen Geerk[1], Alexander Zaitsev[1], and Hilbert von Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe

We report on a progress in the *in situ* preparation of superconducting MgB_2 thin films by thermal evaporation of Mg combined with B sputtering. By sputtering the boron from a red-hot sintered target we were able to increase the substrate temperature up to 550°C. The film properties, like T_c and the residual resistivity, significantly improved compared to films deposited at lower substrate temperatures. In the negative second derivative of the current-voltage characteristic measured on sandwich-type crossed-strip tunnel junctions on MgB_2 films with a T_c of 35 K, theoretically predicted fine structures could be resolved which were missing in our former tunnelling experiments using films with a lower T_c of 32 K. Better crystalline order within the MgB_2 grains is evidently the key to the details of the electron-phonon

coupling.

TT 15.43 Tue 14:00 Poster B

Effect of a dc magnetic field on the microwave losses in MgB_2 thin films — •Roland Hott[1], Alexander G. Zaitsev[1], Rudolf Schneider[1], Thorsten Schwarz[2], and Jochen Geerk[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O. Box 3640, D-76021 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Synchrotronstrahlung, P.O. Box 3640, D-76021 Karlsruhe, Germany

The microwave surface impedance ($Z_s = R_s + iX_s$) of in situ MgB_2 thin films was measured as a function of temperature and parallel dc magnetic field at several frequencies between 5.7 and 18.5 GHz using a dielectric resonator technique. The results are consistent with the expectations for a classical type-II superconductor and, consequently, quite different from those of the high-T_c cuprates. The films cooled in zero field revealed a clear indication of the lower critical field B_{c1}, with a small hysteresis around $B \leq B_{c1}$. In higher fields ($B > B_{c1}$), the losses followed the Coffey-Clem and Brandt model, including the frequency dependences, whereas high-T_c Y-Ba-Cu-O films did not show a reasonable agreement with this model. Both the relatively high values of $\Delta X_s/\Delta R_s$ ratio and their frequency dependence indicate a weak effect of flux creep on the measured microwave loss in MgB_2 films. The temperature dependence of $\Delta X_s/\Delta R_s$ ratio can be described by a microscopic pinning model for BCS superconductors.

TT 15.44 Tue 14:00 Poster B

Static and time-resolved vortex dynamics in a-$Nb_{0.7}Ge_{0.3}$ — •Florian Otto[1], Martin Frisch[1], Ante Bilušić[1], Dinko Babić[2], Christoph Sürgers[3], and Christian Strunk[1] — [1]Inst. for Exp. and Appl. Physics, Univ. Regensburg, Germany — [2]Dept. Physics, Univ. Zagreb, Croatia — [3]Phys. Inst. and DFG Center for Funct. Nanostr. (CFN), Univ. Karlsruhe, Germany

We investigate the motion of vortices in amorphous $Nb_{0.7}Ge_{0.3}$. Because of the very low pinning in this high-κ type-II superconductor, we are able to measure local and non-local transport in the flux-flow regime over large parts of the B-T-phase diagram [1]. Interestingly, there is a finite non-local response close to T_c, even when the applied magnetic field is zero. This points towards the presence of spontaneously formed vortex-antivortex pairs above the Berezinskii-Kosterlitz-Thouless transition. In addition, we report first non-local transport measurements in the time domain, using a boxcar averaging technique.

[1] A.Helzel et al., Phys. Rev. B **74**, 220510 (R) (2006)

TT 15.45 Tue 14:00 Poster B

Unexpected temperature-dependence of the critical current in NbN-microbridges — •Andreas Engel[1], Holger Bartolf[1], Luis Gomez[1], Andreas Schilling[1], Konstantin Il'in[2], Michael Siegel[2], Alexei Semenov[3], and Heinz-Wilhelm Hübers[3] — [1]Physics Institute, University of Zürich, Winterthurerstr. 190, CH-8057 Zürich — [2]Institute of Micro- and Nano-Electronic Systems, University of Karlsruhe, Hertzstr. 16, 76187 Karlsruhe — [3]DLR e.V. Institute of Planetary Research, Rutherfordstr. 2, 12489 Berlin

Superconducting micro- and nanostructures made from NbN ultra-thin films are key elements of THz hot-electron bolometer mixers and single-photon detectors for the visible and near-infrared. Their detection mechanisms require operation with a biasing current close to but below the device's critical current I_c at temperatures well below their critical temperature. We studied the temperature-dependence $I_c(T)$ of up to 10 nm thick NbN bridges with widths between 100 nm and 10 μm. The temperature-dependence of the critical-current density j_c of sub-micrometer wide bridges is well described by the de-pairing j_c. They remain free of magnetic vortices due to a geometrically enhanced Bean-Livingston barrier. Micrometer-wide bridges show a cross-over from de-pairing to de-pinning j_c with decreasing temperature. Moreover, at low temperatures, when I_c is determined by the de-pinning of magnetic vortices due to the self-field of the applied current or small external magnetic fields, $I_c(T)$ may exhibit non-monotonic behavior, *i.e.* reduced I_c at lower temperature. We present experimental data of these unexpected features and discuss their possible reasons.

TT 15.46 Tue 14:00 Poster B

Flux dynamics in HT-superconductor thin films influenced by a surface acoustic wave — •Munise Rakel[1], Arno Wirsig[1], Carsten Hucho[1], and Joachim Albrecht[2] — [1]Paul-Drude-Institut, 10117 Berlin, Germany — [2]Max-Planck-Institut für Metallforschung, 70569 Stuttgart, Germany

We report on magneto-optic investigations of the influence of a traveling strain wave on the magnetic flux density distribution in a type-II superconductor. The investigations are performed on a thin film of YBCO on a piezoelectric substrate using a custom-made magneto-optical microscope. The strain wave is generated by interdigital transducers on the piezoelectric substrate. An external magnetic field applied perpendicular to the surface enters the polycrystalline superconductor depending on the pinning properties. Strain-wave induced pinning-changes or SAW-induced depinning is reported to result in changes in the flux dynamics. We analyze magneto-optic greyscale images of films with dynamically altered pin-state to yield information on the influence of the combined dynamic strain- and electric field on the pinning behavior of the superconducting film.

TT 15.47 Tue 14:00 Poster B

Reconstruction of the electric field distributions for flux dynamics studies in superconducting thin films — •Carolina Romero-Salazar[1], Omar Augusto-Flores[2], and Christian Jooss[1] — [1]Institut fuer Materialphysik, Friedrich Hund Platz 1, 37077 Goettingen, Germany — [2]Instituto de Fisica, Universidad Autonoma de Puebla, Apdo. Post. J-48, Puebla, Mexico

It is well known that in type-II superconductors there are electric fields due to vortex motion. The space-resolved study allows for insights into the mechanism of vortex dynamics and the occurrence of local losses. This is an important and challenging problem for the development of high-current carrying applications with low electromagnetic losses. The electric field in high- T_c superconducting films is reconstructed employing magneto-optical imaging of the magnetic induction $B_z(r)$ distributions. We developed a consistent method to calculate both dynamic and static contributions of the electric field, for a thin film in the so called perpendicular geometry. We investigate the contrasts between our technique, which employs magnetic relaxation measurements, and the theoretical scheme which requires an effective material law, $E = \rho J$, obtained from current transport experiments. Understanding the vortex dynamics in homogeneous superconducting films, provides a necessary background to study materials with complicate structures as patterned holes or inhomogeneous pinning.

TT 15.48 Tue 14:00 Poster B

Nernst effect of Ni-doped $NdBa_2Cu_3O_{7-\delta}$ — •Niko Johannsen[1], Thomas Wolf[2], Alexander V. Sologubenko[1], Thomas Lorenz[1], Axel Freimuth[1], and John A. Mydosh[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Forschungszentrum Karlsruhe, Germany

The mechanism of high-temperature superconductivity is still unsolved. Possible relations to other phenomena such as the pseudogap may play a key role towards an understanding of this mechanism. Using the Nernst effect, we are able to detect vortex-like excitations very sensitively. In $NdBa_2\{Cu_{1-y}Ni_y\}_3O_{7-\delta}$, magnetic Ni-impurities suppress T_c and at the same time enhance the pseudogap. So, this is an ideal system to study possible relations between the pseudogap and superconductivity via the Nernst effect. We present measurements on a series of optimally doped (O_7) and two underdoped ($O_{6.8}$, $O_{6.9}$) samples with Ni contents ranging from y=0 to 0.12. For the optimally doped samples, the onset temperature of the anomalous Nernst signal (T^ν) decreases with increasing Ni content as does T_c. The underdoped ($O_{6.8}$) samples show a slightly different behavior. T^ν is not affected by an increase of the Ni content. The slope of T^ν of the intermediate doping level ($O_{6.9}$) lies between the aforementioned two. None of the detected anomalous vortex Nernst signals shows a relation to the enhanced pseudogap in this system.

TT 15.49 Tue 14:00 Poster B

Proximity Effect in Nb/Au and NbN/Au bi-layers for THz Antenna Structures of HEB Mixers — •Axel Stockhausen[1], Konstantin Il'in[1], Michael Siegel[1], Alexei Semenov[2], Heinz-Wilhelm Hübers[2], Reinhard Schneider[3], and Dagmar Gerthsen[3] — [1]IMS, University of Karlsruhe, Karlsruhe, Germany — [2]DLR e.V. Institute of Planetary Research, Berlin, Germany — [3]LEM, University of Karlsruhe, Karlsruhe, Germany

Hot-electron Bolometer (HEB) mixers are high sensitive heterodyne detectors made from ultra-thin (< 5 nm) NbN film deposited on Si substrate. For proper operation of these devices in THz frequency range a superconducting detecting element is embedded into antenna

structure made from thick Au layer. In systems where a superconducting film with thickness about the coherence length is in contact with a thick normal metal layer superconductivity will be suppressed due to proximity effect. Increasing transparency of superconducting-to-normal metal interface leads to stronger suppression of superconductivity in ultra-thin NbN film. However it allows to decrease RF losses on contact resistance between antenna and detecting element and improve performance of HEB mixer. We have developed processes for deposition of Au antenna structure with superconducting buffer of Nb or NbN. This allows us to avoid deterioration of HEB mixer performance causing by proximity effect even in case of perfectly transparent interface. The superconducting and normal state properties of different Nb and NbN thin films and Nb/Au and NbN/Au bi- and multi-layers will be presented and properties of the interfaces will be discussed.

TT 15.50 Tue 14:00 Poster B

Kinetic Inductance Detectors Based On Quarter Wavelength Resonators — •Gerd Hammer, Stefan Wünsch, Konstantin Ilin, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH), Karlsruhe, Deutschland

Quarter wavelength resonators with high-Q values as core part of a complete readout system for kinetic inductance detectors opens the possibility of a extremely sensitive measurement method for radiation in a wide spectral range. Absorbted radiation causes a change of quasiparticle density and subsequently to a change of kinetic inductance of the resonator. This results in a detuning of the cavity circuit which can be detected by measurement of amplitude or phase. Superconducting thin-film niobium resonators with different geometries in coplanar waveguide topology for 6 GHz were developed, fabricated and measured. Simulation and measurement results of the quality factors Q_R show strong influences of the coupling capacitances and has to be optimized. Measurements at cryogenic temperatures with quality factors Q_R in the range of $10^5 - 10^6$ were achieved in a temperature range of 4 K to 8 K.

TT 15.51 Tue 14:00 Poster B

Response of NbN ultra-thin superconducting films to optical irradiation — •Dagmar Rall[1,3], Konstantin Ilin[2], Stefan Wünsch[2], Felix Glöckler[1], Uli Lemmer[1], and Michael Siegel[2] — [1]Light Technology Institute, University of Karlsruhe, Germany — [2]Institute for Micro- and Nanoelectronic Systems, University of Karlsruhe, Germany — [3]Karlsruhe School of Optics and Photonics, Germany

We study energy relaxation processes in ultra-thin NbN films suitable for development of hot-electron bolometers and superconducting single photon detectors. Improvements of device performance require optimization of material properties of NbN films focussing on increasing of sensitivity and speed of the detector. The NbN thin films with different thickness and stoichiometry are fabricated by dc reactive magnetron sputtering and patterned into narrow strip lines and terminated by the detecting element. Energy relaxation processes in the films are studied using a time domain technique. NbN strips are cooled below critical temperature in a continuous-flow helium cryostat fitted with high-frequency readout electronics and optical window. Femtosecond laser pulse irradiation absorbed in ultra-thin NbN film excites hot-electrons resulting in a voltage pulse. Time propagation of the response pulse is determined by electron energy relaxation processes via inelastic electron-electron and electron-phonon interaction and escape of non-equilibrium phonons from film to substrate. Results on fs-laser pulse response of NbN thin films with different material properties and geometry of the sample will be presented and discussed.

TT 15.52 Tue 14:00 Poster B

Microfabrication of magnetic calorimeters — •Stefan Lausberg, Andreas Pabinger, Andreas Burck, Christian Domesle, Christan Höhn, Sebastian Kempf, Lena Maerten, Christian Pies, Jan-Patrick Porst, Sönke Schäfer, Richard Weldle, Thomas Wolf, Loredana Fleischmann, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg, Germany

Metallic magnetic calorimeters (MMCs) detect the energy of particles by measuring the heat input into a metallic absorber that is thermally well connected to a paramagnetic Au:Er sensor. The sensor is situated in a weak magnetic field. An incident particle deposits energy inside the absorber and heats up the sensor which results in a change of magnetization. This change is proportional to the particle energy and is read out by a SQUID magnetometer. For large area MMCs, the magnetic field is generated by a microstructured meander shaped niobium coil. A persistent current can be frozen in this structure producing an inhomogeneous field in the region of the sensor, which is directly sputtered on top. Both the sputtering of Au:Er sensors with thermodynamical properties that agree with the ones of bulk material as well as the deposition of niobium films with high critical currents are crucial process steps for the microfabrication of MMC detectors with high resolution power. We give a detailed description of the two processes that we presently use for microfabrication of MMC detectors and discuss the achieved results.

TT 15.53 Tue 14:00 Poster B

Development of a Fully Microfabricated Two Pixel Magnetic Calorimeter — •S. Schäfer, A. Burck, C. Domesle, C. Höhn, S. Kempf, S. Lausberg, A. Pabinger, C. Pies, J.-P. Porst, R. Weldle, A. Fleischmann, L. Fleischmann, and C. Enss — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, 69120 Heidelberg

The feasibility to microfabricate single metallic magnetic calorimeter detectors and detector arrays has been studied. These detectors consist of an absorber for x-rays and a paramagnetic temperature sensor placed in a weak magnetic field. At working temperatures below 100 mK any energy deposition in the detector produces a temperature rise which changes the magnetization of the sensor material. By a read out scheme with sensitive low noise SQUID magnetometers, the absorption of single x-ray quanta can be detected and their energy can be measured precisely. The steps of a microfabrication process were developed and optimized which allows for a fabrication of calorimeter arrays with mushroom shaped detectors increasing the sensible area by overhanging absorbers. On a single chip, two detectors were fabricated and read out by two separate circuits. Due to this special setup, it was possible to analyze the crosstalk between both pixels. In addition to measurements in the flux-locked-loop mode, magnetization measurements and spectra were obtained in open-loop mode. In this mode of operation electro-thermal-feedback effects were observed which result in changing the decay times of the pulses. In particular, in this mode faster pulses can be achieved which allows higher count rates.

TT 15.54 Tue 14:00 Poster B

Metallic magnetic calorimeters with superconducting absorbers — •Christian Höhn, Richard Weldle, Jan-Patrick Porst, Andreas Burck, Chriatian Domesle, Sebastian Kempf, Stefan Lausberg, Lena Maerten, Andreas Pabinger, Christian Pies, Sönke Schäfer, Loredana Fleischmann, Andreas Fleischmann, and Christian Enss — KIP, Universität Heidelberg, INF 227, D-69120 Heidelberg, Germany

In metallic magnetic calorimeters (MMCs) the absorbed energy of incoming particles, e.g. X-rays, causes an increase of temperature in the detector which leads to a change of magnetisation in the Au:Er paramagnetic sensor. The resulting change in magnetic flux can be measured with a SQUID-magnetometer. As the flux change depends on the change of temperature which is inversely proportional to the heat capacity, it is attractive to use a superconducting absorber material. The first experiment presented here consists of a rhenium crystal as absorber with a gold foil glued on top that partly covers the surface of the absorber. The different pulse shapes that occur due to X-rays, either hitting directly the rhenium, therefore causing Cooper pairs to break, or the gold, producing a heat signal only phononically coupled to the rhenium, are presented. One idea to reduce the long rise time that occurs when superconductors are used as absorbers is to include magnetic impurities. These impurities reduce the energy gap of the superconductor which may lead to a faster quasiparticle recombination. The results obtained with MMCs having pure Al and Al:Mn absorbers are presented and the differences in pulse shape will be discussed.

TT 15.55 Tue 14:00 Poster B

Electrodeposition of gold absorbers for metallic magnetic calorimeters — •Christian Pies, Stefan Lausberg, Andreas Burck, Christian Domesle, Christian Höhn, Sebastian Kempf, Lena Maerten, Andreas Pabinger, Jan-Patrick Porst, Sönke Schäfer, Richard Weldle, Thomas Wolf, Andreas Fleischmann, Loredana Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg, Germany

Metallic magnetic calorimeters are increasingly used for particle detection. A metallic paramagnetic sensor is situated in a weak magnetic field. Incident particles, like x-rays, dissipate their energy inside a gold absorber which is thermally well connected to the sensor. The temperature rise in the absorber causes a rearrangement of magnetic

moments in the sensor. This change in magnetization is read out by a two-stage SQUID setup.

In order to stop x-rays in the energy range of more than 100 keV, gold absorbers of several hundred microns in thickness are needed. Techniques like sputtering or vapor deposition can effectively produce films of no more than a few microns. Therefore an electrodeposition process was developed to fabricate thick gold layers with high purity and better residual resistivity ratio than sputtered or evaporated films. We use sulfite based gold electrolytes which can produce films of more than 200 microns. In order to control the geometry of the electrodeposited absorbers, we use the SU-8 negative photoresist, which can be structured up to 1 mm in thickness with a high aspect ratio.

TT 15.56 Tue 14:00 Poster B

Microstructured metallic magnetic calorimeter with meander shaped pickup coil — •Sebastian Kempf, Andreas Burck, Christian Domesle, Christian Höhn, Stefan Lausberg, Lena Maerten, Andreas Pabinger, Christian Pies, Jan-Patrick Porst, Sönke Schäfer, Richard Weldle, Thomas Wolf, Andreas Fleischmann, Loredana Fleischmann, and Christian Enss — Kirchoff-Institute for Physics, Heidelberg, Germany

It was recently shown that metallic magnetic calorimeters (MMC) are a promising and powerful tool for many applications. A MMC consists of an absorber for the particles to be detected and a paramagnetic temperature sensor positioned in a weak magnetic field. According to the calorimetric detection principle, the deposition of energy in the detector due to the impact of a massive particle or the absorption of an x-ray photon causes a rise of temperature and results in a change of magnetization of the sensor. This is detected as a change of magnetic flux in a low-noise high-bandwidth dc-SQUID magnetometer and serves as a precise measure of the deposited energy.
We present a fully microstructured MMC which consists of a gold absorber, a 3 μm thick sputter-deposited paramagnetic Au:Er-sensor and a meander shaped niobium thin film pickup coil. By means of temperature dependent measurements of magnetization and detector signal size we will compare the thermodynamic properties of the sputtered sensor material to the properties of bulk material. We discuss the achieved energy resolution, the noise of the detector signal and the shape of the detector response as a function of temperature and magnetic field.

TT 15.57 Tue 14:00 Poster B

Silber-Erbium-Legierungen: Neues Sensormaterial für magnetische Kalorimeter — •A. Burck, S. Kempf, C. Domesle, C. Höhn, S. Lausberg, L. Maerten, A. Pabinger, C. Pies, J. Porst, S. Schäfer, R. Weldle, T. Wolf, A. Fleischmann, L. Fleischmann und C. Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, Heidelberg, Germany

In den meisten der bisher entwickelten magnetischen Kalorimeter wurden paramagnetische Legierungen von Gold und dem Seltenerdmetall Erbium als Temperatursensor eingesetzt. Diese Legierungen stellten einen ausgewogenen Kompromiss zwischen einer schnellen Thermalisierungszeit und einer grossen Signalgrösse dar. Das relativ grosse Kernquadrupolmoment von Gold führt jedoch zusammen mit den elektrischen Feldgradienten in der Umgebung der Erbium-Ionen zu einem nicht vernachlässigbaren Beitrag zur Wärmekapazität, der eine Reduzierung der Signalgrösse zur Folge hat. Dieser ungewollte Beitrag lässt sich eliminieren, indem ein Wirtsmaterial verwendet wird, dessen Kernspin $I \leq 1/2$ ist. Demnach sollte sich Silber ($I = 1/2$) besser als Wirtsmaterial der verdünnten paramagnetischen Legierungen eignen. Wir stellen ein mikrostrukturiertes magnetisches Kalorimeter vor, welches auf einer mäanderförmigen Detektionsspule basiert auf der ein 5um dicker Sensor aus AgEr aufgebracht ist, der eine Erbiumkonzentration von 1300 ppm besitzt. Die Temperatur- und Feldabhängigkeit der Magnetisierung des Sensormaterials, das Rauschen des Detektorsignals, die auftretenden Signalformen, wie auch die Energieauflösung des Detektors werden diskutiert.

TT 16: Symposium: Efficient Classical Simulation of Strongly Correlated Quantum Systems

Time: Tuesday 14:00–17:45 Location: H 0104

Invited Talk TT 16.1 Tue 14:00 H 0104

Density matrix renormalization meets quantum information — •Ulrich Schollwöck — Institut für Theoretische Physik C, RWTH Aachen

In this talk I want to give an overview of the reassessment of the well-established density-matrix renormalization group method for the simulation of low-dimensional quantum systems by the use of quantum information concepts: it is in some sense the first of a set of essentially optimally efficient methods to simulate quantum systems on a classical computer. While this allows to get a very simple picture of the essence of this method which in my view is more adequate than renormalization group perspectives, it also allows to devise a plethora of new simulation techniques that have largely extended the scope of this method. I will give an introduction to these new developments and illustrate them by applications in the field of ultracold atoms and more conventional nanosystems. The purpose of this talk is also to set the stage for further talks on the individual new methods in the session in which it is presented.

TT 16.2 Tue 14:45 H 0104

Time-dependent DMRG: Applications to cold atoms in optical lattices — •Corinna Kollath[1], Andreas Laeuchli[2], and Ehud Altman[3] — [1]Ecole Polytechnique Palaiseau, France — [2]IRRMA Lausanne, Switzerland — [3]The Weizmann Institute of Science, Israel

Ultracold atoms constitute a system to investigate non-equilibrium physics in strongly correlated systems. Their good tunability allows to rapidly change the system parameters and observe the subsequent quantum evolution. For example the non-adiabatic dynamics across the superfluid-Mott-insulating phase transition has been realized in ultracold bosonic gases confined to optical lattices. The theoretical description of these time-dependent phenomena is very involved. We apply the recently developed adaptive time-dependent DMRG method to study the response of these strongly correlated quantum systems to different parameter changes.

TT 16.3 Tue 15:15 H 0104

A Renormalisation-Group Algorithm for Eigenvalue Density Functions of Interacting Quantum Systems — •Tobias Osborne — Royal Holloway, University of London

In this talk I'll describe a certifiable algorithm to calculate the eigenvalue density function – the number of eigenvalues within an infinitesimal interval – for an arbitrary 1D interacting quantum spin system. The method provides an arbitrarily accurate numerical representation for the smeared eigenvalue density function, which is the convolution of the eigenvalue density function with a gaussian of prespecified width. In addition, with the algorithm it is possible to investigate the density of states near the ground state. This can be used to numerically determine the size of the ground-state energy gap for the system to within a prespecified confidence interval. The method exploits a finitely correlated state/matrix product state representation of the propagator and applies equally to disordered and critical interacting 1D quantum spin systems.

15 min. break

Invited Talk TT 16.4 Tue 16:00 H 0104

Projected Entangled Pair States: status and prospects — •Frank Verstraete — Universitaet Wien, Austria

We report on the progress made to extend the density matrix renormalization group to higher dimensions, discuss the underlying theory of projected entangled pair states (PEPS) and illustrate its potential on the hand of a few examples.

TT 16.5 Tue 16:30 H 0104

DMRG and quantum impurity models — •Andreas Weichselbaum and Jan von Delft — Ludwig Maximillians Universität, Arnold Sommerfeld Center, Theresienstr. 37, 80333 München

Quantum impurity models are analyzed routinely and reliably at very low energies using the Numerical Renormalization Group (NRG). Its great benefit of energy scale separation, however, comes at the cost

of reduced resolution at finite energy. By realizing that the algebraic structure underneath NRG is the same as for the density matrix renormalization group (DMRG), namely matrix product states, several strict NRG contraints such as the rigid discretization scheme can be relaxed due to the variational principle of DMRG. Our recent work in that respect will be discussed.

TT 16.6 Tue 17:00 H 0104

Unitary networks to describe quantum many-body systems — •Jens Eisert[1], Chris Dawson[1], Tobias Osborne[2], and Frank Verstraete[3] — [1]Imperial College London, UK — [2]Royal Holloway, University of London, UK — [3]University of Vienna, Austria

To describe strongly correlated quantum many-body systems is typically hard, as the dimension of the underlying state space grows exponentially with the system size. The number of relevant parameters to simulate many-body systems, yet, is typically smaller. This talk will give an overview over variational sets of states which can faithfully grasp ground state properties of quantum lattice systems, which can be described by polynomially many parameters and for which one can efficiently compute local properties. We will introduce a flow approach to varying over such unitary networks, bringing together ideas of Wegner flow with variational methods. Applications to the simulation of two-dimensional lattice systems are outlined.

TT 16.7 Tue 17:30 H 0104

Optimized ensembles in quantum Monte Carlo simulations — •Stefan Wessel[1], Norbert Stoop[2], Emanuel Gull[2], Simon Trebst[3], and Matthias Troyer[2] — [1]Institute for Theoretical Physics, Stuttgart University, Germany — [2]Theoretical Physics, ETH Zurich, Switzerland — [3]Microsoft Research, Station Q, University of California Santa Barbara, USA

We present an adaptive means for improving the efficiency of Monte Carlo simulations of quantum systems in rough free energy landscapes. Such occur e.g. near strongly first-order (quantum) phase transitions, and due to competing interactions. Our approach is based on an extension of the concept of optimized broad-histogram ensembles for classical simulations to the quantum regime. We present examples of this approach within the context of the stochastic series expansion quantum Monte Carlo approach, and indicate the limits of such extended ensemble methods.

TT 17: Matter at Low Temperature: Measuring Devices, Cryotechnique

Time: Tuesday 14:00–15:00 Location: H 2053

TT 17.1 Tue 14:00 H 2053

First Results of the Resonant Inelastic X-Ray Scattering Station at the ADRESS Beamline at the Swiss Light Source — •Thorsten Schmitt[1], Vladimir Strocov[1], Giacomo Ghiringhelli[2], Andrea Piazzalunga[2], Xiaoqiang Wang[3], Justina Schlappa[1], Claudia Dallera[2], Lucio Braicovich[2], Marco Grioni[3], and Luc Patthey[1] — [1]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Politecnico di Milano, Italy — [3]EPFL Lausanne, Switzerland

Resonant inelastic X-ray scattering (RIXS) is a powerful bulk-sensitive probe of the electronic structure of condensed matter with atomic and orbital sensitivity. It is an unique tool for determining the energy and symmetry of charge neutral electronic excitations (e.g. crystal field or spin-flip excitations) in strongly correlated materials. The ADvanced RESonant Spectroscopies (ADRESS) beamline at the Swiss Light Source (SLS) features advanced instrumentation for RIXS. This year it will be complemented by instrumentation for Angle-Resolved Photoelectron Spectroscopy. The RIXS station is equipped with a spectrometer (resolving power $\approx$ 12000 for 1 keV) so-called SAXES (Super Advanced X-ray Emission Spectrograph) based on a variable line spacing spherical grating. The RIXS station is open since spring 2007 and was undergoing the operation tests during the 2nd half of 2007. We report on first results obtained with RIXS on transition metal monoxides (NiO, MnO and CuO) as reference compounds. These results demonstrate the capability of this set-up for RIXS studies on strongly correlated materials with unprecedented ultra-high resolution.

TT 17.2 Tue 14:15 H 2053

Practical SQUID-based noise thermometers for millikelvin temperatures — •Jörn Beyer, Dietmar Drung, Alexander Kirste, and Jost Engert — PTB, Berlin, Germany

We are developing SQUID-based noise thermometers aiming at compact and easy-to-use, linear and fast noise thermometers to cover the temperature range of dilution refrigerators, i.e., from about 10mK to 4K. The two types of thermometers we investigate are the Magnetic Field Fluctuation Thermometer (MFFT) and the Current Sensing Noise Thermometer (CSNT). In both the MFFT and the CSNT the thermally induced motion of charges in a metallic temperature sensor causes thermal magnetic flux noise detected by a SQUID sensor. The temperature of the metal is extracted from the thermal noise signal via the Nyquist theorem. In our MFFT and CSNT implementations the metal temperature sensor and the SQUID sensor are placed at the same temperature stage. In the case of the MFFT, the temperature sensor is a bulk Copper part and thermal magnetic field fluctuations above its surface are measured inductively by a multiloop SQUID-gradiometer. For the CSNT, the temperature sensor in form of a thin film resistor and a SQUID current sensor to measure the resistor current noise are integrated on a silicon chip. We present a comparison of our MFFT and CSNT configurations in terms of their sensitivity, speed, and linearity. We discuss the design of the temperature sensors and SQUID sensors, thermal anchoring and shielding of external interferences for the MFFT and CSNT. Comparison measurements with the Provisional Low Temperature Scale PLTS-2000 will be presented.

Invited Talk TT 17.3 Tue 14:30 H 2053

The centennial of helium liquefaction - a century of low temperature physics — •Dietrich Einzel — Walther-Meißner-Institut für Tieftemperaturforschung, Garching, Germany

The first liquefaction of helium gas by the Dutch physicist Heike Kamerlingh Onnes 100 years ago meant the dawn of a new discipline: low temperature physics. As we all know, this discipline has developed rapidly since that time and led to many important discoveries of new condensed states of matter (metallic superconductivity, superfluidity of liquid ^{4}He and ^{3}He, BEC in alkali gases etc.), which reside almost exclusively at the cold end of the temperature scale. The centennial discovery of liquid helium provides an occasion to review a few milestones in this development. Besides the pioneering work of Heike Kamerlingh Onnes, the contributions of German low temperature physicists (such as Walther Meißner and Robert Doll) to both the cryotechnical and the fundamental side of low temperature physics are emphasized. Hence you can expect a collection of important historical facts, complemented by some insights into the fascinating effects seen at low and ultralow temperatures.

TT 18: Correlated Electrons: Low-dimensional Systems - Materials 2

Time: Tuesday 15:15–18:45 Location: H 2053

TT 18.1 Tue 15:15 H 2053

Charge Ordering in (TMTTF)$_2$X: Evidences for Structural Changes — •Mariano de Souza[1], Alec Moradpour[2], Pascale Foury[2], Jean-Paul Pouget[2], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, Max-von-Laue Str. 1, SFB/TRR49, D-60438 Frankfurt am Main, Germany — [2]Laboratoire de Physique des Solides, Université Paris Sud, CNRS, UMR 8502, 91405 Orsay, France

The (TMTTF)$_2$X family of quasi-1D organic conductors has been the

subject of intensive studies over the last two decades. Recently, NMR spectroscopy studies [1] revealed the existence of a charge-ordered (CO) phase in the X=PF_6 and AsP_6 salts at $T_{CO}\approx$65 and 105 K, respectively. Until now, however, no evidence of structural changes has been reported in the literature and, due to this, the latter has been referred to as a "*structureless*"phase transition. In this contribution, we present directional-dependent high-resolution thermal expansion measurements on the X=PF_6 salt. Our findings reveal strong anisotropic lattice effects at both the Spin-Peierls and the CO transition, with the strongest response along the c^*-axis, along which the stacks are separated by the PF_6^- anions and where the transfer integral t_{c^*} is very weak. For the chain direction (a-axis), less pronounced signatures are observed. These results provide the first evidence for structural effects at the CO transition, indicating both charge and lattice degrees of freedom are involved in this transition.

[1] D.S. Chow *et al.*, Phys. Rev. Lett. **85**, 1698 (2000).

TT 18.2 Tue 15:30 H 2053

Realistic Parameters for the description of the two-dimensional molecular metal Θ-BEDT-TTF — •Andreas Dolfen[1], Erik Koch[1], Laura Cano-Cortes[2], and Jaime Merino[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany — [2]Departamento de Física Teórica de la Materia Condensada,

In order to study correlations in the two dimensional molecular metal Θ-$(BEDT\text{-}TTF)_2I_3$ we employ density-functional theory to calculate realistic parameters for extended Hubbard models.

We evaluate the hopping matrix elements for different angles and distances of two molecules observing a surprising sensitivity with respect to certain molecular orientations. This is because a large part of the molecular orbital is situated next to the sulphur atoms outside the molecules.

The Coulomb parameters, however, are less sensitive. We calculate the on-site as well as the longer range Coulomb repulsion including intra-molecular screening and screening due to all the other molecules (BEDT-TTF and I_3).

TT 18.3 Tue 15:45 H 2053

First principles study of the charge transfer salt κ-$(BEDT\text{-}TTF)_2Cu(CN)_3$ — •Harald O. Jeschke, Hem C. Kandpal, and Roser Valenti — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

The charge transfer salt κ-$(BEDT\text{-}TTF)_2Cu(CN)_3$ has attracted a lot of attention due to experimental evidence that it is a realization of a spin liquid: no magnetic ordering was found down to 20 mK [1]. For a good description of this behaviour, it is crucial to consider the appropriate effective model for this system. Here, we present electronic structure calculations in the frame of density functional theory (DFT) and derive an effective model with the NMTO (N-th order muffin tin orbital) downfolding method and discuss its features. Since from X-ray diffraction, the structure of κ-$(BEDT\text{-}TTF)_2Cu(CN)_3$ has been determined without hydrogen positions, we first prepare a very similar structure including hydrogen atoms and carefully relax it using the projector augmented wave method. This structure is then used for the DFT and NMTO analysis.

[1] S. Ohira, Y. Shimizu, K. Kanoda and G. Saito, J. Low Temp. Phys. **142**, 153 (2006).

TT 18.4 Tue 16:00 H 2053

Extending Grüneisen's relation on systems with two magnetic energy scales — •Andreas Brühl[1], Bernd Wolf[1], Christoph Gross[1], Wolf Assmus[1], Roser Valenti[2], Stefan Glocke[3], Andreas Klümper[3], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, D-60438 Frankfurt(M) — [2]Institut für Theoretische Physik, Universität Frankfurt, D-60438 Frankfurt(M) — [3]Theoretische Physik, Universität Wuppertal, D-42097 Wuppertal

The high-pressure phase of $(VO)_2P_2O_7$ (abbr. HP-VOPO) consists of alternating S=1/2 spin chains with exchange constants J_1 and J_2 of similar size (≈ 120 K). This gives rise to a second, well-separated energy scale in the system, the spin gap $\Delta = 32$ K. Thermal expansion measurements on HP-VOPO reveal distinct anomalies related to these two energy scales. However, the relative size of the low-temperature anomaly, corresponding to the spin gap, is very much enlarged compared to its size in the specific heat. Therefore, the commonly used Grüneisen relation, assuming a proportionality between the magnetic contributions α_{mag} and C_{mag} to thermal expansion and specific heat, does not apply. Instead, an extended form of this relation is presented, which contains an additional term in α_{mag} proportional to the derivative of the magnetic entropy with respect to the spin gap. Using accurate T-DMRG calculations of the required thermodynamic quantities, this leads to a good description of the thermal expansion of HP-VOPO in the whole temperature range. This method could be generalized to cover other spin systems with two or more exchange constants, e. g. to determine their values via thermal expansion measurements.

TT 18.5 Tue 16:15 H 2053

Electron-phonon interaction in the lamellar cobaltate Na_xCoO_2 — •Alexander Donkov[1], 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 Russian Academy of Sciences, 660036 Krasnoyarsk, Russia — [3]Institute für Mathematische und Theoretische Physik, TU Braunschweig, D-38106 Braunschweig, Germany

We study theoretically the dependence of the electron-phonon interaction in Na_xCoO_2 on the sodium concentration, x. For the two phonon modes found in Raman experiments, A_{1g} and E_{1g}, we calculate the matrix elements of the electron-phonon interaction. Analyzing the feedback effect of the conduction electrons on the phonon frequency, ω, we compare the calculated and experimentally observed doping dependence of the A_{1g} mode. Furthermore, due to the momentum dependence of the electron-phonon coupling for the E_{1g} symmetry we find no renormalization of the corresponding phonon frequency which agrees with experiment. Our results shed light on the possible importance of the electron-phonon interaction in this system.

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TT 18.6 Tue 16:30 H 2053

Effect of composition on phonon anomalies in $Na_xCoO_2 \cdot yH_2O$ — •Peter Lemmens[1,2], Dietrich Wulferding[1], Patric Scheib[1], Kwang-Yong Choi[3], Vladimir Gnezdilov[4], Fangcheng Chou[5], Chengtian Lin[2], and Bernhard Keimer[2] — [1]IPKM, TU Braunschweig — [2]MPI-FKF, Stuttgart — [3]NHMFL, Florida — [4]B.I. Verkin Inst. for Low Temp. Phys., NASU, Kharkov — [5]CMSE, MIT, Cambridge, USA

A quantitative analysis of phonon frequencies for nonsuperconducting and superconducting cobaltates $Na_xCoO_2 \cdot yH_2O$ shows pronounced phonon anomalies in the proximity of the charge ordering instabilities in $Na_{0.5}CoO_2$. Furthermore, as function of Na doping a systematic shift of a high energy out-of-plane oxygen phonon is observed in a wide doping range. The corresponding in-plane mode does not show any appreciable anomaly.

Work supported by DFG, ESF-HFM and MRSEC Program of NSF under award number DMR 02-13282.

TT 18.7 Tue 16:45 H 2053

On the metallic conductivity of the delafossites $PdCoO_2$ and $PtCoO_2$ — •Volker Eyert[1,2], Raymond Frésard[1], and Antoine Maignan[1] — [1]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, 6 Boulevard Maréchal Juin, 14050 Caen Cedex, France — [2]Center for Electronic Correlations and Magnetism, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The origin of the quasi two-dimensional behavior of $PdCoO_2$ and $PtCoO_2$ is investigated by means of electronic structure calculations. They are performed using density functional theory in the local density approximation as well as the new full-potential augmented spherical wave method. We show that the electric conductivity is carried almost exclusively by the in-plane Pd (Pt) d orbitals. In contrast, the insulating O–Co–O sandwich layers of octahedrally coordinated Co atoms may be regarded as charge carrier reservoirs. This leads to a weak coupling of the Pd (Pt) layers and causes the strong anisotropy of the electric conductivity.

15 min. break

TT 18.8 Tue 17:15 H 2053

Thermal conductivity of TiOX (X=Br,Cl) — •Nikolai Hlubek[1], Christian Hess[1], Bernd Büchner[1], Michael Sing[2], Ralph Claessen[2], Sander van Smaalen[3], and Paul van Loosdrecht[4] — [1]IFW Dresden, Germany — [2]Experimentelle Physik 4, Universität Würzburg, Germany — [3]Laboratory of Crystallography, Universität Bayreuth, Germany — [4]Zernike Institute for Advanced Materials, University of Groningen, Netherlands

We report experimental results on the thermal conductivity $\kappa(T)$ of

the compounds TiOBr and TiOCl. Below room temperature the compounds undergo two phase transitions T_{c2} and T_{c1}. Above T_{c2} the compounds should contain S=1/2 spin-chains with $J_{Cl} = 676K$ and $J_{Br} = 375K$ respectively formed by direct orbital overlap of the Ti-atoms. Below T_{c1} the chains dimerise to form a non-magnetic ground state. Our data exhibits pronounced anomalies at T_{c2} and T_{c1} confirming the transitions being of second and first order respectively. Surprisingly, $\kappa(T)$ appears to be dominated by phonon heat conduction, since we don't find indications of significant magnetic contributions. This is in contrast to the expectation of a spin chain system. In this context we discuss possible scenarios to understand the unusual behaviour of the thermal conductivity.

TT 18.9 Tue 17:30 H 2053

Competing exchange interactions in the edge-shared chain cuprates $CuCl_2$ and $CuBr_2$ — •Miriam Schmitt[1], Stefan-Ludwig Drechsler[2], and Helge Rosner[1] — [1]MPI CPfS Dresden, Nöthnitzer Strasse 40, D-01187 Dresden — [2]IFW Dresden, P.O.Box 270116, D-01171 Dresden

Low dimensional spin 1/2 chain systems show fascinating phase diagrams with many unusual magnetic ground states as spin-Peierls, spin gap or helically ordered states. These ground states are usually driven by the strong competition between the nearest and next nearest neighbor in-chain interactions. We will present a detailed study of the electronic and magnetic properties based on density functional calculation for the edge shared chain Cu^{2+} compounds $CuCl_2$ and $CuBr_2$. Starting from LDA band structure calculation we developed an effective one-band tight-binding model and mapped it subsequently to a Heisenberg model to evaluate the orbitals and main interactions relevant for the low energy properties. The combination of these results with the exchange integrals from LDA+U total energy differences of different spin configurations leads to reliable microscopic models. For $CuCl_2$ and $CuBr_2$ we find a strong frustration due to competing antiferromagnetic J_2 and ferromagnetic J_1. Unless the significant interchain coupling stabilizes a commensurate ground state we predict that both compounds exhibit a helically ordered state at low temperatures.

TT 18.10 Tue 17:45 H 2053

Electric field gradients in low dimensional cuprates - a comparative study — •Katrin Koch[1], Klaus Koepernik[1,2], and Helge Rosner[1] — [1]MPI-CPFS, Dresden — [2]IFW, Dresden

The theoretical description of strongly correlated systems is still a challenging task. A possible approach to this problem resulting in realistic electron densities is the LSDA+U method where the strong Coulomb repulsion U is treated in a mean field like approximation. Unfortunately the parameter U is not known and needs to be evaluated, i.e. in comparison of calculated properties and experimental measurements.

Here, we present calculations for the electric field gradients (V_{zz}) on the Cu^{2+} sites in strongly correlated low dimensional cuprates. By comparing the calculated V_{zz}(U) with the V_{zz} from NMR experiments for these compounds we can evaluate U. To avoid numerical ambiguity we used two different DFT-band structure schemes: FPLO and WIEN2k. The results are consistent with respect to each other: In part we find good agreement with resulting values of U from other evaluation procedures, especially for strongly distorted Cu^{2+} environment (e.g. $Cu_2P_2O_6CH_2$), though considerable deviation in direction of smaller U values for other compounds (e.g. La_2CuO_4) is obtained. Possible causes for this deviation will be discussed.

TT 18.11 Tue 18:00 H 2053

Temperature dependence of a zero bias anomaly in scanning tunnelling spectra of $Sr_4Ru_3O_{10}$ — •Bernhard Nansseu[1], Tatjana Novgorodov[1], Michael Waelsch[1], Jürgen Hager[1], Jiandi Zhang[2], R. Moore[3], Ward Plummer[3], Zhiqiang Mao[4], and Rene Matzdorf[1] — [1]Universität Kassel, Kassel, Germany — [2]Florida International University, Miami, USA — [3]Oak Ridge National Laboratory and University of Tennessee, USA — [4]Tulane University, New Orleans, USA

We have studied a zero bias anomaly in scanning tunnelling spectra of the layered ruthenate $Sr_4Ru_3O_{10}$. This material shows a dip-like feature in the dI/dV spectra, which has previously observed in the single-layer Sr_2RuO_4 and double-layer $Sr_3Ru_2O_7$ ruthenates. We have studied in particular the temperature dependence of the zero bias anomaly, which is in all three materials different. The triple-layer material shows intergrowth of single and double layers, which have been identified by their spectroscopic fingerprint. Finally, we discuss different effects as possible explanations for the zero bias anomaly.

TT 18.12 Tue 18:15 H 2053

Temperature dependence of the anomalous exponent in $Li_{0.9}Mo_6O_{17}$that reveals Luttinger Liquid behavior — Tatjana Novgorodov[1], Bernard Nansseu[1], Michael Waelsch[1], Jian He[2], Rongying Jin[2], David Mandrus[2,3], and •Rene Matzdorf[1] — [1]Universität Kassel, Kassel, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA — [3]The University of Tennessee, Knoxville, Tennessee, USA

Scanning tunnelling spectroscopy (STS) has been used to study the Luttinger-liquid behavior of the purple bronze $Li_{0.9}Mo_6O_{17}$ in the temperature range 5K¡T¡300K. In the entire temperature range the suppression of density of states at the Fermi-energy could be fitted very good by a model describing the tunneling into a Luttinger liquid at ambient temperature. The power-law exponent extracted from these fits reveals a significant increase above 200K. It changes from alpha=0.6 at low temperature to alpha=1.0 at room temperature.

TT 18.13 Tue 18:30 H 2053

Microscopic simulation and analysis of a spin crossover transition — •Harald O. Jeschke[1], L. Andrea Salguero[1], Badiur Rahaman[2], Christian Buchsbaum[3], Volodymyr Pashchenko[3], Martin U. Schmidt[3], Tanusri Saha-Dasgupta[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — [2]S.N. Bose National Centre for Basic Sciences, JD Block, Sector 3, Salt Lake City, Kolkata 700098, India — [3]Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany

In spin crossover materials, an abrupt phase transition between a low spin state and a high spin state can be driven by temperature, pressure or illumination. Of a special relevance are Fe(II) based coordination polymers where, in contrast to molecular systems, the phase transition shows a pronounced hysteresis which is desirable for technical applications. A satisfactory microscopic explanation of this large cooperative phenomenon has been sought for a long time. The lack of X-ray data has been one of the reasons for the absence of microscopic studies. In this work, we present an efficient route to prepare reliable model structures and within *ab initio* density functional theory analysis and effective model considerations we show that in polymeric spin crossover compounds magnetic exchange between high spin Fe(II) centres is as important as elastic couplings for explaining the considerable cooperativity and thus the width of the hysteresis.

TT 19: Correlated Electrons: Quantum-Critical Phenomena

Time: Tuesday 14:00–18:30 Location: H 3010

TT 19.1 Tue 14:00 H 3010

Non-Fermi liquid metal without quantum criticality — •Christian Pfleiderer[1], Peter Böni[1], Thomas Keller[2,3], Ulrich Rössler[4], and Achim Rosch[5] — [1]Physik-Department E21, Technische Universität München, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, D-85748 Garching, Germany — [4]Leibniz-Institut für Festkörper-und Werkstoffforschung (IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [5]Institute of Theoretical Physics, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

A key question in condensed matter physics concerns whether pure three-dimensional metals can always be described as Fermi liquids. Using neutron Larmor diffraction to overcome the traditional resolution limit of diffraction experiments, we studied the lattice constants of the cubic itinerant-electron magnet manganese silicide (MnSi) at low temperatures and high pressures [1]. We were able to resolve the

nature of the phase diagram of MnSi and to establish that a stable, extended non-Fermi liquid state emerges under applied pressure without quantum criticality. This suggests that new forms of quantum order may be expected even far from quantum phase transitions. [1] C. Pfleiderer, et al., Science **316**, 1871 (2007).

TT 19.2 Tue 14:15 H 3010

Universal ratios of the phase diagram of Pomeranchuk instability: application to $Sr_3Ru_2O_7$ — •HIROYUKI YAMASE — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

We analyze a pure forward scattering model, which exhibits spontaneous d-wave type Fermi surface deformations, the so-called Pomeranchuk instability. The phase diagram is known to be determined by a single energy scale in the weak-coupling limit, and thus dimensionless ratios of different characteristic quantities are universal[1]. We extend such a weak-coupling analysis to the presence of a magnetic field, which is a minimal model for $Sr_3Ru_2O_7$, and compare obtained universal ratios with those provided by experiments[2].

[1] H. Yamase, V. Oganesyan, and W. Metzner, Phys. Rev. B **72**, 035114 (2005).

[2] H. Yamase, Phys. Rev. B **76**, 155117 (2007).

TT 19.3 Tue 14:30 H 3010

Instability of the Quantum-Critical Point of a 2D Weakly Ferromagnetic Fermi Liquid. — •DMITRI EFREMOV[1], JOSEPH BETOURAS[2], and ANDREY CHUBUKOV[3] — [1]TU Dresden — [2]University of St Andrews — [3]University of Wisconsin

We report the study of the stability of a 2D weakly ferromagnetic fermi liquid near to the quantum critical point in the Eliashberg approach. We find that correlations associated with the Landau damping generate a universal negative, nonanalytic $q^{3/2}$ contribution to the static magnetic longitudinal susceptibility $\chi_{zz}(q,0)$ and to the transverse susceptibility $\chi_\perp(q,0)$. It leads towards either incommensurate ordering or first order phase transition. The instability manifests itself also in the free energy. The correlations associated with the Landau damping generate nonanalytic terms in the free energy expansion.

TT 19.4 Tue 14:45 H 3010

Low Temperature Investigations of $YbRh_2Si_2$ doped with Ir and Co — •TANJA WESTERKAMP[1], PHILIPP GEGENWART[2], CORNELIUS KRELLNER[1], CHRISTOPH GEIBEL[1], and FRANK STEGLICH[1] — [1]Max-PIanck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]1. Physikalisches Institut, Georg-August-Universität, Göttingen, Germany

The tetragonal heavy fermion system $YbRh_2Si_2$ shows interesting properties due to its vicinity to an antiferromagnetic quantum critical point (QCP). At zero magnetic field the system becomes antiferromagnetic below $T_N = 70\,\mathrm{mK}$. The system can be tuned through a field-induced QCP at $B_c = 0.05\,\mathrm{T}$ into a Landau-Fermi liquid (LFL) state at $B > B_c$. This state is restricted to temperatures below a scale $T_{LFL}(B)$. Recently, an additional energy scale $T^*(B)$ was found that vanishes at the QCP and was related to the disintegration of the heavy quasiparticles.

We studied the effect of chemical pressure on the phase diagram, using high quality $Yb(Rh_{1-x}M_x)_2Si_2$ single crystals with M = Ir, Co. Here, we present recent results focusing on measurements of the magnetic susceptibility.

TT 19.5 Tue 15:00 H 3010

Anomalous critical behavior at the antiferromagnetic phase transition of $YbRh_2Si_2$ — •CORNELIUS KRELLNER[1], STEFANIE HARTMANN[1], ADAM PIKUL[1], NIELS OESCHLER[1], CHRISTOPH GEIBEL[1], JOCHEN WOSNITZA[2], and FRANK STEGLICH[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]HLD, Forschungszentrum Dresden-Rossendorf, Dresden, Germany

Quantum phase transitions are one of the important topics in the understanding of condensed matter. These transitions are driven by quantum fluctuations in contrast to classical phase transitions which are accompanied by thermal fluctuations. Recently, the heavy-fermion system $YbRh_2Si_2$ was intensively studied, because it is a clean and stoichiometric metal situated on the magnetic side ($T_N = 72$ mK), but very close to a quantum critical point, which can be crossed by applying a tiny magnetic field. Therefore, this system presents both an antiferromagnetic phase transition driven by thermal fluctuations as well as pronounced quantum fluctuations due to the vicinity to the quantum phase transition. In this contribution, we show accurate measurements of the specific heat C around T_N on a single crystal of highest quality (RRR $\sim$ 150). We observe a very sharp peak at T_N with absolute values as high as $C/T = 8\,\mathrm{J/mol\,K^2}$. A detailed analysis of the critical exponent α around T_N reveals $\alpha = 0.37$ which differs significantly from those of the conventional universality classes in the Landau theory $\alpha < 0.11$. We will discuss in detail the analysis and possible mechanisms.

15 min. break

TT 19.6 Tue 15:30 H 3010

Magnetization study of stoichiometric and slightly Ir- Co-doped $YbRh_2Si_2$ — •MANUEL BRANDO[1], LUIS PEDRERO[1], CORNELIUS KRELLNER[1], PHILIPP GEGENWART[2], CHRISTOPH GEIBEL[1], and FRANK STEGLICH[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Georg-August Universität Göttingen, 37077 Göttingen, Germany

Recent results on the heavy fermion compound $YbRh_2Si_2$ point to the presence of multiple vanishing energy scales, $T_N(H)$, $T_{LFL}(H)$ and $T^*(H)$, at the magnetic-field-driven quantum critical point (QCP) [1]. These scales can directly be observed in thermodynamic, transport and magnetic measurements, among them the dc-magnetization M versus the magnetic field H. More precisely, M shows a kink at $T_N(H)$ and a distinct crossover feature at $T^*(H)$ which smears out with increasing temperature.

Slight doping with isoelectronic Co as well as with Ir on the Rh site leads to a volume change, which tunes the strength of the magnetic interaction; this shifts the $T_N(H)$ line in the $T-H$ phase diagram without introducing much disorder in the single crystals. However, little is known about the behavior of the $T^*(H)$ line in the doped compounds.

We present a systematic analysis of different isothermal M vs. H curves for the stoichiometric, Co- (7%) and Ir-doped (6%) samples down to 50 mK to observe whether the two energy scales are still approaching zero at the same point in the doped compounds.

[1] P. Gegenwart *et. al., Science* ***315****, 5814 (2007).*

TT 19.7 Tue 15:45 H 3010

Thermopower investigations of $YbRh_2Si_2$ in the vicinity of an antiferromagnetic quantum critical point — •STEFANIE HARTMANN, NIELS OESCHLER, CORNELIUS KRELLNER, CHRISTOPH GEIBEL, and FRANK STEGLICH — Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The stoichiometric heavy-fermion compound $YbRh_2Si_2$ exhibits an antiferromagnetic (AFM) phase transition at an extremely low temperature of $T_N = 72$ mK. Upon applying a tiny magnetic field the AFM ordering is suppressed and the system is driven towards a quantum critical point (QCP). Furthermore, an additional energy scale at T^* indicating the crossover from local to itinerant character of the $4f$ electron vanishes at the QCP. Here, we report on measurements of the thermoelectric power S of high quality single crystals from 6 K down to 50 mK in fields up to 2 T. $S(T)$ was measured within the easy ab plane of the system, that exhibits a critical field of only 50 mT. In the critical region S/T diverges upon approaching the QCP, while it exhibits a constant value in the Fermi liquid regime at higher fields. The low temperature behavior of the thermopower in $YbRh_2Si_2$ is discussed in detail and compared to available theoretical predictions. Whether the T^* line observed in Hall effect and magnetostriction measurements can also be resolved in the thermopower is a matter of great interest.

TT 19.8 Tue 16:00 H 3010

Low temperature electric transport of $Yb(M_xRh_{1-x})_2Si_2$ M=Co,Ir — •SVEN FRIEDEMANN, NIELS OESCHLER, CORNELIUS KRELLNER, CHRISTOPH GEIBEL, and FRANK STEGLICH — Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany

The heavy-fermion metal $YbRh_2Si_2$ exhibits pronounced non-Fermi liquid behavior due to its vicinity to a quantum critical point (QCP). By applying small magnetic fields, $YbRh_2Si_2$ is driven from an antiferromagnetic (AFM) state to the QCP. At the critical field a second energy scale $T^\star$ vanishes that manifests itself as a crossover in transport and thermodynamic properties, e.g. magnetoresistance. Doping Co (Ir) on the Rh side acts as chemical pressure enhancing (decreasing) the AFM ordering temperature and the critical field of the ordered phase. We here report low temperature resistivity and magnetoresis-

tance measurements on $x = 3,7\%$ Co and $x = 6\%$ Ir doped single crystals. The data are compared with that of the undoped system. Although the ordering temperature is observed to change as expected we find the features associated with $T^\star$ to be robust upon doping.

TT 19.9 Tue 16:15 H 3010

Thermal expansion and magnetostriction measurements on a $CeCu_{5.85}Au_{0.15}$ single crystal — •Stefanie Drobnik[1,2], Kai Grube[1], Roland Schäfer[1], Frédéric Hardy[1], Christoph Meingast[1], Oliver Stockert[3], and Hilbert von Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]MPI für chemische Physik fester Stoffe, 01187 Dresdenm, Germany

A well-studied magnetic quantum critical point (QCP) exists at the onset of antiferromagnetic order in the heavy-fermion system $CeCu_{6-x}Au_x$ with a critical gold concentration of $x_c \approx 0.1$. Due to the instability at the QCP the entropy S shows at finite temperatures a maximum as a function of x, volume, or pressure p. The maximum leads to a sign change of the thermal expansion coefficient, $\alpha = -(1/V)(\partial S/\partial p)$, and of the Grüneisen parameter Γ, the ratio of α and specific heat. This feature and the divergence of Γ at $T \to 0$ are important thermodynamic probes to detect and classify QCPs. We report low-temperature thermal expansion and magnetostriction measurements on a $CeCu_{5.85}Au_{0.15}$ single crystal with a Néel temperature of $T_N \approx 90\,\mathrm{mK}$. The thermal expansion was measured along all orthorhombic axes in a temperature range of $30\,\mathrm{mK} < T < 10\,\mathrm{K}$ in magnetic fields parallel to the c axis of up to 3 T. The results are compared with theoretical predictions and measurements on other heavy-fermion compounds close to a QCP.

TT 19.10 Tue 16:30 H 3010

Breakdown of a valence bond solid in a Heisenberg model with four-spin interaction on honeycomb layers — •Thomas C. Lang[1,2], Anders W. Sandvik[2], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany — [2]Department of Physics, Boston University, Boston, MA 02115, USA

We investigate the scenario of the breakdown of a valence bond solid (VBS) in an $S = 1/2$ quantum antiferromagnet with non-frustrating four-spin interaction on the single and bilayer hexagonal lattice. By means of quantum Monte Carlo in the valence bond basis we find a strong first-order VBS-Néel phase transition in the single layer. In the bilayer the Néel regime separates the VBS and a disordered (zero tilted) phase by a continuous quantum phase transition. A quantum critical point marking a direct VBS-VBS or VBS-disorder transition is absent. This behavior is attributed to the lattice symmetry which allows rigid valence bond configurations to survive while spin-fluctuations are enhanced.

15 min. break

TT 19.11 Tue 17:00 H 3010

Quantum Critical Spin Dynamics of a Cu(II) S=1/2 antiferromagnetic Heisenberg chain studied by ^{13}C-NMR spectroscopy — •H. Kühne[1], H.-H. Klauss[1], J. Litterst[2], S. Grossjohann[3], W. Brenig[3], A.P. Reyes[4], P.L. Kuhns[4], C.P. Landee[5], M.M. Turnbull[5], H.-J. Grafe[6], B. Büchner[6], and J. Haase[6] — [1]Institut für Festkörperphysik, TU Dresden — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig — [3]Institut für Theoretische Physik, TU Braunschweig — [4]NHMFL, FSU, Tallahassee, USA — [5]DPC, Clark University, Worcester, USA — [6]Leibniz-Institut für Werkstoffforschung, Dresden

The antiferromagnetic S=1/2 Heisenberg chain (S=1/2 AFHC) is a model system for quantum many-body physics. It allows a direct comparison between exact theoretical results and experiment for ground state properties and excitations. $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN) is a very good experimental realization of the unperturbed S=1/2 AFHC [1,2]. In this compound we study the low energy spin dynamics by means of NMR. We measured the nuclear spin-lattice relaxation rate T_1^{-1} of ^{13}C as a function of temperature in a wide external magnetic field range from 2T to 28T, with an emphasis on the vicinity of the quantum critical point (QCP) at 14T. The experimental data are in good agreement with Quantum Monte Carlo calculations and clearly show critical behavior at low temperatures, i.e. a divergence of T_1^{-1} at 14T and the linear opening of an energy gap for magnetic excitations with higher external fields. [1] P. Hammar et al., PRB. 59, 1008 (1999). [2] M.B. Stone et al., PRL 91, 037205 (2003).

TT 19.12 Tue 17:15 H 3010

Quantum Critical Dynamics of the S=1/2 AFM Heisenberg Chain in Finite Magnetic Fields: a QMC Study — •Simon Grossjohann[1], Wolfram Brenig[1], Hannes Kühne[2], and Hans-Henning Klauss[2] — [1]Institut für Theoretische Physik, TU Braunschweig — [2]Institut für Festkörperphysik, TU Dresden

We investigate the field driven quantum critical dynamics of the antiferromagnetic S=1/2 Heisenberg chain using Quantum Monte-Carlo techniques (SSE) and analytic continuation by Maximum Entropy methods. Results for the transverse and longitudinal dynamical structure factor $S_{\alpha\beta}(q,\omega)$ will be presented for different temperatures T, with $0.1 \leq T/J \leq 1$ and various magnetic fields below and above saturation field h_c. In the vicinity of h_c, condensation of the elementary excitations of the fully polarized phase induce a diverging longitudinal NMR relaxation rate $1/T_1$. Such quantum critical slowing down has been observed in recent experiments on $Cu(C_4H_4N_2)(NO_3)_2$ and agrees very well with our theoretical findings. In addition our spectra will be shown to be consistent with sum rules for the static structure factor and static susceptibility.

TT 19.13 Tue 17:30 H 3010

Dynamical Scaling Properties of a Doped Quantum Heisenberg Antiferromagnet in Two Dimensions — •Marcello Silva Neto, Juergen Falb, and Alejandro Muramatsu — Institut für Theoretische Physik III, Pfaffenwaldring 57, 70550, Stuttgart, Germany

We study the dynamical scaling properties of an effective quantum field theory for the magnetic degrees of freedom of the $t-t'-t''-J$ model, which is believed to be the relevant model for the physics of cuprate superconductors. We find that, at the lowest doping, where the Fermi surface for the doped holes is composed of very small hole pockets at special points in the magnetic Brillouin zone, damping due to the scattering of magnons from particle-hole excitations is *absent* and the dynamical critical exponent is $z = 1$. As doping increases, however, a nonzero damping term is present. In this case, we find that: i) for the case of Landau damping (clean limit), such term does not modify the dynamical exponent which remains at $z = 1$ for a large portion of the phase diagram, in agreement with experiments; ii) for the case of diffusive damping (dirty limit), such term changes the dynamical exponent from $z = 1$ to $1 < z \leq 2$, and for even larger doping a crossover to a Fermi liquid regime is expected. We compare our findings to previous discussions available in the literature and we discuss the relevance of our results to the physics of high-Tc superconductors.

TT 19.14 Tue 17:45 H 3010

Critical Properties of an Effective Field Theory for 2D Doped Antiferromagnets — •Juergen Falb, Marcello Silva Neto, and Alejandro Muramatsu — Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550, Stuttgart, Deutschland

Starting from the $t - t' - t'' - J$ model for high-Tc cuprate superconductors we derive an anisotropic and gauge massive CP^1 effective field theory that describes the low energy magnetic properties at low doping, establishing a link between doped antiferromagnets on a bipartite lattice and frustrated quantum antiferromagnets [1]. We first discuss the generation of mass for the gauge field introduced by doping, and comment on the possible incommensurate phases associated to it. The massive gauge field opens the possibility of deconfined spinons in the symmetric phase. We find a region of stability for the microscopic parameters J, t' and t'' where the theory is valid. Through a renormalization group study of the theory in weak coupling we obtain its phase diagram. The connection between our results and previous works on the literature are also discussed.

[1] J. Falb and A. Muramatsu, arXiv:0705.1918, accepted for publication in Nucl. Phys. B.

TT 19.15 Tue 18:00 H 3010

Probing field-induced quantum criticality in molecule-based low-dimensional spin systems — •Bernd Wolf[1], Yeekin Tsui[1], Ulrich Tutsch[1], Katarina Removic-Langer[1], Andrej Prokofiev[1], Wolf Assmus[1], Roser Valenti[2], Stefan Wessel[3], Andreas Honecker[4], Matthias Wagner[5], and Michael Lang[1] — [1]Physikalisches Institut, JWG-Universität Frankfurt; SFB/TRR49 — [2]Institut für Theoretische Physik, JWG-Universität Frankfurt; SFB/TRR49 — [3]Institut für Theoretische Physik, Univer-

sität Stuttgart — [4]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [5]Institut für Anorganische und Analytische Chemie JWG-Universität Frankfurt; SFB/TRR49

A quantum critical point (QCP) is found in systems where a phase transition at T = 0 is driven by an external control parameter. Although a QCP takes place at T = 0, inaccessible by experiment, it has a significant influence on the physical properties over a wide range of temperature. Here we concentrate on field-induced QCPs in low-dimensional molecule-based spin systems. The molecular approach enables us to generate materials with magnetic exchange coupling constants weak enough for laboratory fields to drive the system into a new ground state. We present data of the magnetocaloric effect across the saturation field of an antiferromagnetic S = 1/2 Heisenberg chain system. These results compare favourably with theoretical predictions. In additon, we report thermodynamic measurements on the field-induced magnetic transition in coupled S = 1/2 dimer systems.

TT 19.16 Tue 18:15 H 3010

Quantum critical scaling behavior of deconfined spinons — •Flavio Nogueira[1], Steinar Kragset[2], and Asle Sudbo[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin — [2]Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway

We perform a renormalization group analysis of some important effective field theoretic models for deconfined spinons. We show that deconfined spinons are critical for an isotropic SU(N) Heisenberg antiferromagnet, if N is large enough. We argue that nonperturbatively this result should persist down to $N = 2$ and provide further evidence for the so called deconfined quantum criticality scenario. Deconfined spinons are also shown to be critical for the case describing a transition between quantum spin nematic and dimerized phases. On the other hand, the deconfined quantum criticality scenario is shown to fail for a class of easy-plane models. For the cases where deconfined quantum criticality occurs, we calculate the critical exponent η for the decay of the two-spin correlation function to first-order in $\epsilon = 4 - d$.

TT 20: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 1

Time: Tuesday 14:00–15:30 Location: EB 202

Invited Talk TT 20.1 Tue 14:00 EB 202

Adiabatic pumping in nanostructures — •Michele Governale — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

A DC current can be driven through a mesoscopic conductor in the absence of an applied transport voltage by changing periodically in time some of the properties of the conductor. This transport mechanism is known as pumping. If the time-dependent parameters vary slowly as compared to the characteristic internal time scales of the system, pumping is adiabatic, and the average transmitted charge per cycle depends only on the area of the cycle but not on its detailed timing.

In this talk we present the main theoretical concepts in the field and describe some recent developments, such as pumping trough interacting systems [1,2] and in hybrid superconducting-normal structures [3].

[1] J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. Lett. **95**, 246803 (2005).

[2] J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. B **74**, 085305 (2006).

[3] M. Governale, F. Taddei, R. Fazio, and F. W. J. Hekking, Phys. Rev. Lett. **95**, 256801 (2005).

TT 20.2 Tue 14:30 EB 202

Cooper pair pumping in presence of dissipation — •Valentina Brosco[1], Alexander Shnirman[1,2], Rosario Fazio[3,4], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, Karlsruhe, Germany — [2]Institut für Theoretische Physik, Universität Innsbruck, Innsbruck, Austria — [3]International School for Advanced Studies (SISSA), Trieste, Italy — [4]NEST-CNR-INFM and Scuola Normale Superiore, Pisa, Italy

In a Cooper pair pump charge transport is obtained via an adiabatic and periodic manipulation of Josephson couplings or gate voltages and it is a coherent process. Several works investigated the connection between Cooper pair pumping and the geometric and topological properties of the pumping cycle in the parameters space [1]. Recently the predicted relation between Berry's phase and pumped charge was demonstrated experimentally [2]. In the present work we analyze the effects of noise on Cooper pair pumping and we show that dissipation may induce a new geometric contribution in the transferred charge. We show that this contribution can be experimentally distinguished both from the usual pumped charge and from the supercurrent contribution and we propose an experiment where the theory can be probed.

[1] M. Aunola and J. J. Toppari, Phys. Rev. B **68**, 020502 (2003); V. Brosco, R. Fazio, F. W. J. Hekking, and A. Joye, cond-mat/0702333.
[3] M.Mottonen, J. J. Vartiainen, and J. P. Pekola, cond-mat/0710.5623.

TT 20.3 Tue 14:45 EB 202

Adiabatic pumping in a quantum dot-Aharonov-Bohm interferometer — •Bastian Hiltscher, Michele Governale, and Jürgen König — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We study adiabatic pumping in Aharonov-Bohm interferometers, where a quantum dot is embedded in one or in both arms. Charge pumping occurs if two parameters are changed periodically in time. The limit of small frequencies defines the adiabatic regime.
For our calculations we use a real-time diagrammatic technique and combine the properties of AB interferometers [1] with the properties of adiabatic pumping [2] for dots with strong Coulomb interaction. By performing a perturbation expansion in the pumping frequency and in the tunnel-coupling strength we calculate the magnetic-flux dependence of the pumped charge and compare it with the results for rectification of an AC voltage, which may yield an effective DC current as well.
We get information about the character of adiabatic pumping, which could be interpreted as peristaltic, but phase-coherent. Furthermore we find, that adiabatic pumping and rectification show different symmetries and, thereby, are distinguishable.

[1]J. König and 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 20.4 Tue 15:00 EB 202

Non-local Andreev reflection in quantum dots — •David Futterer, Michele Governale, and Jürgen König — Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany

We consider a single-level quantum dot attached to one superconducting and two ferromagnetic leads. The transport through this system is influenced by the interplay of proximity effect, spin accumulation, Coulomb interaction and non-equilibrium due to finite bias voltage.

We employ a real-time diagrammatic technique that accounts for coupling both to ferromagnetic[1] and superconducting[2] leads. We perform a systematic expansion in the tunnel-couplings to the leads. In the limit of large superconducting gap, all orders in the tunnel-coupling strength with the superconductor can be resummed. We calculate the transport properties of the system and identify schemes for detection of non-local Andreev reflection.

[1] M. Braun, J. König, and J. Martinek, Phys. Rev. B **70**, 195345 (2004)

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

TT 20.5 Tue 15:15 EB 202

Cross-Correlations in transport through two parallel quantum dots — •Sebastian Haupt[1,2], Jasmin Aghassi[1], Matthias Hettler[2], and Gerd Schön[1,2] — [1]Institut für theoretische Festkörperphysik, Universität Karlsruhe, 76218 Karlsruhe — [2]Forschungszentrum Karlsruhe, INT, Postfach 3640, 76201 Karlsruhe

We study cross-correlations of currents through two parallel quantum dots coupled to four independent electrodes. The quantum dots are coupled by intra-dot Coulomb interactions but tunneling between the

dots is forbidden. The transport is calculated within second-order pertubation expansion in the coupling Γ to the electrodes within a diagrammatic technique. We allow for an intermediate coupling regime up to coupling constants of $\Gamma \sim k_B T$ (where k_b is the Boltzmann constant and the temperature is T). The level energy of the two quantum dots can be independently controlled via gate voltages. [1,2] The cross-correlations show different signs depending on the relation of transport process through the dots. For higher temperatures, the regions of equal sign have a spherical shape, whereas at lower temperature, an anglular "L-shape" is observed. This can be explained by the analysis of the relevant transport processes.

[1] D.T. McClure *et al.*, Phys. Rev. Lett. **98**, 056801 (2007)
[2] J. Aghassi *et al.*, Appl. Phys. Lett. **89**, 052101 (2006), Phys. Rev.B **73**, 195323 (2006)

TT 21: Transport: Graphene and Carbon Nanotubes

Time: Tuesday 15:45–19:00 Location: EB 202

TT 21.1 Tue 15:45 EB 202

Electromagnetic response of graphene. — •Sergey Mikhailov and Klaus Ziegler — Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

Recently discovered new carbon based material - graphene - demonstrates a number of interesting and unusual transport and optical properties. Our recent predictions of a new transverse electromagnetic mode in graphene [1] and of its strongly non-linear electromagnetic behavior [2] shows that this material can be used in terahertz electronics for higher-harmonics generation at microwave and terahertz frequencies. In this work we study the influence of the self-consistent field effects, the radiative decay and the scattering on the non-linear electromagnetic response of graphene, and find the optimal experimental conditions, under which the higher harmonics generation effect can be observed in this material.

[1] S. A. Mikhailov, K. Ziegler, Phys. Rev. Lett. 99, 016803 (2007).
[2] S. A. Mikhailov, Europhys. Lett. 79, 27002 (2007).

TT 21.2 Tue 16:00 EB 202

Diffusion and localization in carbon nanotubes and graphene ribbons — •Norbert Nemec[1], Klaus Richter[1], and Gianaurelio Cuniberti[2] — [1]Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Institute for Material Science, TU Dresden, 01062 Dresden

We study transport length scales in carbon nanotubes and graphene ribbons under the influence of Anderson disorder. We present generalized analytical expressions for the density of states, the elastic mean free path and the localization length in arbitrarily structured quantum wires. These allow us to analyze the electrical response near the van Hove singularities and in particular around the edge state in graphene nanoribbons. Comparing with the results of numerical simulations, we demonstrate that both the diffusive and the localized regime are well represented by the analytical approximations over a wide range of the energy spectrum. In graphene nanoribbons, we find that the zigzag edge state causes a strong reduction of the localization length in a wide energy range around the Fermi energy.

TT 21.3 Tue 16:15 EB 202

Aharonov-Bohm effect and broken valley-degeneracy in graphene rings — •Patrik Recher[1,2], Björn Trauzettel[3], Adam Rycerz[4], Yaroslav Blanter[2], Carlo Beenakker[1], and Alberto Morpurgo[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [4]Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland

We analyze theoretically the electronic properties of Aharonov-Bohm rings made of graphene. We show that the combined effect of the ring confinement and applied magnetic flux offers a controllable way to lift the orbital degeneracy originating from the two valleys, even in the absence of intervalley scattering. The phenomenon has observable consequences on the persistent current circulating around the closed graphene ring, as well as on the ring conductance. We explicitly confirm this prediction analytically for a circular ring with a smooth boundary modelled by a space-dependent mass term in the Dirac equation. This model describes rings with zero or weak intervalley scattering. We compare our analytical model to another type of ring with strong intervalley scattering. For the latter case, we study a ring of hexagonal form with lattice-terminated zigzag edges numerically. We find for the hexagonal ring that the orbital degeneracy can still be controlled via the flux, similar to the ring with the mass confinement.

TT 21.4 Tue 16:30 EB 202

Quantum transport in graphene-based nanosystems — •Jürgen Wurm[1,2], Michael Wimmer[1], Inanc Adagideli[1], Harold Baranger[2], and Klaus Richter[1] — [1]Institut für theoretische Physik, Universität Regensburg, 93040 Regensburg — [2]Department of Physics, Duke University, Durham, NC 27708, USA

We numerically investigate the ballistic transport properties of graphene rings and other graphene-based nanostructures using a recursive Green function algorithm to calculate the conductance. Recently, the first transport experiments in ring systems made of graphene have been reported, and Aharonov-Bohm oscillations in the conductance were observed [1]. While our simulations confirm the Aharonov-Bohm oscillations in rings, as well as other quantum interference phenomena such as weak localization and universal conductance fluctuations in chaotic cavities, we also find effects of conductance suppression that are not present in usual two-dimensional electron gases.

[1] S. Russo, J.B. Oostinga, D. Wehenkel, H.B. Heersche, S.S. Sobhani, L.M.K. Vandersypen, A.F. Morpurgo, cond-mat 0711.1508 (2007)

TT 21.5 Tue 16:45 EB 202

Conductance and mobility of charge carriers in graphene on silicon carbide — •Johannes Jobst[1], Sergey Reshanov[1], Daniel Waldmann[1], Heiko B. Weber[1], Konstantin V. Emtsev[2], and Thomas Seyller[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, 91058 Erlangen, Germany — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany

We have studied the electronic transport properties of few-layer graphene grown by thermal treatment of 6H silicon carbide. Both graphene grown on the carbon face and on the silicon face were investigated. The transport properties of large area films were characterized in van der Pauw geometry. Mobilities up to $7000\,\mathrm{cm}^2/\mathrm{Vs}$ were observed. In addition, micrometer-sized Hall bar structures were fabricated, which allowed for the determination of Hall mobility and density of charge carriers. The size of these structures was reduced to atomically flat terraces of the silicon carbide surface. However, opposite to our expectations, Hall mobilities determined in these structures did not exceed values of $1000\,\mathrm{cm}^2/\mathrm{Vs}$. The role of surface contamination is discussed.

TT 21.6 Tue 17:00 EB 202

Photocurrent and radiation induced suppression of transport in graphene — Konstantin Efetov[1,2], Mikhail Fistul[1], and •Sergey Syzranov[1] — [1]Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia

We study the ballistic transport in graphene subject to the coordinate dependent potential $U(x)$ and irradiated by monochromatic electromagnetic field (EF). The resonant interaction of quasi-particles with an external radiation opens *dynamical gaps* in their spectrum, resulting in a strong modification of current-voltage characteristics of graphene junctions. The gaps' values are proportional to the amplitude of EF. We obtain that the quasi-particle transmission in diverse junctions, e.g. unipolar (p-p or n-n) junctions, is determined by the tunneling through the gap, and can be fully suppressed for large enough radiation powers. In the case of a p-n junction, as the height of the potential $U(x)$ is larger than the photon energy, the directed current (*photocurrent*) flows through the junction without any dc bias voltage applied. Such a photocurrent arises as a result of inelastic quasiparti-

cles' tunneling assisted by one- or two-photon absorption. We calculate current-voltage characteristics of diverse graphene based junctions and estimate their parameters necessary for the experimental observation of the photocurrent and transmission suppression.

15 min. break

TT 21.7 Tue 17:30 EB 202

Spin injection with rough graphene nanoribbons — •Michael Wimmer[1], Inanç Adagideli[1], Savaş Berber[2], David Tománek[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040, Germany — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824-2320, USA

We investigate spin conductance in zigzag graphene nanoribbons and propose a spin injection method based only on graphene. Combining density functional theory with tight-binding transport calculations, we find that nanoribbons with asymmetrically shaped edges show a non-zero spin conductance and can be used for spin injection. Furthermore, nanoribbons with rough edges exhibit mesoscopic spin conductance fluctuations with a universal value of $\mathrm{rms}\, G_\mathrm{s} \approx 0.4e/4\pi$.

[1] M. Wimmer, I. Adagideli, S. Berber, D. Tomanek, K. Richter, arXiv:0709.3244 (2007)

TT 21.8 Tue 17:45 EB 202

Long-range spin interaction between Quantum dots in a Graphene nanoribbon — •Matthias Braun and Guido Burkard — Institut für Theoretische Physik C, RWTH-Aachen, Germany

Recently it was proposed to realize spin qubits in graphene ribbons with semiconducting armchair boundaries [1]. The band gap arising in ribbons does avoid the Klein tunneling i.e., enable a confinement of electrons. Since the band gap is significantly smaller than in conventional semiconductors, RKKY is not necessarily the dominant spin-spin interaction between the qubits. Indeed, we show that a superexchange mechanism can lead to a tunable long-range spin-spin interaction. We model the system by two Anderson impurities coupled by a common lead. We remove all first and second order tunneling processes by a two-stage Schrieffer-Wolff transformation, and integrate out the lead degrees of freedom. At the end we arrive at an effective fourth order spin Hamiltonian. We can identify different kinds of interactions such as RKKY or superexchange. Which interaction dominates the spin dynamics depends on system parameters. We are particularly interested in the superexchange process as this spin interaction can not only couple adjacent quantum dots but also next-to-nearest neighbors.

[1] Nature Phys. **3**, 192 (2007).

TT 21.9 Tue 18:00 EB 202

Orthogonality catastrophe and Kondo effect in graphene — •Martina Hentschel[1] and Francisco Guinea[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain

We analyze Anderson's orthogonality catastrophe in graphene, at energies close to the Dirac point. It is shown that in the clean system, the orthogonality catastrophe is suppressed due to the vanishing density of states at the Dirac point. In the presence of preexisting localized states at the Dirac energy, the orthogonality catastrophe shows features similar to those found in normal metals with a finite density of states at the Fermi level [1]. We argue that, therefore, also the presence or absence of edge states is crucial for the behavior of the system. The implications for the Kondo effect induced by magnetic impurities, and for the Fermi edge singularities in tunneling processes, are also discussed.

[1] M. Hentschel and F. Guinea, Phys. Rev. B **76**, 115407 (2007).

TT 21.10 Tue 18:15 EB 202

Scrutinizing the conductance and noise of ac driven carbon-based nanostructures — •Luis Foa Torres and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany.

Time-dependent excitations provide an opportunity to achieve control through selective excitations, opening an avenue for both fundamental research and practical applications. Due to their outstanding electrical properties, carbon-based nanostructures offer an ideal playground to study such phenomena in low dimensions. Here we focus on the effects of ac driving on the conductance and the shot noise of single walled carbon nanotubes and graphene nanoribbons. Our calculations, which are based on Floquet theory and take into account the full electron dynamics, are aimed to bridge the gap between theory and recent experiments carried out in the Fabry-Perot regime. Numerical results are complemented by analytical calculations based on a simplified model. The effects of decoherence are further explored by using a phenomenological model.

TT 21.11 Tue 18:30 EB 202

Optoelectronic Measurements on Hybrid Systems made out of Carbon Nanotubes (CNTs) and the Photosystem I (PS I) — •Simone Lingitz[1], Markus Mangold[1], Itai Carmeli[2], Ludmila Frolov[2], Chanoch Carmeli[2], Shachal Richter[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut, TUM, Garching, Deutschland — [2]Center for NanoScience, Tel Aviv University, Israel

We examine the Photosystem I (PS I) covalently bound to carbon nanotubes (CNTs) by optoelectronic transport spectroscopy [1]. The PS I is a protein complex located in the thylacoid membrane of plants, algae and cyanobacteria which mediates the light-induced electron transfer in the photosynthetic pathway. As a nano-sized, high-efficient bioenergetic unit, the photosynthetic reaction centre is a promising candidate for applications in molecular nano-optoelectronics. In order to electrically contact the photoactive proteins, a cysteine mutant is generated at one end of the PS I by genetic engineering and to this reactive group the CNTs are covalently bound via chemical self-assembly using carbodiimide chemistry. Due to this combination of an energy transformation and a transport unit, this hybrid nanosystem provides an ideal basis for optoelectronic applications. In my talk, I will present wavelength and power dependent photoresponse measurements on such a CNT-PS I heterostructure in comparison to a pure CNT device. [1] S. Lingitz, M. Mangold, et al. in preparation (2008).

TT 21.12 Tue 18:45 EB 202

Supercurrent through carbon nanotubes with Nb contacts — •Emiliano Pallecchi, Markus Gaass, and Christoph Strunk — University of Regensburg, Germany

We report on low temperature transport measurements on a multi-wall carbon nanotube (MWNT) coupled to niobium leads. We used a very careful filtering scheme which is essential in order to measure small supercurrents. To provide damping at the plasma frequency, we used on chip resistors and capacitors. Depending on the gate voltages the sample shows both, proximity induced supercurrent and Coulomb blockade. The supercurrent showed narrow resonances corresponding to the Coulomb resonances at lower transmission. We found supercurrents up to 30nA, which is, to our knowledge, this is the highest value observed so far. At very low temperature the IV characteristics are characterized by hysteretic switching; when increasing T the hysteresis is gradually suppressed. In the hysteretic regime, we have also measured switching histograms to gain further information on the switching mechanism.

TT 22: Transport: Poster Session

Time: Wednesday 14:00–18:00 Location: Poster B

TT 22.1 Wed 14:00 Poster B

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. This is not only because of the potential application to quantum-computing but also due to the advent of new experiments specifically looking into 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. To this end we numerically solve a quantum master equation (QME) for the many-body density matrix describing the state of the quantum dot system. This allows us to access the time-resolved occupation and the currents flowing through the system. As a first application we show for the non-interacting resonant level model a comparison of our results with non-equilibrium Green function calculations [1]. Furthermore, we revisit a recent experiment [2] with double quantum dots and analyse it by means of the QME. For this purpose we focus on the number of pulse-induced tunneling electrons as a function of pulse length. In addition to numerical results we propose a simple analytical model which allows for the interpretation of the characteristic features observed.

[1] N. S. Wingreen et al., Phys. Rev. **B48**, 8487 (1993)
[2] T. Hayashi et al., Phys. Rev. Lett. **91**, 226804 (2003)

TT 22.2 Wed 14:00 Poster B

Transport through an interacting quantum dot tunnel coupled to a ferromagnet with time-dependent magnetisation — •Nina Winkler, Michele Governale, and Jürgen König — Institut für Theoretische Physik III · Ruhr-Universität Bochum

We study spin and charge transport through a system composed of a quantum dot with Coulomb interaction, weakly tunnel coupled to a normal and a ferromagnetic lead with time-dependent magnetisation. We also allow the level position of the dot and the tunnel coupling to the normal lead to vary in time. In general, this setup works as a quantum pump and we focus on the adiabatic-pumping regime. To calculate the pumped charge and spin we extend a diagrammatic real-time approach to pumping through interacting quantum dots [1] to include ferromagnetic leads with time-dependent magnetisations.

[1] J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. B **74**, 085305 (2006).

TT 22.3 Wed 14:00 Poster B

Influence of spin waves on transport through a quantum-dot spin valve — •Björn Sothmann[1], Jürgen König[1], and Anatoli Kadigrobov[1,2] — [1]Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum — [2]Department of Physics, Göteborg University, SE-412 96 Göteborg

We study transport through a quantum-dot spin valve, i.e. a single-level quantum dot with strong Coulomb interaction tunnel coupled to ferromagnetic leads with non-collinear magnetizations. By applying a bias voltage, a spin on the dot is created, reducing the conductance. Furthermore, there is an exchange field due to the Coloumb interaction. In the case of linear transport this leads to a decrease of the spin valve effect, while in the case of nonlinear transport it gives rise to a negative differential conductance.

In Ref. [1] a real-time diagrammatic technique was developed to describe transport through quantum dot spin valves. We generalize this theory to include the excitation of spin waves in the leads. Thereby we distinguish the regimes of the spin wave energy being comparable or being much larger than the tunnel coupling. By solving a generalized master equation for the system's reduced density matrix, we derive the transport properties of the system in the different regimes in linear and non-linear response.

[1] M. Braun, J. König, J. Martinek, Phys. Rev. B **70**, 195345 (2004).

TT 22.4 Wed 14:00 Poster B

Non-equilibrium proximity effect in quantum dots — •Michele Governale[1], Marco G. Pala[2], and Jürgen König[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]IMEP-LAHC-MINATEC (UMR CNRS/INPG/UJF 5130), BP 257, F-38016 Grenoble, France

We present a real-time diagrammatic theory for transport through interacting quantum dots tunnel coupled to normal and superconducting leads [1]. We apply it to a system made up of a single-level quantum dot with Coulomb interaction, coupled to one normal and two superconducting leads. A finite bias voltage can be applied to the normal lead to drive the dot out of equilibrium. We compute both the Andreev current in the normal lead and the Josephson current between the two superconductors. In the large-superconducting-gap limit, we are able to calculate the non-equilibrium Andreev and Josephson currents to all orders in the tunnel coupling with the superconducting leads. In particular, we show that a spectroscopy of the Andreev bound states in the dot can be performed by measuring the current in the normal lead as a function of the dot level position and of the bias voltage. Furthermore, we identify the regions of bias and gate voltage where the system behaves as a π-junction.

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

TT 22.5 Wed 14:00 Poster B

Super-Poissonian current noise in coupled single-electron transistors — •Björn Kubala[1,2], Göran Johansson[3], and Jürgen König[1] — [1]TP III, Ruhr-Universität Bochum, Germany — [2]Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, 80333 Munich, Germany — [3]MC2, Chalmers University Göteborg, Sweden

Non-Poissonian noise has been explored theoretically and experimentally in a variety of systems. We investigate zero-frequency noise and current-current crosscorrelations in networks of coupled single-electron transistors (SETs) within a real-time diagrammatic theory [1]. Calculating all noise contributions up to second order in the coupling strength, we include sequential and standard cotunneling processes, but also renormalization processes and cotunneling involving several transistor islands. For a single SET we find the familiar suppression of noise in double-barrier systems and reproduce results of orthodox and cotunneling theories.

A setup, where two SETs are capacitatively coupled, provides an inside into novel correlation effects, e.g., bunching of electrons as similarly found in semiconductor systems [2]. We identify a number of different mechanisms causing super-Poissonian noise, which could be experimentally investigated in coupled SETs.

[1] B. Kubala, G. Johansson, and J. König, Phys. Rev. B **73**, 165316 (2006).
[2] A. Cottet, W. Belzig, and C. Bruder, Phys. Rev. B **70**, 115315 (2004); S. S. Safonov *et al.*, Phys. Rev. Lett. **91**, 136801 (2003).

TT 22.6 Wed 14:00 Poster B

An iterative real-time path integral method for an Anderson dot with metallic leads — •Jens Eckel, Stephan Weiss, Michael Thorwart, and Reinhold Egger — Institut für Theoretische Physik IV, Heinrich-Heine-Universität Düsseldorf

We present a newly developed method based on an iterative non-equilibrium real-time path integral approach, which is numerically exact since no perturbative approximations are involved [1]. The convergence procedure [2] allowing to eliminate the discretization errors within the method (e.g., (i) a finite memory length of the lead correlator and the interaction self-energy, and (ii) a discretization error due to a Trotter breakup) is illustrated in detail and physically motivated to show the universal validity of the method. The method is applied to a single level Anderson dot attached to metallic leads, where we take into account a finite bias voltage as well as an external magnetic field. The full dI/dV characteristics is computed numerical exact without any perturbative limitation for various experimentally relevant parameters, e.g., the gate voltage and the temperature of the system.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, submitted.
[2] J. Eckel, S. Weiss, and M. Thorwart, Eur. Phys. J. B **53**, 91-98 (2006).

TT 22.7 Wed 14:00 Poster B

Signatures of Aharonov-Bohm effect in the charge transfer statistics of the interacting quantum dot — •Stefan Maier[1] and Andrei Komnik[1,2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [2]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

We study the electron transport statistics of an Aharonov-Bohm interferometer with an embedded single level quantum dot under non-equilibrium conditions. Special emphasis is placed on the interplay of Aharonov-Bohm interferences and Coulomb on-site interaction. To this end we model the system by an Anderson impurity coupled to two metallic electrodes, between which a direct tunnelling is possible. By means of perturbative expansion in interaction amplitude we are able to identify the relevant effects in the generating function of the charge transfer statistics. We see a pronounced magnetic field dependence of the latter and investigate the evolution of the emerging Fano resonances as the electrode-dot as well as electrode-electrode couplings are changed.

TT 22.8 Wed 14:00 Poster B

State Dependent Full Counting Statistics and Statistics of State Changes in a Quantum Dot — •Ansgar Pernice and Wal-

ter T. Strunz — Physikalisches Institut der Universität Freiburg, Herrmann-Herder-Str. 3, 79104 Freiburg, Germany

We consider a quantum dot in the Coulomb blockade regime, coupled to source and drain. Making use of the quantum jump representation of the density operator, we derive a state dependent formula for the full counting statistics (FCS) of electrons entering the quantum dot. In the steady state our result reduces to the one obtained by Bagrets and Nazarov [1] as well as de Jong [2]. Furthermore, we investigate the "Full Statistics of State Changes" on the dot. Remarkably, for this novel quantity an analytical expression can be found in the time domain which turns out to be highly sensitive to the coupling symmetry of the quantum dot to the leads.

[1] D.A. Bagrets and Yu.V. Nazarov. Full Counting Statistics of Charge Transfer in Coulomb Blockade Systems. Phys. Rev. B, 67(8):085316, 2003.

[2] M.J.M. de Jong. Distribution of transmitted charge through a double-barrier junction. Phys. Rev. B, 54(11):8144-8149,1996.

TT 22.9 Wed 14:00 Poster B

Excited states in the conductance of a double dot — Georg Begemann, •Andrea Donarini, and Milena Grifoni — University of Regensburg, Germany

We study the linear transport through two coupled interacting quantum dots in series at temperatures smaller than the tunneling rate, though still larger than the Kondo temperature.

In this regime the sequential tunnelling picture breaks down and the conductance is not uniquely determined by ground states transitions. Coulomb blockade is partially lifted due to transitions to excited states and also the resonances acquire a dependance on the tunnelling coupling to the leads.

We adopt in our calculation the equation of motion technique and systematically compare different truncation schemes unified under a general formalism.

TT 22.10 Wed 14:00 Poster B

Effects of the intershell tunneling in the spectrum of incommensurate DWNTs — •Magdalena Marganska, Shidong Wang, and Milena Grifoni — Institut of Theoretical Physics, University of Regensburg, 93047 Regensburg

In calculations involving multi-wall nanotubes and taking into account the inter-wall coupling, some form of that coupling must be adopted. We study the effects which the choice of a particular expression for the inter-shell electron tunneling has on the calculated electronic spectrum of an incommensurate double-wall carbon nanotube (DWNT). We examine the level statistics and the fractal dimensions of the spectra obtained using different forms of the coupling. The former quantity can determine whether the system is chaotic or regular, the latter may be an indicator of the nature of the transport in the system. We find that the more localized is the tunneling, the more pronounced are the fractal features of the spectrum and the chaotic nature of the system. Therefore when investigating e.g. the transport characteristics in incommensurate DWNTs, different results may be obtained depending on the choice of the inter-shell tunneling.

TT 22.11 Wed 14:00 Poster B

Dynamics of a qubit in a linear/nonlinear structured environment — •Carmen Frammelsberger, Johannes Hausinger, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg

The understanding of the main dephasing and relaxation mechanisms is crucial for the realization of efficient solid state qubits. In this contribution we focus on the case in which the qubit is coupled to a driven linear or non-linear oscillator which in turn interacts with a dissipative environment. This situation mimicks the case of flux qubits read-out by a DC-SQUID, the latter being a linear or non-linear oscillator, or a Cooper-pair box in a resonant electromagnetic cavity.

In our work we adopt the point of view that the oscillator is part of the environment itself. In the linear oscillator case, this amounts to consider a spin-boson problem with a structured spectral density. Generalizing [1] to the case of a finite bias, we show that analytic solutions for the dynamics can be obtained, at arbitrary detuning and finite temperatures, in the case of large Q-factors of the oscillator. One, two or more dominating oscillation frequencies of the qubit can be observed as a consequence of the entanglement with the oscillator. In the nonlinear case we show, using a mapping procedure which is exact in the linear case, that the problem can be approximated to a spin-boson model whose spectral density is proportional to the imaginary part of the nonlinear susceptibility of a quantum Duffing oscillator.

[1] F Nesi, M Grifoni and E Paladino, New J. Phys. 9, 316 (2007).

TT 22.12 Wed 14:00 Poster B

Spin-dependent tunneling current in magnetic tunnel junctions — •Niko Sandschneider and Wolfgang Nolting — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

The tunneling current through a hybrid structure where a confined nonmagnetic insulator is sandwiched between two ferromagnetic metals is calculated within the non-equilibrium Keldysh formalism. The metals are assumed to be band ferromagnets, such as Co, and are described by the single-band Hubbard model. Special emphasis is made to explain the tunneling current features in terms of the quasiparticle density of states of the materials. Also the relationship between the current and the inter-layer exchange coupling is discussed.

Furthermore we show how a generalization of the model presented here can be used to model current-induced switching of magnetization in a self-consistent way.

TT 22.13 Wed 14:00 Poster B

Tunable transmission via quantum state evolution in oval quantum dots — •Daniel Buchholz[1], Panagiotis Drouvelis[3], and Peter Schmelcher[1,2] — [1]Theoretische Chemie, Universität Heidelberg, INF 229, 69120 Heidelberg, Deutschland — [2]Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland — [3]Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Deutschland

We explore the quantum transmission through open oval shaped quantum dots. The transmission spectra show periodic resonances and, depending on the geometry parameter, a strong suppression of the transmission for low energies. Applying a weak perpendicular magnetic field changes this situation drastically and introduces a large conductance. We identify the underlying mechanisms being partially due to the specific shape of the oval that causes a systematic decoupling of a substantial number of states from the leads. Importantly a pairwise destructive interference of the transmitting states is encountered thereby leading to the complete conductance suppression. Coupling properties and interferences can be tuned via a weak magnetic field. These properties are robust with respect to the presence of disorder in the quantum dot.

TT 22.14 Wed 14:00 Poster B

Theoretical and experimental investigations of Coulomb blockade in coupled quantum dot systems — •Franz J. Kaiser[1], Sigmund Kohler[1], Peter Hänggi[1], Marcin Malecha[1], Jens Ebbecke[1,2], and Achim Wixforth[1] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK

We investigate the electron transport through coupled quantum dots in a ratchet like geometry. Our experimental observations of the 'Coulomb diamonds' at low temperatures are supported by a theoretical description, where we compare the results from scattering theory with those of a master equation approach for strong interaction [1]. Moreover, we characterize in each case the shot noise by the Fano factor and identify our experimental findings of sub structures in the Coulomb diamonds as being related to the orbital degrees of freedom. We find very good agreement for the strongly interacting case.

[1] F.J. Kaiser, M. Strass, S. Kohler, and P. Hänggi, Chem. Phys. **322**, 193 (2006)

TT 22.15 Wed 14:00 Poster B

Effective capacitance of charge qubits undergoing Landau-Zener transitions — •Georg Reuther, Peter Hänggi, and Sigmund Kohler — Institut für Physik, Universität Augsburg, 86135 Augsburg

A Cooper pair box in the charging regime has been used for the implementation of solid-state qubits in various experiments. The state of such a qubit can be probed by a weak rf signal. At the charge degeneracy point, the phase of the reflected signal depends sensitively on the effective capacitance of the qubit which, in turn, depends on the energy of the qubit state. For an ac-driven qubit undergoing multiple Landau-Zener transitions, the tunnelling dynamics has been monitored in this way [1]. Relating the measured data to the qubit state, however,

was based on the assumption that the qubit relaxation is either very slow or very fast. We work beyond this limit and study the effective capacitance in the crossover regime of intermediate relaxation times. Our results allow for relating the measured phase shift to the actual state of the qubit and to estimate the measurement fidelity.
[1] M. Sillanpää et al, Phys. Rev. Lett. 96, 187002 (2006)

TT 22.16 Wed 14:00 Poster B

Landau-Zener tunneling in circuit QED at finite temperatures — •David Zueco, Sigmund Kohler, and Peter Hänggi — Institut für Physik, Universität Augsburg, Augsburg, Germany

A possibility to generate single photons in a transmission line coupled to a superconducting charge qubit relies on Landau-Zener transitions between different dressed states [1,2]. Photon losses in the transmission line influence the transition probability and, moreover, limit the photon lifetime.

We study these limitations by taking the coupling of the circuit QED to its electromagnetic environment into account. The environment is integrated out within Born-Markov approximation which yields a master equation for the reduced density operator of the qubit and the transmission line. Its numerical solution provides the final occupation of both the oscillator and the spin-flip probability, as well as the conditions on the loss rate and the temperature which still allow a reliable single-photon generation.

[1] K. Saito, M. Wubs, S. Kohler, P. Hänggi and Y. Kayanuma Europhys. Lett v 76 pp. 22-28 (2006)

[2] M. Wubs, S. Kohler and P. Hänggi Physica E 40, 187ž013197 (2007)

TT 22.17 Wed 14:00 Poster B

Relaxation of Josephson qubits due to bistable fluctuators — •Clemens Müller[1], Alexander Shnirman[1], and Gerd Schön[2] — [1]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [2]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Decoherence is a major problem for the use of superconducting Josephson qubits in quantum information processing. Recent measurements of the relaxation time T_1 of Josephson charge qubits reveal strongly nonmonotomic behavior as a function of the energy splitting (e.g. [1], [2]), the origin of which is not understood.
As a possible model we study the relaxation time T_1 of a Josephson qubit coupled to an environment of bistable fluctuators (TLF) in the case that the TLFs are coupled between each other. We show new features of T_1 due to the interaction between TLFs. Two methods were used for calculation, succesive use of Golden Rule and Bloch-Redfield equations for the density matrix. The validity of the widely used Golden Rule method was studied.
[1] G. Ithier et al., Phys. Rev. B **72**, 134519 (2005)
[2] O. Astafiev et al., Phys. Rev. Lett. **93**, 267007 (2004)

TT 22.18 Wed 14:00 Poster B

Fabrication of sub-μm Nb/Al-AlO$_x$/Nb Josephson Junctions with Electron Beam Lithography for Qubit Applications — •Christoph Kaiser, Konstantin Il'in, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe (TH), D-76187 Karlsruhe

We fabricated sub-μm Josephson Junctions in Nb/Al-AlO$_x$/Nb trilayer technology. The shape of the junctions was defined by electron beam lithography and reactive ion etching. The junctions were electrically insulated by a layer of anodically oxidized Niobium as well as a SiO layer. The SiO film was deposited in a lift off process via thermal evaporation and its contact windows were also defined by electron beam lithography. Samples with different critical current densities were characterized at low temperatures in order to examine their suitability for qubit experiments.

TT 22.19 Wed 14:00 Poster B

Superconducting Quantum Circuits: Building Blocks for cQED experiments — •Thomas Niemczyk, Elisabeth Hoffman, Achim Marx, and Rudolf Gross — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaftem, Garching

There have been numerous promising advancements in the field of quantum information processing (QIP) since its conception. Coupling *superconducting (SC) qubits* to high-Q SC resonators opens the fascinating field of circuit quantum electrodynamics (cQED). Recent experiments with SC *charge qubits* have demonstrated the fundamental interaction of these 'artificial atoms' with a single microwave photon. In our work we are concentrating on the development of SC *flux-qubits* and the required building blocks for cQED. We present designs and realizations of different SC coplanar waveguide resonators for cQED experiments with quality factors up to $2.3 \cdot 10^5$. Furthermore, we present measurements on high-transparency Al/AlO$_x$/Al Josephson-Junctions (JJ). The JJs were characterized at 500 mK and exhibit E_J/E_C ratios of 30 - 70 with critical current densities J_c larger than 1000 A/cm^2. Finally, we present measurements on different realizations of microstrip hybrid rings, which act as a beam splitter in the microwave regime. The hybrid rings were characterized at 4.2 K and 1.5 K and exhibit isolation (S_{31}) and coupling (S_{23}) spectra suitable for a quantum homodyne measurement scheme for the detection of single microwave photons.
Financial support by the DFG via SFB 631 and the Excellence Initiative via NIM is gratefully acknowledged.

TT 22.20 Wed 14:00 Poster B

Observation of coherent oscillations in a superconducting qubit with π-junction — •Jürgen Lisenfeld[1], Stefano Poletto[1], Alexey Feofanov[1], Anna N. Rossolenko[2], Vladimir A. Oboznov[2], Vitaly V. Bolginov[2], Alexander Lukashenko[1], Valery V. Ryazanov[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut III, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432 Russia

Flux qubits consist of superconducting loops interrupted by Josephson junctions. It has been theoretically proposed that embedding a π-junction into the loop allows to realize a 'quiet' qubit, which does not require applying any external magnetic field for biasing at the optimum operation point. When the phase drop across the π-junction with high critical current is set to π, a circulating current spontaneously emerges and stabilizes the qubit at the working point.
We incorporated a superconductor-ferromagnet-superconductor π-junction in the loop of a phase qubit made by conventional Nb technology. We observed Rabi oscillations and measured the qubit decay from the excited state. We found no difference between the decoherence times of otherwise identical qubits with and without π-junctions. The short decay of the order of several nanoseconds is limited in both cases by the decoherence sources in the on-chip dielectrics rather than by dissipation induced by the ferromagnetic π-junction phase shifter. This promising first result supports the feasibility of designing self-biased 'quiet' flux qubits.

TT 22.21 Wed 14:00 Poster B

Dispersive Readout of Josephson Phase Qubits — •Tobias Wirth[1], Jürgen Lisenfeld[1], Alexander Lukashenko[1], Alexander Zhuravel[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut III, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]B. Verkin Institute for Low Temperature Physics & Engineering, National Academy of Sciences of Ukraine, Kharkov, Ukraine

Solid-state quantum bits based on current-biased Josephson junctions require appropriate isolation from the bias leads which can be achieved by using superconducting transformers. A superconducting loop with a tunnel junction allows to prepare an asymmetric double-well potential, where the discrete quantum levels in the shallow well form the qubit states. State-dependent tunneling to the deeper well changes the magnetic flux in the qubit, which is measured by a dc-SQUID. In our ongoing experiments, we use a high-frequency readout based on a non-dissipative measurement of the dc-SQUID Josephson inductance, which in turn depends on the qubit flux. The measurement is done by detecting either the resonance shift of the LC-circuit, which consists of the dc-SQUID with a shunt capacitor, or the phase change of the reflected probe signal. We observed the periodic dependence of the reflected microwave amplitude and phase on externally applied magnetic flux. By using a low temperature scanning laser microscope, we map the microwave current distribution in our circuit. Current experiments are focused on a pulsed rf-readout and the use of an IQ-mixer to detect the phase change of the reflected signal.

TT 22.22 Wed 14:00 Poster B

Experiments with two-cell flux qubits — •Alexey K. Feofanov and Alexey V. Ustinov — Physikalisches Institut III, Universität Erlangen-Nürnberg, Erlangen, Germany

A two-cell flux qubit with four Josephson junctions has an advantage over conventional single-cell three-junction flux qubits that it features orthogonal controls of both the potential barrier height and its symme-

try.This aspect facilitates reliable initialization of the qubit and offers additional fast gate control. Changing the potential barrier height allows for moving the qubit operation point away from parasitic resonances and makes it possible to realize tuneable coupling to common bus. Our two-cell qubits feature asymmetric dc-SQUID readout and on-chip flux controls. To bias the qubit at the optimal working point we use a passive pi-shifter in the superconducting bar separating two cells. The readout is performed by standard pulse sequence consisting of short switching and long latching pulses. Experimental results on testing these devices will be reported.

TT 22.23 Wed 14:00 Poster B

Modeling of quasiparticle transitions in Josephson charge-phase qubits — •Jens Könemann, Hermann Zangerle, Brigitte Mackrodt, Ralf Dolata, and Alexander B. Zorin — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Superconducting circuits, based on the tunneling of single Cooper pairs, enable remarkable charge-phase qubits. The qubit operation relies on the coherent superposition of the macroscopic quantum states, but the unwanted tunneling of unpaired electrons (quasiparticles) changes instantly the charge state and thus, the working point of the qubit.

Recently we have investigated quasiparticle transitions in an Al charge-phase qubit [1] inducing a dynamic change of the qubit states. Non-equilibrium quasiparticles tunnel stochastically on and off the island and may excite the qubit. The relaxation of the qubit by releasing a single quasiparticle to the leads becomes the dominating relaxation mechanism. In this work, we present a numerical modeling of these transitions. Moreover, we discuss the effect of microwave irradiation on the quasiparticle-induced transitions.

[1] J. Könemann *et al.*, Phys. Rev. B **76**, 134507 (2007).

TT 22.24 Wed 14:00 Poster B

Finite-temperature Bell test for quasiparticle entanglement in the Fermi sea — •Wolf-Rüdiger Hannes[1], Mikhail Titov[1,2], and Wolfgang Belzig[1] — [1]Universität Konstanz, Fachbereich Physik, D-78457 Konstanz — [2]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK

Theoretical predictions of the presence of quantum entanglement in solid-state devices commonly make use of Bell-type inequalities formulated in terms of currents and current-current cross correlators. We demonstrate [1] that no such Bell-test can be performed at finite temperatures in the vast majority of setups proposed previously for entanglement generation. This fundamental difficulty originates in a finite probability of quasiparticle emission from Fermi sea detectors. The feedback problem can be overcome by a resonant coupling of the detectors and an additional detector cooling. Application of this simple improvement to a generic beam splitter setup constitutes a device that can be used to determine the critical temperature for the entanglement produced in the absence of fermionic interactions.

In the future we will try to access the temperature dependent entanglement generation of an electronic beam splitter by investigating its full counting statistics.

[1] W.-R. Hannes and M. Titov, Preprint arXiv:0710.0348v1

TT 22.25 Wed 14:00 Poster B

Numerical analysis of shaped coherent pulses — •Peter Karbach, Stefano Pasini, Götz S. Uhrig, and Joachim Stolze — TU Dortmund - Theoretische Physik I

Recently we presented analytical results on the optimization of coherent pulse shapes based on the Magnus-expansion (arXiv:0709.0588, submitted to PRA). The expansion parameter is the pulse duration τ_p. The coefficients for the linear and the quadratic order have been obtained. Depending on the pulse shapes certain coefficients vanish and the resulting pulses are better suited than the plain pulses (i.e. with constant amplitude) for the coherent control of small quantum systems in general and for single quantum bits in particular.

These analytical results are tested numerically for the proposed piecewise-constant pulses in different coupling geometries. It is confirmed that the analytical calculations are valid for a large parameter range (coupling constants, number of spins in the bath).

The numerical results are presented and the limitations of the analytical findings are discussed.

TT 22.26 Wed 14:00 Poster B

Non-equilibrium states in graphene rings driven by ultrashort light pulses — •Andrey Moskalenko and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Graphene became a hot topic since the demonstration of its fabrication because of the quasi-relativistic properties of its band structure. Mesoscopic effects are of a particular interest as they exhibit features unusual for metallic or semiconductor mesoscopic structures. Recently, mesoscopic graphene rings were fabricated. The properties of the Aharonov-Bohm effect were investigated theoretically and experimentally. We investigate non-equilibrium mesoscopic effects in graphene rings excited by picosecond asymmetric electromagnetic pulses. Ultrafast generation of charge-polarized and current-carrying states is demonstrated and illustrated for the experimentally relevant parameters of the graphene ring.

TT 22.27 Wed 14:00 Poster B

Conductance through a strongly interacting region – LDA versus exact results — •Stefan Schenk, Michael Dzierzawa, Ulrich Eckern, and Peter Schwab — Universität Augsburg

Density functional theory within the local density approximation is the method of choice for calculations of the electronic structure of complex materials. In recent years the method has been adapted to transport problems, in particular to transport through systems of molecular size.

Here we study a one-dimensional model of spinless fermions. This has the advantage that the density matrix renormalization group provides numerically exact results for the conductance. We find that although for weak electron-electron interaction the local density approximation gives reasonable estimates for the location of conductance resonances, the method strongly overestimates the conductance in the non-resonant case. The discrepancies arise from the insufficient accuracy of the ground state density obtained within the local density approximation. Dynamic effects that can be captured within the time-dependent density functional theory are only of minor importance.

TT 22.28 Wed 14:00 Poster B

Resistance measurements on Bismuth nanowire arrays at low temperatures — •Thomas Kaupp[1], Christoph Kaiser[2], Georg Weiss[1], Thomas Cornelius[3], and Reinhard Neumann[3] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Universität Karlsruhe, 76187 Karlsruhe, Germany — [3]Gesellschaft für Schwerionenforschung, 64291 Darmstadt, Germany

Our sample fabrication started with creating nanoporous templates by exposing polymeric foils to heavy ion radiation. Into these templates, single- and poly-crystalline bismuth nanowires were electrochemically deposited. Resistance and magnetoresistance of arrays of these nanowires were studied at temperatures down to 50 mK. Additionally, aged samples of single-crystalline nanowires could be studied.

We observed a reduction of the resistance below 0.5 K of about 3 to 20 percent depending on the type of sample. The magnetoresistance of single-crystalline samples in this temperature range showed a linear behaviour up to 50 mT and then follows a power law with an exponent of 3/2 as previously reported. A linear magnetoresistance was observed for the poly-crystalline sample. The size of the linear increase up to 50 mT corresponds to the temperature dependent resistance reduction below 0.5 K.

Presently the interpretation of our observations is unclear. We discuss both the role of localization effects as well as the possibility that parts of the nanowires become superconducting.

TT 22.29 Wed 14:00 Poster B

Switching Dy break junctions by a magnetic field — •Marc Müller[1], Richard Montbrun[1], Christoph Sürgers[1,2], and Hilbert v. Löhneysen[1,2,3] — [1]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — [2]Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

In search for conductance steps in rare-earth-metal atomic contacts, we study the low-temperature electronic transport properties of mechanically controlled Dy break junctions. The junctions are prepared from Dy wires cut from a dentritic polycrystal which are broken insitu by means of a three-point bending mechanism. Magnetic fields are applied along the wire axis. In a mechanically pre-adjusted and fixed position of the two electrodes, the contact can be reproducibly opened and closed by variation of the applied magnetic field. The

switching, i.e. the change in resistance vs. contact distance, shows a hysteretic behavior and presumably arises from the large magnetostriction of ferromagnetic Dy. Preliminary measurements show steps in the conductance-distance characteristics which are, however, much larger than one conductance quantum $G_0 = 2e^2/h$.

TT 22.30 Wed 14:00 Poster B

Point contact spectroscopy of quench-condensed Ag films — •Torben Peichl, Marcel Spurny, Michael Burst, and Georg Weiss — Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany

We report on the progress in fabricating nanostructured point contacts as a result of our structural characterization studies. The point contacts are defined by electron beam lithography on top of silicon nitride membranes. Then the bottom side is covered with a layer of Au before a SF_6 plasma etching from the top side is used to obtain nano-sized holes in the membrane. Finally, a highly disordered Ag layer is prepared by quench-condensing Ag films at low temperatures <10 K on the top side. This results in metallic point contacts with diameters <50 nm and resistances between 1 and 10 Ω.

Electronic transport properties of these point contacts were studied at temperatures from 1.5 to 8 K by measuring the differential resistance using lock-in methods. Within sample series we find reproducible results, in particular a distinct minimum of the differential resistance which we identify as a zero-bias minimum shifted by a DC offset of yet unknown origin. This minimum becomes narrower at increasing temperatures and vanishes at 8 K. Similarly, the minimum diminishes continuously with magnetic field until it vanishes completely at about 2 T. Low energy excitations as well as coulomb blockade effects might be responsible for the observed behavior. Additionally, slight oscillations of the differential resistance curves are reminiscent of weak localisation effects.

TT 22.31 Wed 14:00 Poster B

Charge transport properties of biphenyl molecules and tetrathiafulvalene — •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, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

We study theoretically the charge transport properties of single molecule junctions. For this, we use a combination of density functional theory and Green's-function techniques [1]. In our analysis, we consider different types of molecules, namely biphenyl molecules and tetrathiafulvalene. For the biphenyl molecules, the tilt angle of the phenyl rings is changed continuously by means of alkyl chains of varied lengths. We investigate the dependence of both the tilt angle and the conductance on this chain length. In addition, we examine the conductance of tetrathiafulvalene.

[1] F. Pauly, Ph.D. Thesis, Universität Karlsruhe (2007).

TT 22.32 Wed 14:00 Poster B

In-situ fabrication of nanobridges under ultra-high vacuum conditions — •Dominik Stöffler[1], Hilbert v. Löhneysen[1,2], and Regina Hoffmann[1] — [1]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

Contacting single molecules with nanostructured metallic leads remain a challenge, in spite of numerous attempts. We investigate nanocontact formation by thermally assisted electromigration of gold nanowires. The nanowires are prepared by electron beam lithography. An automatic feed-back allows to follow a line of constant dissipated power at the nanocontact, which leads to a gradual thinning of the wire until a small gap is formed. The fabricated gaps are smaller than 10 to 20 nm. By following the line of constant power, we estimate an increase of the temperature of the contact from 350 K in the thermal regime at the beginning, to 650 K in the ballistic regime at the end of the overall electromigration process. Due to the lithography process, leftovers such as PMMA remain on the metallic contacts, which eventually affect transport measurements with molecules. We introduce a promising alternative method to fabricate and contact clean metallic nanostructures, using evaporation through a mask under ultra-high vacuum. These structures can eventually be separated by electromigration to accommodate single molecules.

TT 22.33 Wed 14:00 Poster B

Conductance measurements on palladium breakjunctions with superconducting leads — •Stefan Egle, Cécile Bacca, Christian Schirm, and Elke Scheer — Department of Physics, University of Konstanz

We will present our recent results of palladium nanobridges connected by superconducting leads of aluminium. The structures are fabricated by using electron beam lithography and two-step shadow evaporation. By means of the mechanically controllable break junction (MCBJ) technique we are able to open the bridges to a one-atom contact and close again repeatedly at low temperatures, thus obtaining conductance histograms. Studying the properties of these palladium atomic point contacts at 270mK, we show the influence of the superconducting leads onto the electronic properties of palladium (proximity effect) by measuring the differential resistance. As expected, we observe a decrease of the dV/dI for voltages $|V| \leq 120\mu\text{V} < \Delta_{Al} = 180\mu\text{V}$ which increases again when either the external magnetic field or the temperature is raised. Investigating the disappearence of this effect, we determine the critical values B_c and T_c.

TT 22.34 Wed 14:00 Poster B

Reversible Switching Effect in Atomic-Size Contacts — •Christian Schirm, Hans-Fridtjof Pernau, and Elke Scheer — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

We investigate electromigration effects in atomic-size contacts of aluminum fabricated with the mechanically controllable break junction technique at $T \leq 1.5$K. We observe current-driven conductance changes ΔG and analyze their influence on the conductance histogram. In particular situations a reversible switching between two conductance values is observed (> 100 repetitions) which attribute to the formation of preferred atomic configurations. A correlation between these configurations and conductance channels shall be established via the analysis of MAR in the superconducting state [1].

[1] E. Scheer et al., Phys. Rev. Lett. **78** (1997) 3535-3538

TT 22.35 Wed 14:00 Poster B

Breakjunctions on Membranes — •Reimar Waitz, Olivier Schecker, and Elke Scheer — Universität Konstanz, Germany

A so-called "mechanically controlled breakjunction" is made of a metallic wire with a suspended constriction. This constriction can be elongated until having - just before breaking - a diameter of one atom. In this project we developed a new kind of breakjunctions on silicon membranes. The wire is made by electron-beam lithography on top of a 600x600 micrometer crystalline silicon membrane with a thickness of a few hundred nanometers. In contrast to the "standard" breakjunction technique, we use the strain of the membrane to control the elongation of the wire. In our poster we present the process of sample fabrication and a mechanism for controlled breaking, which has successfully been used to measure the conductance of single atom contacts.

TT 22.36 Wed 14:00 Poster B

Bias-dependent electronic transport in nanowires — •Neng-Ping Wang and Stefan Heinze — Institute of Applied Physics, University of Hamburg, Jungiusstrass 11, 20355 Hamburg, Germany

Transport of electrons in nanoscale structures is of interest from a fundamental as well as an application point of view. Often nanoscale systems display nonlinear current-voltage characteristics, which make them interesting for device applications. Here, we report first principles calculations of bias-dependent ballistic transport in nanowires using the non-equilibrium Greens function method. The system under consideration is divided into a central scattering region attached to semi-infinite left and right leads. First, we use density functional theory (DFT) to calculate the electronic structure of the system. The DFT eigenstates are then transformed into a set of maximally localized Wannier functions (WFs). Using the WFs as localized orbitals, we construct the Hamiltonian of scattering region and leads, which is used for transport calculation. The coupling of the scattering region to the semi-infinite leads is described by the self-energies of the leads which we obtain with the particularly efficient decimation technique. We solve for the Green function of the system and calculate the transmission and current at low bias voltages.

As a first application of our approach, we study the I-V characteris-

tics of Cu wires with a stretched bond as a function of the bond length. In order to explain the transport characteristics, we analyze the potential drop and non-equilibrium charge distribution as a function of the applied bias voltage.

TT 22.37 Wed 14:00 Poster B

Synthesis of Opto-Electronic Compounds from Carbon Nanotubes and Photosystem I — •Markus Mangold[1], Simone Lingitz[1], Itai Carmeli[2], Ludmila Frolov[2], Chanoch Carmeli[2], Shachar Richter[2], and Alex Holleitner[1] — [1]Walter Schottky Institut, TU München, Deutschland — [2]Center for Nanoscience, Tel Aviv University, Israel

The photosystem I (PS I) reaction center is a chlorophyll protein complex located in the thylakoid membranes of chloroplasts and cyanobacteria. PS I mediates a light induced electron transfer through a serial of redox reactions and is central for the photosynthesis in plants and bacteria. Utilizing a unique cysteine (Cys) mutation at the end of PS I, we demonstrate a four-step chemical procedure based on carbodiimide chemistry for covalent binding of PS I proteins to carbon nanotubes (CNTs) [1]. This procedure resulted in linear, circular, and T- shaped CNT-PS I hybrids, which are ideally suited for the integration of the PS I into optoelectronic circuits. We present first measurements of an opto-current generated in the hybrid structures upon illumination with visible light.

We gratefully acknowledge financial support by CeNS and the Nanosystems Initiative Munich, the DFG grant HO-3324/1, and the DFG SFB 486 TP A1.

[1] I. Carmeli, M. Mangold, et al. Advanced Materials, in press (2007).

TT 22.38 Wed 14:00 Poster B

Quantum conductance from the irreducible polarization function — •Swantje Heers, Arno Schindlmayr, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The standard approach to quantum transport, which involves a combination of *ab initio* density-functional theory and the Landauer formula, successfully describes the conductance of nanojunctions at a qualitative level, but it remains unclear how the Coulomb interaction can best be incorporated into this single-particle picture of ballistic transport. An alternative approach proposed by P. Bokes *et al.* [Phys. Rev. B **69**, 245420 (2004); **76**, 125433 (2007)] that uses a relation between the polarization function and the conductance formally includes such noncoherent effects. In order to demonstrate its applicability in numerical calculations for a semi-infinite scattering setup with proper boundary conditions we investigate transport through model metal-vacuum-metal interfaces with a piecewise constant potential varying in one dimension only. Starting from the non-interactiong Green function we calculate the polarization function and then the conductance. The necessary extrapolation to zero frequency and the dependence on relevant convergence parameters are demonstrated. In the first instance we neglect the electron-electron interaction and find that the conductance in the single-particle picture coincides with the Landauer formula. This scheme is hence a promising avenue to take exchange and correlation effects into account in future transport calculations.

TT 22.39 Wed 14:00 Poster B

Quantum Transport Through Nanowires: Ab Initio Studies Using Plane Waves and Supercells — •Björn Oetzel, Martin Preuss, Frank Ortmann, Karsten Hannewald, and Friedhelm Bechstedt — European Theoretical Spectroscopy Facility and Institut für Festkörpertheorie und -optik, 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. As a first example for the usefulness of the method, we present DFT calculations of transmission functions for various one-dimensional Au nanowires. The results are discussed with respect to future extensions to metal-molecule-metal nanojunctions.

TT 22.40 Wed 14:00 Poster B

Non-Equilibrium Energy Gaps and Inelastic Transport in Carbon Nanotubes: Role of Phonon Symmetries — •Luis Foa Torres[1], Rémi Avriller[2], and Stephan Roche[2] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany. — [2]DSM/DRFMC/SPSMS/GT, Commissariat à l'Energie Atomique, 17 rue des Martyrs, 38054 Grenoble, France.

We report on a theoretical study of inelastic basckscattering and transport in metallic carbon nanotubes. A Peierls-type mechanism due to electron-phonon interaction with longitudinal optic as well as K point modes [1] in armchair tubes is shown to induce non-equilibrium energy gaps, which in turn manifest as plateaus in the current-voltage characteristics as soon as optic modes are activated. The precise features of these plateaus depend on the specifics of the coupling with the environment through the thermalization rate of the phonons. These phenomena are unveiled by using a full quantum description of the joined processes of tunneling and phonon-assisted transport and can be seen as the removal of degeneracies in Fock space. Further generalizations to tubes of arbitrary helicity are also outlined [1] thereby giving a much broader reach to previously reported results [2].

[1] L. E. F. Foa Torres, R. Avriller and S. Roche, submitted.

[2] L. E. F. Foa Torres and S. Roche, Phys. Rev. Lett. 97 (2006) 076804.

TT 22.41 Wed 14:00 Poster B

Tunable transport by controlling the structure of an STM molecular junction — •Florian Pump[1], Michael Rohlfing[2], Bo Song[1], Ruslan Temirov[3], Adam Lassise[4], Olga Neucheva[3], Stefan Tautz[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — [2]Department of Physics, University of Osnabrück, D-49069 Osnabrück, Germany — [3]Institute of Bio- and Nanosystems (IBN), Institute 3: Institute of Thin Films and Interfaces 3 (IBN3), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [4]Jacobs University Bremen, School of Engineering and Science, D-28725 Bremen, Germany

In molecular junctions, the coupling between the electric contacts and the actual molecule is of great importance. Scanning tunneling microscopy (STM) techniques allow, in addition to their imaging possibilities at a high resolution, the option to mechanically manipulate the bonding properties between molecules and metal surfaces and provide the feasibility to subsequently measure transport effects through the molecule. Based on recent experiments studying the lifting of a single PTCDA molecule from an Ag surface, we present the results of our Density Functional Theory based calculations. We discuss the variation of the energies of the molecular levels and the device substrate coupling during the peeling process and describe its effects on the transport properties through the molecule.

TT 22.42 Wed 14:00 Poster B

Dynamical effects in the conductance properties of short DNA molecular wires: a combined study using molecular dynamics and model Hamiltonians — Benjamin Woiczikowski[1], •Rodrigo Caetano[2], Rafael Gutierrez[2], Tomas Kubar[1], Marcus Elstner[1], and Gianaurelio Cuniberti[2] — [1]Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany — [2]Institute for Materials Science, Dresden University of Technology and Max Bergmann Centre of Biomaterials, D-01062 Dresden, Germany

The potential applications of DNA oligomers in molecular electronics makes of crucial importance to understand the microscopic mechanisms of charge migration. Experimental studies provide very striking results, which range from insulating to superconducting behavior. Theoretically, it is very important to take into account dynamical effects, since DNA is known to be a flexible molecule. In this work, we study charge transport through short Poly(G)-Poly(C) molecules within a minimal tight binding Hamiltonian model. The model parameters are extracted from snapshots along molecular dynamic trajectories and thus effectively include internal and external (soventmediated) dynamical effects. We perform a statistical analysis of the time-dependent onsite energies and electronic hopping integrals and show that they can be fitted to Gaussian functions. We use Green's function techniques in order to calculate the linear conductance and the current-voltage characteristics and demonstrate how the average quantities do depend on the charge tunneling time.

TT 22.43 Wed 14:00 Poster B

Numerical Renormalization Group Calculation of Electronic Transport in the Anderson Holstein Model — •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

Since their recent first realizations, molecular transistors attract more and more interest in nanoelectronics due to their rich transport properties. They consist of a molecule connecting two leads where a gate electrode can be used to tune the charge on the molecule. An important point in describing their transport behaviour is the understanding of electron-phonon interactions. We investigate these interactions using an Anderson Holstein Model [1,2] where a single impurity is linearily coupled to a harmonic osillator describing the vibrational degrees of freedom of the molecule. In our work we use the Numerical Renormalization Group [3] to calculate transport properties of the molecular transistor.

[1] P.W.Anderson, Phys. Rev. **124**, 41 (1961)
[2] T.Holstein, Ann. Phys. **8**, 325 (1995)
[3] K.Wilson, Rev. Mod. Phys. **47**, 773 (1975)

TT 22.44 Wed 14:00 Poster B

Time-resolved electron transport of surface state electrons on helium in confined geometry — •Marc Schmid and Paul Leiderer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

We report on an investigation of the transport of surface state electrons on liquid helium films in restricted geometry. For this purpose we use a source-gate-drain structure, similar to a field effect transistor, which is lithographically prepared on a silicon substrate. The electron densities on both source and drain are determined by an optical measurement of the underlying helium film, whose thickness depends on the surface charge density. For time-resolved measurements, a pulse of electrons from a small filament is first collected on the source area, and then the passage of this pulse through the channel of the split gate towards the drain is monitored. This allows to determine the electron transport of surface state electrons in channels of various dimensions and for a wide range of electron densities.

TT 22.45 Wed 14:00 Poster B

Influence of chopped laser light onto the electronic transport through atomic-sized contacts — •Kerstin M. C. Hans, Daniel C. Guhr, Dennis Rettinger, Johannes Boneberg, Artur Erbe, Paul Leiderer, and Elke Scheer — Universität Konstanz, Konstanz, Germany

In our experiment we investigate the influence of laser irradiation onto the electrical conductance G of Au nanocontacts established with the mechanically controllable breakjunction (MCB) technique [1]. We concentrate on the study of reversible G changes which can be as high as 50%. We compare results of samples fabricated on different substrate materials. On metal substrates, with high reflectivity in the visible light range and insulated from the MCB, we observe an enhancement of G under almost all conditions [2]. In contrast to this, on pure insulating and full light-absorbing substrates we additionally observe a decrease of G, depending on the position of the laser spot on the sample. Within one series of measurements we have also varied intensity, the polarisation and the wavelength. We discuss several physical mechanisms which might contribute to the observed effect including thermal expansion and photon-assisted transport (PAT) [3]. From the analysis of our data we conclude that PAT is the dominating effect in our experiment on metal substrates and thermal expansion on the insulating substrates. First results with Pt structures on insulated metal substrates will also be shown.

[1] J. M. van Ruitenbeek et al., Rev.Sci. Instrum. 67, 108 (1996)
[2] D. C. Guhr et al., PRL 99, 086801 (2007)
[3] J. K. Viljas and J. C. Cuevas, PRB 75, 075406 (2007)

TT 22.46 Wed 14:00 Poster B

Electronic Transport Measurements on Mass-Selected Silicon Clusters — •Jochen Grebing, Rainer Dietsche, Gerd Ganteför, and Elke Scheer — Dept. of Physics, University of Konstanz

We present electronic transport measurements on mass-selected silicon clusters, in particular Si_4 which are supposed to be magic [1].

These clusters are being created using a magnetron sputter source. After mass separation they are soft-landed onto adjustable metallic electrodes fabricated with a MCB technique [2]. Following the deposition a single or a few clusters may be contacted, and their transport properties are being investigated *in situ* by recording conductance histograms and current voltage curves.

The histograms show significant changes in their characteristics after deposition of ≈ 0.1ML of Si_4 clusters. To further investigate whether transport occured through single or few clusters IV-curves have been measured. Calculations predict nonlinearities for a bias $\gtrsim 0.25$V for Si_4 contacted with Au leads [3].

[1] M. Grass et al., Appl. Phys. Lett **81**, 3810 (2002)
[2] MCB: **M**echanically **C**ontrollable **B**reakjunction
[3] C. Roland et al., Phys. Rev. B **66**, 035332 (2002)

TT 22.47 Wed 14:00 Poster B

Effects of curvature on the electronic transport in graphene — •Sebastian Gattenlöhner[1], Mikhail Titov[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz — [2]School of EPS - Physics Department, Heriot-Watt University Edinburgh

As was recently shown experimentally [1], free-standing graphene is not entirely flat but is intrinsically curved. The low-energy electronic excitations in graphene can be described by a Dirac-like Hamiltonian, where the curvature manifests itself in form of additional vector and scalar potentials. We study the effect of these potentials on the electronic transport properties of graphene.

[1] J. C. Meyer et al., The structure of suspended graphene sheets, Nature **446** (2007) 60-63.

TT 22.48 Wed 14:00 Poster B

Electrical Characterization of Molecular Monolayers using Micro-Transfer Printing — •Christian Kreuter, Artur Erbe, Stefan Bächle, and Elke Scheer — Department of Physics, University of Konstanz, D-78457 Konstanz

The formation, characterization and understanding of metal-molecule contacts are necessary preconditions for the development of future molecular-electronic devices. Although in the past 20 years various techniques of contacting single molecules and layers of molecules have been developed, establishing a stable metal-molecule contact is still a challenge. Another serious problem is to separate artifacts which arise from to the used contacting technique from molecule-based properties.

Here we demonstrate a Micro-Transfer Printing (μTP) Technique to contact a molecular monolayer of thiol molecules on GaAs and other substrates. We also present measurements of the current-voltage(I-V) characteristics of a monolayer of dithiolated molecules as a function of temperature and light. At low temperatures, we find asymmetries in the IV-characteristics which can be ascribed to the specific influence of the molecules. Further on, it is shown that the current flow through the device can be strongly affected by light. The dependence of the conductance in relation to the area of contact (typically about 20-100 μm^2) is studied in order to understand the quality of the metal-molecule contact.

TT 22.49 Wed 14:00 Poster B

Conductance through Metal–Molecule Contacts in Solution — •Thomas Kirchner[1], Uta Eberlein[1], Simon Verleger[1], Thomas Huhn[2], Artur Erbe[1], and Elke Scheer[1] — [1]FB Physik, Universität Konstanz, Germany — [2]FB Chemie, Universität Konstanz, Germany

Lithographically defined Mechanically Controllable Break Junctions (MCBJ) are employed to establish metal-molecule contacts at room temperature. Using a liquid cell containing a molecule solution, and a solvent re-filling system the molecules are kept in a tetrahydrofuran-based solvent throughout the measurement. We investigate oligo phenylene ethynylenes (OPE) with various end groups including pyridine. The conductance can be measured while slowly varying the distance between the electrodes, thus revealing preferred conductance values by statistical analysis. Furthermore, current-voltage characteristics are determined at a constant distance.

TT 22.50 Wed 14:00 Poster B

Electronic transport through C_{60} — •Tobias Böhler, Achim Edtbauer, and Elke Scheer — Universität Konstanz FB Physik

The electronic transport through a single or a few C_{60} molecules is studied experimentally with the help of the mechanically controllable break-junction (MCB) technique [1,2]. The tip electrodes of the MCB are fabricated of Al. The molecule is evaporated onto an opened break-junction under UHV conditions and at low temperatures (10 K). The experiment shows evidence for excitations of Al phonons in the differential conductance. By varying the electrode position we can shift the phonon energy. From the development of the energy we find evidence

for longitudinal and transversal phonon modes. With C_{60} between the contacts we observe additional features in the d^2I/dV^2 which we tentatively attribute to vibronic modes of C_{60} previously observed for C_{60} with gold contacts [2]. Furthermore the dI/dV's of Al-C_{60}-Al contacts reveals a Kondo behaviour with a characteristic temperature of approximately 70 K.

[1] T. Böhler et al. Nanotechnology 15 (2004) 465
[2] T.Böhler et al. PRB 76 (2007) 125432

TT 22.51 Wed 14:00 Poster B

Influence of defects on universal conductance fluctuations in diffusive metallic nanowires — •Thomas Schluck[1], Michael Wolz[1], Vojko Kunej[1], Christian Debuschewitz[2], and Elke Scheer[1] — [1]Univ. of Konstanz, Dep. of Phys. — [2]attocube AG

One of the most common methods to study quantum interference effects in diffusive nanostructures is the recording of magneto-resistance curves which exhibit reproducible variations of the resistance due Universal Conductance Fluctuations (UCF). The UCF pattern depends on the configuration of scattering centers for electron wave functions. The question arises how the UCF pattern changes when small artificial defects are added to the scattering configuration and whether a partial correlation between the patterns persists. Therefore we investigate metallic nanowires in the diffusive regime and achieved reproducible UCF patterns at $T = 4.2$K and $T = 2.2$K for magnetic fields up to 5T. To add artificial defects to the metallic nanowires a homebuilt, low-temperature and non-magnetic STM is in use [1]. For positioning the STM-tip with respect to the sample, the STM is equipped with two slip-stick tables. The nanowire structures were fabricated by electron beam lithography, reactive ion etching, wet etching and shadow evaporation (Au, Au/Cu)[2]. With a focussed ion beam we add smooth search patterns to the sample layout as a guide to the nanowire in STM mode. UCF measurements and first successful manipulations of a nanowire are presented.

[1] C. Debuschewitz et al., J. Low Temp. Phys. **147** (2007), p.525
[2] T. Hoss et al., Europhys. Lett. **54** (2001), p.654

TT 22.52 Wed 14:00 Poster B

Fluctuation Correction to Andreev Transport — •Fabian Mohn[1], Wolfgang Belzig[1], and Yuli V. Nazarov[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz — [2]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

The quantum mechanical nature of electronic transport at low temperatures is reflected in fluctuations of physical properties due to wave interference in a disordered environment. The superconducting proximity effect describes the superconductivity in the normal parts of a heterostructure induced by the presence of a superconductor and is a consequence of the macroscopic phase coherence. Studying the interplay between this macroscopic interference and the microscopic interference underlying mesoscopic fluctuations is of fundamental interest.

Recently a method to treat quantum corrections to the circuit theory in normal metals was developed by Campagnano and Nazarov [1]. The circuit theory of mesoscopic transport provides an efficient and controlled way to include e.g. superconducting and spin-transport properties. We generalize the method to include superconducting terminals and use it to investigate the quantum corrections to the proximity density of states and the Andreev conductance.

[1] G. Campagnano and Yu. V. Nazarov, Phys. Rev. B **74**, 125307 (2006)

TT 22.53 Wed 14:00 Poster B

Observation of Coulomb blockade in diamond-like carbon films — •Savcho Tinchev[1], Evgenia Valcheva[2], and Sashka Alexandrova[3] — [1]Institute of Electronics, Bulgarian Academy of Sciences, Tzarigradsko Chaussee 72, 1784 Sofia, Bulgaria — [2]Physics Department, Sofia University, J. Bourchier 5, 1164 Sofia, Bulgaria — [3]Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko Chaussee 72, 1784 Sofia, Bulgaria

Coulomb blockade of tunneling is a phenomenon observed in low capacitance tunnel junctions usually at low temperatures. To fabricate single electron devices operating at room temperatures it is essential to obtain nano-sized quantum dots or nanostructures with sizes below 10 nm, because the charging energy can overcome the thermal energy only in such small structures. Dimensions below 10 nm are, however, below the resolution limit of the electron beam lithography. Therefore self-organization processes are promising candidates for preparing electron devices operating at room temperatures.

We report here on observation of Coulomb blockade in diamond-like carbon (DLC) films at room temperature. Diamond-like carbon films used in our experiments were amorphous hydrogenated carbon films (a-C:H) made by DC PECVD from a mixture of benzene and argon. Nonlinear current voltage characteristics with a threshold voltage of about 3 volts and in some cases also step-like structures, known as Coulomb staircase were observed in diamond like carbon films. We interpret this observation as a clear manifestation of Coulomb blockade found for the first time in these films.

TT 22.54 Wed 14:00 Poster B

Influence of dephasing to the intrinsic spin Hall effect — •Pei Wang — Institut für Physik, Universität Augsburg und LMU München

The intrinsic spin Hall effect has attracted much attention in recent years, because it can be used to generate spin-polarized currents in paramagnetic semiconductors electronically. In the spin Hall effect, a longitudinal electric field creates a transverse motion of spins with the spin-up and spin-down carriers moving in opposite directions, which leads to a transverse spin current perpendicular to the external electric field. I will introduce the intrinsic spin Hall effect in a 2DEG with Rashba spin-orbit coupling and in p-type semiconductors described by a Luttinger Hamiltonian. The spin Hall conductivity in the presence of nonmagnetic and magnetic impurities is calculated. The critical influence of dephasing (inelastic scattering) to the spin Hall effect is discussed.

TT 22.55 Wed 14:00 Poster B

Quantum transport in ferromagnetic Permalloy wires and films — •Daniel Neumaier, Anton Vogl, and Dieter Weiss — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Germany

We investigated the transport properties of mesoscopic Permalloy wires and films at milikelvin temperatures. The samples have been fabricated using electron beam lithography and lift-off techniques.

In wires with a width of 40 nm, a thickness of 15 nm and a length of 140 nm and 340 nm we found mesoscopic conductance fluctuations, originating from the electrons wave nature. These fluctuations reveal a phase coherence length of approx. 200 nm at 20 mK and decrease rapidly with increasing temperature.

To search for weak localization we fabricated arrays of wires to suppress conductance fluctuations. The arrays consist of 4 wires in parallel with a length of 4 micron, a width of 20 nm and a thickness of 15 nm. Below 1 K the conductance of the wire array is decreasing with decreasing temperature without an influence of an applied magnetic field. This behaviour can be explained by electron-electron-interaction, a contribution due to weak localization could not be found. In extended films with a thickness of 15 nm also a conductance decrease due to electron-electron interaction and no contribution due to weak localization was observed.

TT 22.56 Wed 14:00 Poster B

A spin ratchet effect in dissipative systems with spin-orbit coupling — •Sergey Smirnov[1], Dario Bercioux[1,2], Milena Grifoni[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Physikalische Institut, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany

A possibility to generate fully polarized pure spin currents, a hot topic in modern spintronics, is studied. The idea is to create such spin currents using a spin ratchet effect if it exists. We investigate this question in an ac driven quasi-one-dimensional periodic structure with Rashba's spin-orbit interaction [1] and strong dissipative coupling to an external environment. It is analytically proven that when the quantum transport of electrons is restricted within the sub-bands below the barrier and originating from the same Bloch band, the charge transport is totally absent. In contrast we analytically show that the stationary spin current vanishes for symmetric periodic potentials while it can be finite for asymmetric ones. This confirms the existence of the spin ratchet effect in our system. Moreover, we rigorously show that for a harmonic confinement only one component of the spin current is non-zero, that is the spin current is fully polarized.

[1] S. Smirnov, D. Bercioux, and M. Grifoni, Europhys. Lett. 80, 27003 (2007).

TT 22.57 Wed 14:00 Poster B

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

We investigate phase coherent transport through a quasi two-dimensional hole gas in p-doped III-V semiconductors. The problem is treated within a 4-band Luttinger Hamiltonian in a quasi two-dimensional approximation. The transport properties are calculated in an effective tight-binding approximation by means of the Green function method. We consider the influence of coupling between heavy-holes and light-holes in the diffusive regime and ballistic cavities to point out their effect on weak localization.

TT 22.58 Wed 14:00 Poster B

Shot noise in graphene three terminal ballistic devices — •Miriam del Valle[1] and Gianaurelio Cuniberti[2] — [1]Institute of Theoretical Physics, Universität Regensburg — [2]Institute for Materials Science, TU Dresden

Graphene is in the focus of an immense scientific interest due to remarkable quantum properties which may emerge already at room temperature. We present here a study of electronic transport in single-layer graphene ribbons in three-terminal configuration set-ups, where the finite-size effects become of importance. These systems are characterized by much more complex stability diagrams than their nanotube (CNT) counterparts. A symmetry-related suppression of transmission of some states is responsible for the Fabry-Pérot interference patterns obtained for CNT devices, whereas these "dark states" become conducting for graphene. This additional complexity is investigated by analizing shot noise properties.

TT 22.59 Wed 14:00 Poster B

Optimal control of current and shot noise in molecular wires using femtosecond laser pulses — •Guangqi Li[1], Michael Schreiber[2], and Ulrich Kleinekathöfer[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

The tunneling of electrons through a molecular junction weakly coupled to two leads in the presence of a time-dependent external field is studied using using a master equation approach [1-4]. By combining the theory of optimal control and by using a predefined target current, a laser field can be obtained which does generate a predefined current pattern. The same technique can be applied to control also the shot noise in the system in order to minimize it. For a tight-binding approximation of the molecular wire we show how to compute the laser pulses to switch on and off the current through the wire . With this approach the current flow pattern in time can be chosen in an almost arbitrary fashion.

[1] S. Welack, M. Schreiber, and U. Kleinekathöfer, J. Chem. Phys. **124**, 044712 (2006).
[2] U. Kleinekathöfer, G.-Q. Li, S. Welack, and M. Schreiber, Europhys. Lett. **75**, 139 (2006).
[3] G.-Q. Li, M. Schreiber, and U. Kleinekathöfer EPL **79**, 27006/1-6 (2007).
[4] S. Kohler and P. Hänggi, Nature Nanotech. **2**, 675 (2007)

TT 22.60 Wed 14:00 Poster B

General relation between diffusive transport and current-autocorrelation function — •Jochen Gemmer — Universität Osnabrück, Osnabrueck, Germany

The (regular) conductivity relates a current to an external force field. Within linear response theory this coductivity is given by the Kubo formula, i.e., essentially the current-autocorrelation function. The diffusion constant relates a current to a spatial density gradient. We investigate from first principles if and in which sense the diffusion constant can also be calculated from the current-autocorrelation function. In other words, we aim at verifying a generalized Einstein relation on basic quantum mechanical grounds.

TT 22.61 Wed 14:00 Poster B

Approach to transport in modular quantum systems by modelling of reservoirs — •Marcel Ogiewa and Jochen Gemmer — University of Osnabrueck, Osnabrueck, Germany

We investigate the transport behavior in a special class of quantum models, which are essentially of the periodic one-particle type but may nevertheless exhibit regular transport. To induce a current these systems are coupled to different baths at each ending.

The corresponding Lindblad Master Equation is solved by a Monte Carlo stochastic unraveling method in order to find the quasi-stationary state.

Hence we verify the existence of diffusive transport (in a certain parameter range) according to Fourier's law and extract the conductivity. The results are compared to other findings for the same systems derived by entirely different methods.

TT 22.62 Wed 14:00 Poster B

Investigations on transport properties of modular quantum systems based on a perturbative expansion of the current-autocorrelation function — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany

The dynamics of the spatial variance of the deviation of some density (particles, energy, etc.) from equilibrium can be expressed in terms of the dynamics of the current-autocorrelation function, that also appears in the Kubo formula (see also talk J. Gemmer). We present a systematic perturbation expansion for the current-autocorrelation function whose leading order is based on the diagonalization of finite parts of the system.

Additionally, we introduce a numerically feasible approximation for the next higher order to estimate if and for what times the leading order can be expected to give an adequate description. The analysis is supported by numerical calculations for concrete models.

TT 22.63 Wed 14:00 Poster B

Transport in randomly coupled many-particle quantum systems — •Robin Steinigeweg and Jochen Gemmer — Physics Department, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Although models for non-interacting particles in ideally ordered structures are rather simple examples of quantum systems, the complete characterization of the available types of transport often remains an unsolved problem. However, such a characterization has recently been done for a certain class of randomly coupled but translational invariant single-particle models [1]. In particular, a transition from diffusive to ballistic transport has been found in the limit of both small and large length scales, e.g., the long-time dynamics always is ballistic for a sufficiently large system. We discuss whether or not these transitions also appear in similarly structured many-particle quantum systems which naturally are much more complex. To this end we correspondingly consider a randomly coupled, translational invariant model and compare the theoretical predictions with the numerical solution of the full time-dependent Schrödinger equation for a range of accessible model sizes.

• [1] R. Steinigeweg, H.-P. Breuer, and J. Gemmer, Phys. Rev. Lett. **99**, 150601 (2007)

TT 23: Correlated Electrons: (General) Theory

Time: Wednesday 14:00–18:45 Location: H 0104

TT 23.1 Wed 14:00 H 0104

Multigrid Hirsch-Fye quantum Monte Carlo solver for dynamical mean-field theory — •Nils Blümer — Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz

The dynamical mean-field theory (DMFT) is a nonperturbative approach to Hubbard-type models in which an impurity model has to be solved self-consistently. This is possible nonperturbatively using the Hirsch-Fye quantum Monte-Carlo (HF-QMC) algorithm which introduces an imaginary-time discretization $\Delta\tau$. The associated Trotter error impacts all "raw"HF-QMC results including phase boundaries, Green functions, spectra, and scalar observables such as energies and quasiparticle weights. Unbiased estimates of scalar observables can be derived from HF-QMC data by extrapolation $\Delta\tau \to 0$, with high precision and efficiency [1]. However, this *a posteriori* correction of the Trotter error is problematic close to phase boundaries and could so far

not be applied to Green functions and spectra.

In this talk, I show how numerically exact Green functions can be extrapolated from HF-QMC estimates and construct a multigrid HF-QMC algorithm which eliminates the discretization error within the DMFT self-consistency cycle. In contrast to conventional HF-QMC, the multigrid algorithm converges to the numerically exact fixed point(s) and allows for the direct determination of phase boundaries without further extrapolation. It extends the useful range of $\Delta\tau$ values and yields unbiased estimates of observables with high precision and efficiency, even close to phase transitions.

[1] N. Blümer, to appear in Phys. Rev. B [arXiv:0708.1749v3].

TT 23.2 Wed 14:15 H 0104

Bath-symmetries and hybridization sum-rules for CDMFT and DCA — •Erik Koch[1], Giorgio Sangiovanni[2], and Olle Gunnarsson[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

In the Hamiltonian formulation of CDMFT and DCA, the point symmetries of the cluster imply 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. As examples we discuss calculations for the Hubbard model in one-dimension and for 2×2 clusters.

TT 23.3 Wed 14:30 H 0104

Dual Fermion Approach to Susceptibility of Correlated Lattice Fermions — •Sergey Brener[1], Hartmut Hafermann[1], Alexey N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute of Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands

We show how the two-particle Green function can be obtained within the framework of the recently developed Dual Fermion approach. This facilitates the calculation of the susceptibility in strongly correlated systems where long-ranged non-local correlations cannot be neglected. We formulate the Bethe-Salpeter equations for the full vertex in the particle-particle and particle-hole channels and introduce an approximation for practical calculations. The scheme is applied to the two-dimensional Hubbard model at half filling. The spin-spin susceptibility is found to strongly increase for the wavevector $\mathbf{q} = (\pi, \pi)$, indicating the antiferromagnetic instability. Combining this approach with the cluster dual formalism and applying it to the Hubbard model at finite doping we get the possibility to capture all the essential physics of HTSC.

TT 23.4 Wed 14:45 H 0104

Cluster Dual Fermion Approach to Nonlocal Correlations — •Hartmut Hafermann[1], Sergey Brener[1], Alexey N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute of Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands

We formulate a cluster generalization to the recently developed Dual Fermion approach to nonlocal correlations in crystals.

The scheme allows the treatment of long-range correlations beyond the cluster DMFT and nonlocal effects in realistic calculations of multiorbital systems. It is shown that in the simplest approximation one exactly recovers the free-cluster DMFT. Recent results are presented, among them the application to the one-dimensional Hubbard model. Already the first dual fermion correction to the free cluster leads to a drastic improvement of the calculated Green function.

TT 23.5 Wed 15:00 H 0104

Competing Instabilities in One Dimension - Functional Renormalization Group With Symmetry Breaking Terms — •Matthias Ossadnik[1,2] and Carsten Honerkamp[1] — [1]Universität Würzburg — [2]ETH Zürich

Fermionic renormalization group flows often lead to strong coupling, i.e. certain components of the interactions diverge at low energy scale and temperatures. By including appropriate types of symmetry-breaking via counterterms in the initial conditions of the flow, the divergence can however be avoided and properties of the low-temperature state can be computed. Here we show for a one-dimensional example that this approach allows us to describe competing order and quantum phase transitions between ground states with different symmetries, in qualitative agreement with bosonization analysis.

15 min. break

TT 23.6 Wed 15:30 H 0104

Understanding Supersolids — Andre Stoffel and •Miklos Gulacsi — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We model the newly discovered supersolid phase of 4He by a hard-core bosonic quantum lattice model in 3 dimension including nearest and next-nearest neighbor interactions. As hard-core Boson exhibit the same algebra as spin-1/2 operators there exists a one-to-one correspondence to the anisotropic Heisenberg model in an external field. To solve this Heisenberg model we used the Tyablikov Green's function technique and in order to obtain a closed set of equations we used a cumulant decoupling scheme. The obtained Green's functions have been used to study the properties of the system. Here, we are particularly interested in the normal-solid (NS) and supersolid (SS) phases as well as the corresponding phase transition. It was long proposed that vacancies and defects may play a crucial role in the formation of the supersolid phase. Hence we studied the incommensurability which is a measure of the net fraction of vacancies. For the NS phase we re-obtained the well-known thermal activation theory. However, the incommensurability in the SS displays a rather different behavior, which also suggests that the NS to SS transition is a commensurate-incommensurate transition.

TT 23.7 Wed 15:45 H 0104

Plateaux and supersolid phases in $SrCu_2(BO_3)_2$ — •Kai P. Schmidt, Julien Dorier, and Frederic Mila — Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

In a magnetic field, $SrCu_2(BO_3)_2$ displays magnetization plateaux at fractional fillings 1/8, 1/4 and 1/3. This work aims at a microscopic description of these plateaux, and investigate the behavior around these plateaux focussing on possible supersolid phases.

Using series expansion techniques, we have derived a realistic hard-core boson model which is dominated by long-range repulsive interactions and correlated hopping. We investigate the properties of this model by a classical approximation based on a spin representation. While the long-range interactions stabilize solid phases at fractional fillings (magnetization plateaux), the correlated hopping favours supersolid phases. This interplay between interactions and kinetics leads to a rich phase diagram with solid, superfluid, and supersolid competing phases.

TT 23.8 Wed 16:00 H 0104

Non-equilibrium Hubbard Model in an external, time-dependent field — •Andreas Lubatsch and Johann Kroha — Physikalisches Institut, Universitaet Bonn, Germany

Mott-Hubbard insulating materials have the potential to be used for ultrafast electric switches, driven by an external laser field, because of the short relaxation times characteristic for strongly correlated systems. We consider the Hubbard model at half filling, driven by an external, stationary laser field. This electromagnetic field couples to the dipole moment of the charge distribution in the system, i.e. it induces an extra contribution to the hopping amplitude in the Hubbard Hamiltonian, periodic in time (photo-induced hopping). We generalize the dynamical mean-field theory (DMFT) to this non-equilibrium situation, employing a Floquet expansion of the electron density in terms of higher harmonics of the time-periodic hopping amplitude within the Keldysh formalism. We calculate the non-equilibrium electron distribution function, the density of states and the DC conductivity in the presence of the external laser field for laser frequencies above and below the Mott-Hubbard gap. The results demonstrate that the system can be switched from a Mott-Hubbard insulating state to a conducting state by the external field, which corresponds to photo-induced excitations into the upper Hubbard band.

TT 23.9 Wed 16:15 H 0104

Real-time evolution of the nonequilibrium Hubbard model

— •Michael Möckel and Stefan Kehrein — LMU München, Department für Physik und Arnold Sommerfeld Center for Theoretical Physics, Theresienstraße 37, 80333 München

Recent experiments with cold atomic gases loaded onto optical lattices have opened up a new line of research into nonequilibrium properties of closed quantum systems. Motivated by these results we study the Hubbard model in infinite dimensions for a weak two-particle interaction $U\Theta(t)$ which is switched on instantaneously in time. We address the question of its real-time evolution by means of the flow equation technique and calculate the time-dependent momentum distribution function. After an initial buildup of a correlated distribution on a time scale set by U^{-1} a nonequilibrium transient state extends on a long time scale proportional to U^{-4}. It resembles an interacting Fermi liquid at zero temperature but its quasiparticle residuum mismatches the value for the correlated equilibrium state.

TT 23.10 Wed 16:30 H 0104

Non-thermal steady states after an interaction quench in the Falicov-Kimball model — •Martin Eckstein and Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

We present the exact solution of the Falicov-Kimball model after a sudden change of its interaction parameter using non-equilibrium dynamical mean-field theory. For different interaction quenches between the homogeneous metallic and insulating phases the system relaxes to a non-thermal steady state on time scales on the order of $\hbar$/bandwidth, showing collapse and revival with an approximate period of h/interaction if the interaction is large. We discuss the reasons for this behavior and provide a statistical description of the final steady state by means of generalized Gibbs ensembles.

TT 23.11 Wed 16:45 H 0104

Relaxation of a one-dimensional Mott insulator after a quantum quench — •Marcus Kollar and Martin Eckstein — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

We obtain the exact time evolution for a one-dimensional integrable fermionic Hubbard model after a sudden change of its interaction parameter, starting from either a metallic or a Mott-insulating state. In all cases the system relaxes to a new steady state, showing that the presence of the Mott gap does not inhibit relaxation. The properties of the final state are described by the fully constrained Gibbs ensemble. We discuss under which conditions such ensembles provide the correct statistical description of integrable systems in general.

15 min. break

TT 23.12 Wed 17:15 H 0104

Inhomogeneous solutions of the charge rotationally invariant Gutzwiller approach for the Hubbard model — •Falk Günther and Götz Seibold — BTU Cottbus, PO BOX 101344, 03013 Cottbus

We present a charge rotationally invariant Gutzwiller approach for the attractive Hubbard model. It is shown the formalism can be used to calculate homogeneous and inhomogeneous charge-ordered (CDW) and superconducting (SC) structures. Our formalism reproduces the correct degeneracy between CDW and SC phase in the half filled system. Restricting to on-site attraction we find that inhomogeneous structures e.g. anti-phase domain walls with regard to the SC order are only excitations of the system but never constitute the ground state of the model. In addition we present results for the Gutzwiller approximated extended Hubbard model including nearest neighbor repulsion, which allows for a competition between inhomogeneous CDW and SC textures.

TT 23.13 Wed 17:30 H 0104

Gutzwiller approach to phonon renormalization in the correlated SSH Model — •Ernst von Oelsen — Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany

The SSH Model [1] is supplemented with a Hubbard repulsion term in order to study the influence of electronic correlations on transitive phonon excitations. Our investigations are based on the time-dependent Gutzwiller approximation [2] and we restrict to the undimerized case. Eliminating double occupancy fluctuations via an anti-adiabaticity condition we obtain the quadratic fluctuations in the phonon and electronic density fields. Already on this level we find correlation-induced softening for small wave vectors which eventually induces an instability in addition to the Peierls nesting mechanism. In addition we show that inclusion of a Hubbard repulsion creates additional couplings between electrons and phonons beyond the bare transitive interaction. Finally we calculate the phonon self-energy which is compared with the uncorrelated case.

[1] W. P. Su and J. R. Schrieffer and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980)

[2] G. Seibold and J. Lorenzana, Phys. Rev. Lett. **86**, 2605 (2001)

TT 23.14 Wed 17:45 H 0104

Rotationally invariant slave-boson formalism and momentum dependence of the quasiparticle weight — •Frank Lechermann[1], Antoine Georges[2], Gabriel Kotliar[3], and Olivier Parcollet[4] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]CPHT, École Polytechnique, Palaiseau, France — [3]Serin Physics Laboratories, Rutgers University, NJ, USA — [4]Service de Physique Théorique, CEA Saclay, Gif-Sur-Yvette, France

The rotationally invariant formulation of the slave-boson formalism is generalized to multiorbital models, with arbitrary interactions, crystal fields, and multiplet structure [1]. This allows for the study of multiplet effects on the nature of low-energy quasiparticles. Nondiagonal components of the matrix of quasiparticle weights can be calculated within this framework. When combined with cluster extensions of dynamical mean-field theory, this method renders it possible to address the effects of spatial correlations, such as the generation of the superexchange and the momentum dependence of the quasiparticle weight. The method is illustrated on several examples, including a two-dimensional single-band Hubbard model (within a two-site cellular dynamical mean-field approximation).

[1] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, PRB **76** 155102 (2007).

TT 23.15 Wed 18:00 H 0104

Absence of fermionic quasi-particles in the BEC regime of the attractive Fermi gas — •Nils Lerch, Lorenz Bartosch, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

We calculate the effect of order parameter fluctuations on the fermionic single-particle excitations of the attractive Fermi gas in the BEC regime where the binding energy of the s-wave bound state is the largest energy scale. We show that in dimensions $D = 3$ the singular interaction between the fermions mediated by the gapless Bogoliubov-Anderson mode prohibits the existence of well-defined quasi-particles. We explicitly calculate the single-particle spectral function and show that in this case the quasi-particle residue and the density of states are logarithmically suppressed.

TT 23.16 Wed 18:15 H 0104

Self-masking of Fermi surface symmetry breaking in layered materials — •hiroyuki yamase — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Recently, a new type of spontaneous symmetry breaking, the d-wave type Fermi surface deformation (dFSD), the so-called Pomeranchuk instability, was found in various two-dimensional (2D) models such as t-J, Hubbard, and extended Hubbard. Such 2D systems are often realized in layered materials, where a small interlayer coupling exists. In this contribution, employing the bilayered model with a pure forward scattering interaction driving the dFSD instability, we study the stacking of the dFSD state along the z axis. Since the dFSD is characterized by breaking of the Ising symmetry, there are two possibile stacks, (+,+) and (+,–). We find that the latter "antiferromagnetic"configuration is usually favored and thus bulk symmetry breaking is hidden.

TT 23.17 Wed 18:30 H 0104

Influence of electronic correlations on the ground-state properties of CeN. — •Elena Voloshina[1] and Beate Paulus[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

The electron-correlation effects on the ground-state properties of CeN were studied by *ab initio* quantum-chemical methods. The $4f$-states of cerium were treated with $4f$-in-core pseudopotential derived by M. Dolg *et al.* for trivalent cerium (Ce^{11+}-PP) [1]. The approach which was used consists in the combination of two separate steps: 1) the

ground-state Hartree-Fock calculations for the crystal; 2) application of the method of increments [2] to the studied system, which allows an expansion of bulk properties using the information from quantum-chemical calculations performed for finite cluster, in connection with the size-extensive coupled-cluster method. As it can be expected, for CeN correlation play a significant role: with Hartree-Fock method only a half of the experimental cohesive energy has been covered, whereas after correlation corrections the ground-state properties were shown to be in good agreement with the experimental data found in literature. The computed ground-state properties of CeN are compared with corresponding values obtained for LaN and GdN [3].

[1] M. Dolg, P. Fulde, W. Küchle, *et al.* J. Chem. Phys. 94, 3011 (1991). [2] H. Stoll, Phys. Rev. B 46, 6700 (1992). [3] S. Kaldova, M. Dolg, H.-J. Flad, *et al.* Phys. Rev. B 57, 2127 (1998).

TT 24: Correlated Electrons: Low-dimensional Systems - Models

Time: Wednesday 14:00–19:00 Location: H 2053

TT 24.1 Wed 14:00 H 2053

Particle-hole symmetry and the Pfaffian state — •Bernd Rosenow, Michael Levin, and Bertrand I. Halperin — Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

The Moore-Read Pfaffian (Pf) state is believed to be a strong candidate for the observed quantum Hall plateau at filling fraction $\nu = 5/2$. This possibility is particularly exciting since the quasiparticle excitations in this state carry non-abelian statistics. Much work has been devoted to understanding the basic physical properties of the Pf state. However, one aspect of the Pf state has not been addressed - namely, its behavior under particle-hole (PH) conjugation of electrons in the spin-aligned partially occupied second Landau level. This issue is important because, to a good approximation, the Hamiltonian of the $\nu = 5/2$ FQH system is symmetric under this PH conjugation.

We show that the particle-hole conjugate of the Pfaffian state - or "anti-Pfaffian" state - is in a different universality class from the Pfaffian state, with different topological order. The two states can be distinguished by both their bulk and edge physics though the difference is most dramatic at the edge: the edge of the anti-Pfaffian state has a composite structure that leads to a different thermal Hall conductance and different tunneling exponents than the Pfaffian state. At the same time, the two states are exactly degenerate in energy for a $\nu = 5/2$ quantum Hall system in the idealized limit of zero Landau level mixing. Thus, both are good candidates for the observed $\sigma_{xy} = \frac{5}{2}(e^2/h)$ quantum Hall plateau.

TT 24.2 Wed 14:15 H 2053

Emergent fermions and anyons in the Kitaev model — •Kai P. Schmidt[1], Sebastien Dusuel[2], and Julien Vidal[3] — [1]Institute of Theoretical Physics, Ecole Polytechnique Federal de Lausanne, CH-1015 Lausanne, Switzerland — [2]Lycee Louis Thuillier, 70 Boulevard de Saint Quentin, 80098 Amiens Cedex 3, France — [3]Laboratoire de Physique Theorique de la Matiere Condensee, CNRS UMR 7600,

We study the gapped phase of the Kitaev model on the honeycomb lattice using perturbative continuous unitary transformations. The effective low-energy Hamiltonian is found to be an extended toric code with interacting anyons. High-energy excitations are emerging free fermions which are composed of hardcore bosons with an attached string of spin operators. The excitation spectrum is mapped onto that of a single particle hopping on a square lattice in a magnetic field. The present approach yields analytical perturbative results in the thermodynamical limit and gives a simple description of the spectrum without using the Majorana or the Jordan-Wigner fermionization initially proposed to solve this problem.

TT 24.3 Wed 14:30 H 2053

Novel many-body states on the honeycomb lattice — •Carsten Honerkamp — Theoretische Physik, Universität Würzburg

We apply a functional renormalization group scheme to search for interesting many-body states of electrons on the honeycomb lattice, interacting by onsite and up to second nearest-neighbor terms. Near half band-filling, critical minimal interaction strengths are required for instabilities toward antiferromagnetic or charge-density wave order. A strong second-nearest neighbor repulsion drives the system into a quantum-spin-Hall insulating state. Away from half filling, f-wave triplet pairing and $d+id$ singlet pairing instabilities are found to emerge out of density-wave regimes.

TT 24.4 Wed 14:45 H 2053

Dynamic structure factor of Luttinger liquids — •Peyman Pirooznia[1], Florian Schütz[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt, Germany — [2]Department of Physics, Brown University, Providence, RI 02912, USA

We calculate the dynamic structure factor $S(\omega, q)$ of non-relativistic fermions with quadratic energy dispersion and long-range density-density interaction, assuming that the Fourier transform f_q is the interaction is dominated by momentum transfers $q \lesssim q_c \ll k_F$, where k_F is the Fermi momentum. Using functional bosonization and the known properties of symmetrized closed fermion loops, we obtain an expansion of the inverse irreducible polarization $\Pi_*^{-1}(q, \omega)$ to second order in the small parameter q_c/k_F. In contrast to conventional bosonization and to direct fermionic perturbation theory, in our approach we do not generate unphysical mass-shell singularities. We then show that for $q \ll q_c$ the width w_q of the single-pair particle-hole continuum on the frequency axis scales as q^2/m. However, for $q \to 0$ most of the spectral weight is carried by the collective zero sound (ZS) mode, whose damping γ_q is parametrically smaller than w_q. For sharp cutoff in momentum space, $f_q = f_0\Theta(q_c - q)$, we find to order $(q_c/k_F)^2$ that the ZS mode is not damped at all. For smooth cutoff the ZS damping scales as q^n with $n \geq 3$ for $q \to 0$, where the value of n depends on the functional form of f_q. We also comment on previous attempts to calculate the damping γ_q of the ZS peak in Luttinger liquids.

TT 24.5 Wed 15:00 H 2053

Towards Experimental Verification of Luttinger Liquid Behavior — •Peter Wächter[1], Volker Meden[2], and Kurt Schönhammer[1] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]Institut für Theoretische Physik, RWTH Aachen, Germany

Luttinger Liquid (LL) behavior of metallic one-dimensional (1d) electron systems is well established as a theoretical concept. It manifests itself e.g. in the power law scaling of a variety of physical observables as functions of external parameters with exponents depending on a single parameter, the LL parameter K. However, experiments revealing clear indications of LL behavior are very rare. One major difficulty is to convincingly exclude any other source than LL physics for the observed scaling. To cope with this problem we propose a scheme to extract K from two different observables as functions of two different external parameters p_1 and p_2. Consistency of the findings in an experiment, that means $K(p_1) \approx K(p_2)$, would provide strong evidence for LL physics.

TT 24.6 Wed 15:15 H 2053

Effects of dissipation on disordered Luttinger liquids — •Zoran Ristivojevic and Thomas Nattermann — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We study theoretically the low energy properties of 1D Luttinger liquids in the presence of dissipation and disorder. Both the case of a single impurity (Kane-Fisher) and that of gaussian randomness (Giamarchi-Schulz) are considered in a renormalization group approach. We show that dissipation drastically changes the phase diagram and the conductance/conductivity in both cases. The approach is an extension of recent work of Cazallila et al. (Phys. Rev. Lett. 97, 076401 (2006)).

15 min. break

TT 24.7 Wed 15:45 H 2053

Density Distribution in Finite One-Dimensional Interacting Fermion Systems — •Stefan Soeffing and Sebastian Eggert — FB Physik, TU Kaiserslautern, 67663 Kaiserslautern

We numerically investigate the ground state density distribution of the Hubbard model with open boundary conditions by means of the Density Matrix Renormalization Group (DMRG). In addition to the expected Friedel oscillations with wave vector $2k_F$, we also observe $4k_F$ Wigner crystal oscillations which are in certain cases the dominant contribution.

We systematically analyze the amplitude of the density oscillations as a function of system length, lattice filling and interaction strength. The decay of the standing waves with respect to the distance from the boundaries is compared with the predicted power laws from Luttinger Liquid theory.

TT 24.8 Wed 16:00 H 2053

Local Density of States of a Finite Quantum Wire: Numerical Results from DMRG in Comparison with Bosonization Results — Imke Schneider and •Sebastian Eggert — FB Physik, TU Kaiserslautern, 67663 Kaiserslautern

We consider a finite quantum wire, modeled by a one-dimensional system of locally interacting Fermions. We are able to numerically obtain the local density of states (LDOS) with the help of the density matrix renormalization group (DMRG). We believe this is the first time that the LDOS was calculated energy and spatially resolved for an interacting lattice model. We are able to compare to analytic expressions for individual energy levels in systems with open boundary conditions from Luttinger Liquid theory.

In this way, a detailed understanding of the LDOS for each individual energy level can be obtained in both fermionic and bosonic pictures. Certain degeneracies of the Luttinger Liquid spectrum are lifted in the lattice model by band curvature and interaction effects, leading to a large number of states and energy levels in the LDOS.

TT 24.9 Wed 16:15 H 2053

The magnetic polaron in the one-dimensional Kondo lattice model away from half filling — •Sebastian Smerat[1,2], Ian P. McCulloch[3], Ulrich Schollwöck[2], and Herbert Schoeller[1] — [1]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Deutschland — [2]Institut für Theoretische Physik C, RWTH Aachen, D-52056 Aachen, Deutschland — [3]School of Physical Sciences, the University of Queensland, QLD 4072, Australia

Recent progress in the fabrication of nanosized materials may in the near future allow to load nanotubes with, e.g., fullerenes. We expect the magnetic and transport properties of such materials to be adequately described by a one-dimensional Kondo lattice model. This motivates our numerical analysis of the model. Our main focus is on the properties of magnetic polarons, which previously have been argued to exist in both the limit of a half-filled and an empty conduction band. Using a state-of-the-art numerical method, the density matrix renormalization group algorithm, we compute the spectral functions of the model as a function of filling. As a main result, we provide clear evidence for the existence of the magnetic polaron away from half filling. A careful analysis of the spectral functions allows us to determine lower bounds for the quasi-particle life-time.

TT 24.10 Wed 16:30 H 2053

Hybrid approach for quantum antiferromagnets in a uniform magnetic field: Method — •Andreas Kreisel, Francesca Sauli, Nils Hasselmann, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

The properties of ordered quantum antiferromagnets can be calculated by an expansion in inverse powers of the spin quantum number S via the Holstein-Primakoff transformation of the underlying Heisenberg model, or by a renormalization group approach to the non-linear sigma model (NLSM). The relation between these descriptions can be made precise by expressing the canonical magnon operators in the spin-wave approach in terms of hermitian field operators which represent the uniform and staggered components of the spin operators. An effective action for the staggered spin fluctuations (low energy degrees of freedom) has been derived for the case of vanishing magnetic field [1]. We now generalize the approach to quantum antiferromagnets in a uniform magnetic field and discuss the resulting interaction vertices in comparison with those of the NLSM and the conventional $1/S$ expansion.
[1] N. Hasselmann and P. Kopietz, Europhys. Lett. **74**, 1067 (2006)

TT 24.11 Wed 16:45 H 2053

Hybrid approach for quantum antiferromagnets in a uniform magnetic field: Application — •Francesca Sauli, Andreas Kreisel, Nils Hasselmann, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We use a hermitian parameterization of the canonical magnon operators obtained from the usual Holstein-Primakoff transformation and combine it with a $1/S$-expansion of the Heisenberg model to acquire the effective action for quantum antiferromagnets (QAF). Integrating over the fields associated with the uniform spin fluctuations yields a field theory for the staggered spin fluctuations on a lattice but avoids the cutoff ambiguities of the non-linear sigma model (NLSM). Using this effective lattice action for the staggered spin-fluctuations of a QAF subject to a uniform magnetic field we explicitly calculate the leading $1/S$-corrections to the spin wave velocity as well as the damping of the staggered spin fluctuations.

TT 24.12 Wed 17:00 H 2053

Two particle excitations of projected wavefunctions. — •Tejaswini Dalvi and Claudius Gros — ITP, J.W. Goethe University, Frankfurt

The study of projected wavefunctions involves extensive use of Gutzwiller approximation (GA), along with Variational Monte Carlo (VMC), to study ground state properties. Recent studies include, study of properties of elementary excitations in doped Mott-Hubbard systems in detail by Renormalized Mean Field Theory (RMFT) and VMC. Important progress has been made in extending the technique of GA to calculate matrix elements in partially projected wavefunctions.

This generalization has allowed construction of normalized projected excitations for Fermi sea and BCS wavefunctions and evaluation of matrix elements between ground state and excited states. We here propose to study the particle-particle, hole-hole and particle-hole scattering for projected particle and projected hole state by generalised GA and VMC. This aims at laying foundation for a "Projected Fermiliquid Theory".

15 min. break

TT 24.13 Wed 17:30 H 2053

Doped ladders under magnetic field — •Guillaume Roux[1], Edmond Orignac[2], Steven R. White[3], and Didier Poilblanc[4] — [1]Institut für theoretische Physik C, RWTH Aachen, Aachen, Germany — [2]Laboratoire de Physique de l'École Normale Supérieure de Lyon, ENS-Lyon, CNRS UMR5672, Lyon, France — [3]Department of Physics and Astronomy, University of California, Irvine, USA — [4]Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier, CNRS UMR5152, Toulouse, France

We study the effect of the magnetic field on doped two-leg ladders by means of density-matrix renormalization group (DMRG) and bosonization techniques. It is shown that the Zeeman effect induces a magnetization plateau controlled by hole doping and a FFLO phase. This latest is associated with an exceeding of Pauli limit which can help with the interpretation of experiments. Furthermore, superconducting non-polarized triplet fluctuations are also found to emerge at high magnetic field. In addition, the orbital effect is included and the transverse current correlations are shown to be commensurate with the charge density ones as soon as the magnetic field is turn on. Lastly, the diamagnetic susceptibility probes the commensurate phases appearing for commensurate dopings.

TT 24.14 Wed 17:45 H 2053

Effect of shell structure on Anderson orthogonality catastrophe — •Swarnali Bandopadhyay and Martina Hentschel — Max Planck Institute for the Physics of Complex Systems, N{\"o}thnitzer Str. 38, 01187 Dresden, Germany

We study the Anderson orthogonality catastrophe (AOC) for parabolic quantum dots (PQD). AOC is one of the many-body responses leading to Fermi-edge singularities in, e.g., the photo-absorption cross-section of metals. We use rank-one perturbation to model the static impurity created by an x-ray exciting a core electron into the conduction band. A PQD is characterized by an inherent shell structure. The degeneracy in a shell is slightly lifted in presence of a weak magnetic field. The behavior of a PQD is governed by two energy-scales: The inter-shell spacing (set by the oscillator's bare frequency) and the intra-shell level spacing (set by the magnetic field). We study the statistics of the Anderson overlap for an uniform as well as a realistic mesoscopic PQD as a function of perturbation strength, position of the localized impurity, number of electrons and system size. The clustering of levels gives rise

to an oscillatory behavior in Anderson overlap as a function of filling of the PQD levels. In particular, we find a pronounced AOC, related to the quasi-degeneracy of levels, whenever a new shell is opened up. This inherent shell structure survives in the presence of mesoscopic fluctuations, when we observe the Anderson overlap to remain unchanged despite adding several electrons to the system. A similar bunching phenomenon has been observed in transport measurements on quantum dots by Zhitenev et. al.[PRL,79, 2308 (1997)].

TT 24.15 Wed 18:00 H 2053

Konkurrenz von Coulomb-Abstoßung und Elektron-Phonon-Wechselwirkung in einem eindimensionalen Elektron-Phonon-System — •Gerd Zschaler, Steffen Sykora und Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

Wir untersuchen ein verallgemeinertes Su-Schrieffer-Heeger Modell mit zusätzlicher Coulomb-Abstoßung zwischen nächsten Nachbarn. Während die Elektron-Phonon-Wechselwirkung eine Dimerisierung auf den Bonds favorisiert, führt die Coulomb-Abstoßung zu einer Ladungsdichtewelle (CDW). Mit Hilfe der projektiven Renormierungsmethode (PRM) werden beide Wechselwirkungen sukzessive eliminiert, so dass ein renormiertes, entkoppeltes Elektron-Phonon-System resultiert. Der Einfluss der konkurrierenden Wechselwirkungen auf die renormierten Einteilchenenergien wird untersucht.

TT 24.16 Wed 18:15 H 2053

Entanglement percolation at quantum phase transitions in random quantum magnets — •Yu-Cheng Lin[1], Ferenc Igloi[2,3], and Heiko Rieger[1] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany — [2]Research Institute for Solid State Physics and Optics, H-1525 Budapest, Hungary — [3]Institute of Theoretical Physics, Szeged University, H-6720 Szeged, Hungary

We study the scaling of the entropy quantifying the degree of quantum entanglement between two regions in a bipartite random quantum Ising model in two dimensions, using an asymptotically exact renormalization group treatment [1]. This system undergoes a quantum phase transition at a certain transverse field strength, at which point the von Neumann entanglement entropy of a subsystem violates the "area law", providing evidence for non-trivial and long-range quantum entanglement in the ground state. The entanglement entropy per surface area of a subsystem diverges in a double logarithmic form, arising from a type of percolation of the critical ground state that is fundamentally different from classical percolation. The latter can be found in an analogous quantum system with random bond dilution; here the area law is valid at the quantum critical point, which implies that entanglement cannot be regarded as an indicator of quantum criticality for higher dimensional systems in the way as for one-dimensional cases.

[1] Y.-C. Lin, F. Iglói and H. Rieger, Phys. Rev. Lett. 99, 147202 (2007).

TT 24.17 Wed 18:30 H 2053

Spin-orbit coupling and electron correlations in quantum wires — •Jens Eiko Birkholz[1] and Volker Meden[2] — [1]Institut für Theoretische Physik, Universität Göttingen, D- 37077 Göttingen, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, D-52056 Aachen, Germany

We investigate the influence of the spin-orbit coupling on the transport properties of mesoscopic quantum wires. For a continuum model we discuss the effect of the spin-orbit interaction resulting from the lateral potential necessary to confine the two-dimensional electron gas, ocurring at a semiconductor hetero junction, to a quasi one-dimensional wire geometry. The spin polarization at a potential step in the presence of a magnetic field is analyzed. We introduce a lattice model which shows similar low-energy physics. For this lattice model we use the functional renormalization group method to investigate the role of the two-particle interaction (Coulomb interaction). The interplay of spin-orbit coupling, potential barriers, and electron correlations leads to interesting phenomena in the low-energy physics regime.

TT 24.18 Wed 18:45 H 2053

Single hole and vortex excitations in the doped Rokhsar-Kivelson quantum dimer model on the triangular lattice — •Hugo Ribeiro[1,2], Samuel Bieri[2], and Dmitri Ivanov[2] — [1]Institute of theoretical physics C, RWTH Aachen, Germany — [2]Institute of theoretical physics, EPF Lausanne, Switzerland

We consider the doped Rokhsar-Kivelson quantum dimer model on the triangular lattice with one mobile hole (monomer) at the RK point. The motion of the hole is described by two branches of excitations: the hole may either move with or without a trapped Z2 vortex (vison). We perform a study of the hole dispersion in the limit where the hole hopping amplitude is much smaller than the inter-dimer interaction. In this limit, the hole without vison moves freely and has a tight-binding spectrum. On the other hand, the hole with a trapped vison is strongly constrained due to interference effects and can only move via higher-order virtual processes.

TT 25: Superconductivity: Heterostructures, Andreev Scattering, Proximity Effect, Coexistence

Time: Wednesday 14:00–15:30 Location: H 3010

TT 25.1 Wed 14:00 H 3010

Andreev bound state spectrum in half-metallic ferromagnets — •Matthias Eschrig — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe

Half-metallic ferromagnets are important for potential applications in spintronics and as sources of completely spin-polarized currents. In heterostructures with superconductors they introduce new effects in the interface regions, like spin-mixing and triplet rotation. A triplet supercurrent trough a half metal has been prediced [1] and experimentally verified [2]. Another interesing question regards the question how the density of states is modified in the half-metallic region. Here we present results of the Andreev bound state spectrum in a half-metal/superconductor proximity structure. We discuss the dependence on the interface parameters that enter the interface scattering matrix of the heterostructure. We discuss the role of odd-frequency pairing amplitudes in the proximity structure [3]. We also study the modification of the Andreev bound state spectrum in a superflow.

[1] M. Eschrig et al., Phys. Rev. Lett. **90**, 137003 (2003).
[2] R.S. Keizer et al., Nature, **439**, 825-827 (2006).
[3] M. Eschrig, T. Löfwander, submitted to Nature Physics.

TT 25.2 Wed 14:15 H 3010

Transport through ferromagnet-superconductor contacts — •Georgo Metalidis and Matthias Eschrig — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe

Rapid advances in nanofabrication techniques have made it possible to create high quality ferromagnet-superconductor heterostructures. Apart from potential device applications, a variety of fundamental physical phenomena make such structures interesting both from the experimental and theoretical point of view. The behavior of hybrid ferromagnet-superconductor devices is largely determined by the phenomena proximity effect and Andreev scattering. In the present work, we make use of the quasiclassical theory of superconductivity in order to study Andreev reflection processes at ferromagnet-superconductor interfaces. We address the role that impurities play in the phenomenon of crossed Anreev reflection.

TT 25.3 Wed 14:30 H 3010

Non-local Andreev reflection in superconducting quantum dots — •Dmitry Golubev and Andrei Zaikin — Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021, Karlsruhe, Germany

With the aid of the Keldysh technique we develop a microscopic theory of non-local electron transport in three-terminal NSN structures consisting of a chaotic superconducting quantum dot attached to one superconducting and two normal electrodes. Our theory fully accounts for non-equilibrium effects and disorder in a superconducting terminal. We go beyond perturbation theory in tunneling and derive a general expression for the system conductance matrix which remains valid in both weak and strong tunneling limits. We demonstrate that the proximity effect yields a decrease of crossed Andreev reflection (CAR). Beyond weak tunneling limit the contribution of CAR to the non-local conductance does not cancel that of direct electron transfer between

two normal terminals. We argue that temperature dependence of the non-local resistance of NSN devices is determined by the two competing processes – Andreev reflection and charge imbalance – and it has a pronounced peak occurring at the crossover between these two processes. This behavior is in a good agreement with recent experimental observations.

TT 25.4 Wed 14:45 H 3010

Superconducting spin valve structures grown on epitaxial [Fe/V]-(001) superlattices — •Gregor Nowak[1], Hartmut Zabel[1], Björgvin Hjörvarsson[2], and Kurt Westerholt[1] — [1]Experimentalphysik /Festkörperphysik, Ruhr - Universität Bochum, Germany — [2]Department of Physics, University of Uppsala, Sweden

In a superconducting F1/S/F2 spin valve trilayer structure a superconducting layer (S) is imbedded by a ferromagnetic layer F1 and F2. Model calculations based on the F/S proximity effect have shown that with suitable parameters for the thicknesses and correlations lengths of the F and S-layers the superconductivity can be switched off and on by rotating the magnetization of F1 and F2 from a parallel to an antiparallel orientation. Experimentally, however, it turned out to be challenging to optimize the F1/S/F2 device and until now only very small differences of the superconducting (SC) transition temperature Ts between the parallel and antiparallel orientation has been observed. We have prepared epitaxial F1/S/F2 spin valve systems using an [Fe/V] superlattice as F1, V as the superconducting layer S and Co, Fe(1-x)V(x) layer as F2. The epitaxial quality in this kind of heterostructures reduces the impurity and surface electron scattering so that the superconducting coherence length approaches the thickness of the V-layer. We observe a well pronounced spin valve effect, especially in the system with the Fe(1-x)V(x)-alloy layers, which can be as high as tens of mK.

TT 25.5 Wed 15:00 H 3010

Josephson Effect in Hybrid Oxide Heterostructures with an Antiferromagnetic Layer — •Philipp Komissinskiy[1,2,3], Gennady Ovsyannikov[2,3], Igor Borisenko[2], Yulii Kislinskii[2], Sandra Heinz[1], Dag Winkler[3], and Lambert Alff[1] — [1]Department of Materials Science, Darmstadt University of Technology, 64287 Darmstadt, Germany — [2]Institute of Radio Engineering and Electronics Russian Academy of Sciences, 125009 Moscow, Russia — [3]Department of Microtechnology and Nanoscience, Chalmers University of Technology, 41296 Gothenburg, Sweden

Josephson coupling between an s- and d-wave superconductor through $Ca_{1-x}Sr_xCuO_2$ antiferromagnetic layer was observed for the hybrid $Nb/Au/Ca_{1-x}Sr_xCuO_2/YBa_2Cu_3O_{7-\delta}$ heterostructures and investigated as a function of temperature, magnetic field and applied millimeter-wave electromagnetic radiation [1]. Values of the Josephson characteristic voltage $V_c = I_cR_N \sim 100-200\,\mu$V were demonstrated in the Nb/Au/CSCO/YBCO junctions with up to 50 nm thick CSCO AF layer. The ac Josephson effect is manifested in multiple Shapiro steps, which are well fitted by the RSJ Josephson junction model. The magnetic field dependence of the supercurrent $I_c(H)$ exhibits anomalously rapid oscillations, which is the first experimental evidence of the theoretically predicted giant magneto-oscillations in Josephson junctions with antiferromagnetic interlayers.

[1] P. Komissinskiy, G. A. Ovsyannikov, I. V. Borisenko, Yu.V. Kislinskii, K.Y. Constantinian, A.V. Zaitsev, and D. Winkler, Phys. Rev. Lett. **99**, 017004 (2007).

TT 25.6 Wed 15:15 H 3010

Inhomogeneous vortex distribution and magnetic coupling in oxide superconductor-ferromagnet hybrids — •Joachim Albrecht[1,2], Märit Djupmyr[1], Soltan Soltan[3], Hanns-Ulrich Habermeier[3], Malcolm Connolly[2], and Simon Bending[2] — [1]MPI für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — [2]Department of Physics, University of Bath, Bath BA2 7AY, UK — [3]MPI für Festkörperforschung, Heisenbergstr.1, 70569 Stuttgart

Hybrid systems of thin films of oxide ferromagnets and high-temperature superconductors have been investigated by Scanning Hall Probe Microscopy to analyze the local magnetic flux density distribution at low temperatures [1]. In addition to the intrinsic properties of the films themselves such structures exhibit novel phenomena due to complex interactions arising at the interface between them. As a consequence the distribution of vortices in the superconductor is strongly influenced by the magnetic background arising from the ferromagnet. The local magnetic information obtained from Scanning Hall Probe Microscopy images provides clear evidence for the presence of a magnetic dipolar interaction between the magnetic domains of the ferromagnetic component and the vortex ensemble in the superconductor.

[1] J Albrecht et al., New Journal of Physics **9**, 379 (2007)

TT 26: Superconductivity: Vortex Dynamics, Vortex Phases, Pinning

Time: Wednesday 15:45–18:15 Location: H 3010

TT 26.1 Wed 15:45 H 3010

General critical state in type-II superconductors with longitudinal currents — •Ernst Helmut Brandt[1] and Grigorii Mikitik[1,2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]B. Verkin Institute for Low Temperature Physics and Engineering, NUAS, Kharkov, Ukraine

The concept of the Bean critical state has been very successful in superconductors with vortex pinning. It states that the current density $|\mathbf{j}|$ is either zero or j_c, the critical current density, and it thus predicts sharp spatial jumps of $\mathbf{j}$. However, this usual critical state model applies only when $\mathbf{j}$ is perpendicular to the vortex lines everywhere. We generalize this model to the frequent situation when $\mathbf{j}(\mathbf{r})$ is at arbitrary angle with respect to the induction $\mathbf{B}(\mathbf{r})$, by postulating that only the perpendicular component $j_\perp$ (which causes the Lorentz force) is critical, $j_\perp \le j_c$. Surprisingly, even for the simple example of a slab in rotating magnetic field such that no flux cutting occurs, the resulting spatial profiles of $\mathbf{j}(x)$ and $\mathbf{B}(x)$ in the critical state are now smooth, diffusion like, and do not exhibit the expected sharp fronts.

[1] E. H. Brandt and G. P. Mikitik, Phys. Rev. B **76**, 64526 (2007).

TT 26.2 Wed 16:00 H 3010

Vortex Matter and Vortex Manipulation in Mesoscopic Superconducting Systems — •Roger Wördenweber[1], Eugen Hollmann[1], Jürgen Schubert[1], Rolf Kutzner[1], Konstantin Ilin[2], and Michael Siegel[2] — [1]Institute for Bio- and Nanosystems and cni - Center of Nanoelectronic Systems for Information Technology, Research Center Jülich — [2]Institute for Micro- and Nano-Electronic Systems, University of Karlsruhe

The understanding of the properties of Abrikosov vortices in mesoscopic superconducting systems that are exposed to low and high-frequencies electric fields is of interest for basic aspects of vortex matter and for potential application of superconductivity in fluxonic devices. We report on theoretical aspects and new experiments on vortex matter in patterned superconducting films. The impact of micropatterns on the vortex mobility and vortex manipulation is examined for frequencies ranging from dc to 20GHz. Conventional superconducting films (Nb and NbN) as well as HTS films (YBCO) are examined. The manipulation of the vortices in thin films is achieved either by patterning with various hole arrays (antidots of different size and geometry) or by adding nanodots. The mobility and the manipulation of the direction of vortex motion by the micro and nanostructures are analyzed as function of frequency. Vortex diodes are generated by asymmetric pinning or an additional vortex driving potential provided by a dc current. The diode effect is demonstrated for different frequency regimes.

TT 26.3 Wed 16:15 H 3010

Commensurability effects in Nb thin films with randomly diluted pinning arrays — •Daniel Bothner[1], Matthias Kemmler[1], Konstantin Ilin[2], Michael Siegel[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena, Universität Tübingen, Germany — [2]IMS, Universität Karlsruhe, Germany

We study experimentally the critical depinning current I_c versus applied magnetic field B in Nb thin films, which contain 2D arrays of circular antidots arranged in randomly diluted triangular lattices.

For measurements of electric transport close to the Nb transition temperature T_c, the sample temperature is controlled and stabilized via an optical, very low noise heating system.

We investigate samples with fixed lattice constant as well as such with fixed antidot-density and compare dilutions between 0% and 80%. Our results show some interesting features in the $I_c(B)$ patterns as commensurability effects at nonmatching fields and a significant suppression of vortex channeling for higher magnetic fields as predicted by Reichhardt *et al.* [1].

[1] C. Reichhardt and C.J. Olson Reichhardt, Phys. Rev. B **76**, 094512(2007)

TT 26.4 Wed 16:30 H 3010

Self-generated vortices in NbN ultra-thin film structures — •Konstantin Ilin[1], Michael Siegel[1], Andreas Engel[2], Holger Bartolf[2], Andreas Schilling[2], Alexei Semenov[3], and Heinz-Wilhelm Huebers[3] — [1]Institute of Micro- and Nano-Electronic Systems, University of Karlsruhe, Germany — [2]Physics Institute, University of Zurich, Switzerland — [3]DLR e.V. Institute of Planetary Research, Berlin, Germany

Detectors of electro-magnetic radiation made from NbN ultra-thin superconducting films find their application in different fields: astronomy, optical and THz spectroscopy, imaging and security. The detecting element of these devices is typically a micrometer or submicrometer wide superconducting strip operating at temperatures well below the critical temperature. The bias current required for proper operation of detectors is about the critical value. We present results on study of a current-generated critical state in 3-5 nm thick NbN structures with different width. The critical current of micrometer wide strips of ultra-thin NbN film is almost independent of temperature below 6 K. This is typically caused by de-pinning of self-generated magnetic vortices in current carrying superconductors. A reduction of the strip width leads to an increase of the critical current density approaching the value of de-pairing critical current for 300-400 nm wide stripes, which are much larger than the coherence length in NbN films. We describe the obtained results in term of the three-current model considering an enhancement of the Bean-Livingston edge barrier for vortex penetration with decreasing width of superconducting strip.

TT 26.5 Wed 16:45 H 3010

Vortex structures in ultra high purity niobium revealed by neutron scattering — •Sebastian Muehlbauer[1,2], C. Pfleiderer[1], P. Boeni[1], A. Wiedenmann[3], R. Kampmann[4], E. M. Forgan[5], and G. Behr[6] — [1]Physik-Department E21, Technische Universität München, D-85748 Garching — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, FRM II, D-85748 Garching — [3]Hahn-Meitner-Institut, D-14109 Berlin — [4]Geesthacht Neutron Facility, GKSS, D-21502 Geesthacht — [5]School of Physics and Astronomy, Birmingham UK — [6]IFW Dresden , D-01171 Dresden

Small angle neutron scattering (SANS) directly maps the vortex lattice (VL) of type II superconductors and gives valuable information on both the underlying Fermi surface and the mechanism of the superconducting pairing. But the symmetry of the VL is also mainly influenced by pinning and impurity effects. Recent studies of the VL in ultra pure samples of the classical superconductor Niobium with field applied along the four-fold (100) axis are showing frustration between the six-fold VL and four-fold crystal symmetry. Four-fold VL patterns additionally breaking the crystal symmetry have been identified in Niobium, which can be partially explained by non-local corrections in the Eilenberger model (1). The symmetry breaking transition is vanishing at a specific rotation angle of the magnetic field versus the (100) axis. As this angle also shows specific features in magnetoresistance, a direct link between the Fermi symmetry and VL symmetry maybe drawn. First experiments benefiting from time-of-flight SANS on VL will be presented. (1) M. Laver et al, Phys. Rev. Lett. 96, 167002 (2006)

15 min. break

TT 26.6 Wed 17:15 H 3010

Critical Currents in $YBa_2Cu_3O_{7-\delta}$/$La_{2/3}Ca_{1/3}MnO_3$ Hybrid Structures — •Märit Djupmyr[1], Soltan Soltan[2], Hanns-Ulrich Habermeier[2], and Joachim Albrecht[1] — [1]MPI für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — [2]MPI für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

The local critical current density in hybrid structures of high-temperature superconducting $YBa_2Cu_3O_{7-\delta}$ and ferromagnetic $La_{2/3}Ca_{1/3}MnO_3$, grown on vicinal cut substrates is measured with high accuracy using a spatially resolved magneto-optical method. A detailed study of the temperature dependence of the critical current in the film gives information about the flux pinning mechanisms. In YBCO thin films different pinning mechanisms has been found depending on temperature and microstructure of the film. We have studied what influence the ferromagnetic layer has on these pinning mechanisms and the critical current. Found were a substantial modification of the critical current that could be explained by a transfer of an inhomogeneous magnetic induction distribution from the ferromagnet to the superconductor

TT 26.7 Wed 17:30 H 3010

Signatures of the quantum zero-point motion of vortices in the cuprate superconductors — •Lorenz Bartosch[1] and Subir Sachdev[2] — [1]Institut für Theoretische Physik, Universität Frankfurt — [2]Department of Physics, Harvard University

We explore the experimental implications of a recent theory of the quantum dynamics of vortices in two-dimensional superfluids proximate to Mott insulators [L. Balents, L. Bartosch, A. Burkov, S. Sachdev, and K. Sengupta, Physical Review B **71**, 144508 (2005)]. The theory predicts modulations in the local density of states in the regions over which the vortices execute their quantum zero point motion. We use the spatial extent of such modulations in scanning tunneling microscopy measurements on the vortex lattice of BSCCO to estimate the inertial mass of a point vortex. We also discuss the influence of the quantum zero-point motion of a vortex on the electronic quasiparticle spectra and give a possible explanation for the origin of the 7 meV peaks which were observed in STM studies of the electronic structure of the vortex core in BSCCO.

TT 26.8 Wed 17:45 H 3010

Flux dynamics in superconductors with columnar array of artificial defects — •Carolina Romero-Salazar[1], Omar Augusto-Flores[2], and Christian Jooss[1] — [1]Institut fuer Materialphysik, Friedrich Hund Platz 1, 37077 Goettingen, Germany — [2]Instituto de Fisica, Universidad Autonoma de Puebla, Apdo. Post. J-48, Puebla, Mexico

In this work we extend the analysis of the dynamic properties in thin film superconductors to more complicate materials, with patterned holes or areas with locally enhanced pinning. Understanding how interactions of ensembles of vortices with artificial holes or inhomogeneous pinning take place have implications for possible technological applications, based on controlled-transport of vortices. Employing our electric field reconstruction method, we perform experimental and theoretical studies on BSSCO single crystals, where columnar defects (strong vortex attractors) are presented in cylindrical regions of $100\mu m$ diameter. The columnar defects were created by high-energy ion irradiation [1] A better understanding of vortex dynamics in presence of inhomogeneities is necessary to learn about local losses. We observe that in inhomogeneous superconductors, the vector velocity is not strictly parallel to the Lorentz force.

[1] S.S Banerjee *et al Phys. Rev. Lett.* **93** 097002 (2004).

TT 26.9 Wed 18:00 H 3010

Effect of planar defects on the stability of the Bragg glass phase of type-II superconductors — •Aleksandra Petković[1], Thorsten Emig[1,2], and Thomas Nattermann[1] — [1]Institut für Theoretische Physik der Universität zu Köln — [2]Laboratoire de Physique Théorique et Modèles Statistiques, CNRS UMR 8626, Bât. 100, Université Paris-Sud, 91405 Orsay cedex, France

It is shown that the Bragg glass phase can become unstable with respect to planar defects. A single defect plane that is oriented parallel to the magnetic field as well as to one of the main axis of the Abrikosov flux line lattice is always relevant, whereas we argue that a plane with higher Miller index is irrelevant. A finite density of parallel defects with random separations can be relevant even for larger Miller indices. Defects that are aligned with the applied field restore locally the flux density oscillations which decay algebraically with distance from the defect. We calculate the current voltage relation. The theory exhibits some similarities to the physics of Luttinger liquids with impurities.

TT 27: Symposium: Circuit QED

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

Invited Talk TT 27.1 Thu 9:30 H 0104

Single artificial-atom maser — •Yasunobu Nakamura[1,2,3], Oleg Astafiev[1,2], Kunihiro Inomata[2], Antti O. Niskanen[3,4], Tsuyoshi Yamamoto[1,2,3], Yuri A. Pashkin[1,2], and Jaw-Shen Tsai[1,2,3] — [1]NEC Nano Electronics Research Laboratories — [2]RIKEN Frontier Research System — [3]CREST-JST — [4]VTT Technical Research Centre of Finland

Masers and lasers usually involve ensemble of atoms to be excited and stimulated for emission. As those atoms are only weakly coupled to the cavity mode, a large number of atoms and strong pumping are needed for lasing in order to overcome the cavity loss and the relaxation of atoms due to spontaneous emission into other modes. However, when the coupling becomes strong even a single atom is enough for lasing, as have been demonstrated with atoms in microwave/optical cavities. We have realized an analogous single artificial-atom maser in a superconducting circuit. Josephson-junction charge qubit is used as an artificial atom with a large dipole. The qubit is coupled to a superconducting Nb coplanar-waveguide resonator at around 10 GHz and with a quality factor of 7600. The coupling strength between the qubit and the resonator is 80 MHz. Population inversion is generated by current injection: A current is injected through a voltage-biased electrode attached to the charge qubit via a highly resistive tunnel junction. In the so-called Josephson-quasiparticle process, the qubit is pumped incoherently to the upper state and emits photon into the cavity. Reference: O. Astafiev et al., Nature 449, 588 (2007).

Invited Talk TT 27.2 Thu 10:00 H 0104

Sisyphus cooling and amplification by a superconducting qubit — •Evgeni Il'ichev[1], M. Grajcar[1,2], S.H.W. van der Ploeg[1], A. Izmalkov[1], H.-G. Meyer[1], A. Fedorov[3], A. Shnirman[4], and Gerd Schoen[5] — [1]Institute of Photonic Technology, Albert-Einsteinstr 9, 07745, Jena, Germany — [2]Department of Experimental Physics, Comenius University, SK-84248 Bratislava, Slovakia — [3]Quantum Transport Group, Delft University of Technology, 2628CJ Delft, The Netherlands — [4]Institut für Theoretische Physik, Universität Innsbruck, Austria — [5]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany

Recently superconducting qubits have been shown to act as artificial two-level atoms, demonstrating many different quantum effects known in quantum optics. Coupling such qubits to resonators is quite natural extension of this analogy. Similar to laser cooling of the atomic motion we demonstrate here Sisyphus cooling of a low frequency LC oscillator coupled to a near-resonantly driven flux qubit. The analogy to the quantum optics is obvious: the LC oscillator plays the role of the mechanical degree of freedom of an atom, while the qubit mimics the electronic, laser driven, transition. We also demonstrate the counterpart of the Sisyphus cooling, namely, Sisyphus amplification.

TT 27.3 Thu 10:30 H 0104

Quantum Computation and Quantum Optics with circuit QED — •Jens Koch — Departments of Physics and Applied Physics, Yale University, New Haven, Connecticut 06520, USA

The idea of harnessing superconducting circuits to act as artificial atoms, and coupling them to microwave transmission line resonators has come a long way since its first realization in 2004. This architecture, termed circuit quantum electrodynamics (QED), has been successfully employed in a number of experiments probing fundamental aspects of quantum mechanics and quantum optics, and has enabled impressive progress towards quantum computing. At the same time, circuit QED constitutes an appealing testbed for the theoretical understanding and modeling of driven open quantum systems. This talk will give an introduction to the basics of circuit QED, and a discussion of recent results obtained with the new transmon qubit, an improved Cooper pair box immune to 1/f charge noise.

Work done in collaboration with L. S. Bishop, A. Blais, J. M. Chow, L. Frunzio, J. M. Gambetta, A. A. Houck, B. Johnson, J. Majer, J. Schreier, D. I. Schuster, A. Wallraff, T. Yu, M. Devoret, S. M. Girvin, and R. J. Schoelkopf.

TT 27.4 Thu 10:55 H 0104

Engineering coherent quantum states in superconducting systems — •Raymond W Simmonds — National Institute of Standards and Technology, Division 817.03, 325 Broadway St. Boulder, CO 80305 USA

Recently, we have taken the first step towards creating and controlling quantum information using superconducting circuits. We have observed for the first time a coherent interaction between two superconducting "atoms" (quantum bits or qubits) and an LC cavity formed by a 7 mm long coplanar waveguide resonant at approximately 9 GHz. When either qubit is resonant with the cavity, we observe the vacuum Rabi mode splitting of the qubit's spectral line. In a time-domain measurement, we observe coherent vacuum Rabi oscillations between either qubit and the resonator. Using controllable shift pulses, we have shown coherent transfer of a arbitrary quantum state. We prepare the first qubit in a superposition state, then this state is transferred to the resonant cavity and then after a short time, we transfer this state into the second qubit. These experiments show that developing custom designed quantum systems on chip is possible, opening up new possibilities for studying quantum mechanics and information science.

15 min. break

TT 27.5 Thu 11:35 H 0104

Observation of Berry's Phase in a Superconducting Qubit Embedded in a Cavity — •Peter Leek[1], Johannes Fink[1], Alexandre Blais[2], Romeo Bianchetti[1], Martin Goeppl[1], Jay Gambetta[3,4], David Schuster[4], Luigi Frunzio[4], Robert Schoelkopf[4], and Andreas Wallraff[1] — [1]Department of Physics, ETH Zürich, Switzerland — [2]Département de Physique, Université de Sherbrooke, Québec, Canada — [3]Institute for Quantum Computing, University of Waterloo, Canada — [4]Departments of Applied Physics and Physics, Yale University, USA

In quantum information science, the phase of a wavefunction plays an important role in encoding information. While most experiments in this field rely on dynamic effects to manipulate this information, an alternative approach is to use geometric phase, which has been argued to have potential fault tolerance [1]. Here we demonstrate the controlled accumulation of a geometric phase, Berry's phase, in a superconducting qubit, manipulating the qubit geometrically using microwave radiation, and observing the accumulated phase in an interference experiment [2]. This is achieved using the excellent phase coherence and qubit control possible in Circuit QED [3]. We find excellent agreement with Berry's predictions, and also observe a geometry dependent contribution to dephasing.

[1] J.A. Jones *et al.*, Nature 403, 869 (2000). [2] P.J. Leek *et al.*, Science, 22 November 2007 (10.1126/science.1149858). [3] A. Wallraff *et al.*, Nature 431, 162 (2004).

TT 27.6 Thu 12:00 H 0104

Strong squeezing in a solid state system — •Michael Marthaler[1], Alexander Shnirman[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128, Germany — [2]Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

A Superconducting Single Electron Transistor (SSET) coupled to an anharmonic oscillator can be used to create a strongly squeezed distribution of photon number states. The transitions caused by quasiparticle tunneling in the SSET have a sharp cut-off, resulting from the vanishing density of states inside the gap. This creates a strong nonlinearity in the rates which increase the number of photons in the oscillator. If the dissipation in the oscillator is low we produce a nearly pure Fock state.

TT 27.7 Thu 12:15 H 0104

Dissipation in circuit QED — •Stephan André[1], Valentina Brosco[1], Gerd Schön[1], and Alexander Shnirman[1,2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, Germany — [2]Institut für Theoretische Physik, Innsbruck, Austria

Recently many experimental and theoretical works realized concepts originally introduced in the field of quantum optics [1,2]. In the present

work, we study the dynamics of a flux qubit coupled to a slow LC-oscillator in presence of noise. The qubit is driven to perform Rabi oscillations, and the Rabi frequency is tuned to resonance with the oscillator. When the qubit driving frequency is blue-detuned, the system exhibits lasing behaviour; for red detuning, the qubit cools the oscillator. We analyze the effects of different types of environment on the dynamics of this system. We show that there is a remarkable dependence of the lasing and cooling on the noise spectrum acting on the qubit.

[1] E. Il'ichev et al., Phys. Rev. Lett. **91**,097906 (2003).
[2] J.Hauss et al. cond-mat/0701041

TT 27.8 Thu 12:30 H 0104

Quantum Zeno Effect in Detection of Itinerant Microwave Photons — •Ferdinand Helmer[1], Matteo Mariantoni[2], Enrique Solano[1], and Florian Marquardt[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, Department für Physik, Center for NanoScience, Ludwig-Maximilians-Universität Müunchen, Germany — [2]Walther Meissner Institut, Bayerische Akademie der Wissenschaften, Garching b. München, Germany

We propose and analyze a scheme for detecting single microwave photons traveling along a superconducting transmission line on a chip. The setup exploits a nonlinear coupling between different modes in a transmission line resonator, brought about by the interaction with a superconducting qubit (as demonstrated in recent experiments). The backaction produced by the measurement device may produce a fundamental limit for the fidelity of photon detection in any such scheme. This is a consequence of the Quantum Zeno effect, and we discuss both analytical estimates and quantum trajectory simulations of the measurement process.

TT 27.9 Thu 12:45 H 0104

Single Photon Generation in Superconducting Microwave Cavities — •Giuseppe Mangano[1,2], Jens Siewert[1,2], and Giuseppe Falci[1] — [1]MATIS CNR-INFM & DMFCI, Università di Catania, I-95125 Catania, Italy — [2]Institute für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Circuit quantum electrodynamics (circuit QED) in superconducting nanocircuits provides a new system analogous to quantum-optical cavity QED. A particular advantage of circuit QED is the flexibility with respect to system parameters that allow to drive the setup in various regimes. Thus, it opens a playground to test in this solid-state system many effects that have been predicted in quantum optics. One particularly interesting problem is the generation and detection of non-classical cavity states such as photon number states (despite the fact that up to date there is no single-photon detector for these microwave photons). In a recent experiment, generation of single photons relied on spontaneous emission events has been demonstrated in a circuit QED architecture [1]. Here we propose an alternative method to trigger the emission of a single photon into the cavity by applying the stimulated Raman adiabatic passage (STIRAP) invoking a third level of the Cooper-pair box. The method requires a leaky cavity [2], otherwise the STIRAP protocol could not generate single photons as in circuit QED the capacitive atom-cavity coupling is fixed.

[1] A. A. Houck, et al. Nature 449, 328-331 (2007).
[2] A. Kuhn, et al. Appl. Phys B 69, 373 (1999).

TT 28: Correlated Electrons: Metal-Insulator Transition 1

Time: Thursday 9:30–12:45 Location: H 2053

TT 28.1 Thu 9:30 H 2053

Surface Effects on Oxide Heterostructures — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Perovskite heterostructures have attracted recent interest due to the discovery of metallic interlayers in an otherwise insulating structure. The physical properties of such a multilayer structure hence are not present in either of its constituents. For example, at the contact between the two band insulators $LaAlO_3$ and $SrTiO_3$ a quasi 2D electron gas with very high carrier density is formed. However, it was shown that the $LaAlO_3$ surface layer must reach a critical thickness of 4 unit cells for the interface to be conducting.

We report on surface effects on the electronic properties of interfaces in epitaxial $LaAlO_3/SrTiO_3$ heterostructures. Our results are based on DFT calculations for well-relaxed multilayer configurations, terminated by a thin $LaAlO_3$ surface layer. On varying the thickness of this layer, we find that the interface conduction states are subject to almost rigid band shifts due to a modified Fermi energy. Confirming experimental data, the electronic properties of heterointerfaces therefore can be tuned systematically by alterating the surface-interface distance.

TT 28.2 Thu 9:45 H 2053

Hubbard Model on the Bethe lattice with next-nearest neighbor hopping — •Robert Peters and Thomas Pruschke — Friedrich-Hund-Platz 1, 37077 Göttingen

We investigated the Bethe lattice with nearest-neighbor and next-nearest neighbor hopping t_1 and t_2 within dynamical mean-field theory using Wilson's numerical renormalization group as impurity solver. We study this model for various values of t_2 including $t_2 = t_1$ and $t_2 < 0$. We especially discuss the interplay between antiferromagnetism and the paramagnetic metal-insulator-transition at half-filling. For the doped model the existence of ferromagnetism depending on the value of U is analyzed.

TT 28.3 Thu 10:00 H 2053

Optical conductivity and specific heat anomalies in the proximity of the Mott-Hubbard transition — •Alessandro Toschi[1], Massimo Capone[2,3], Claudio Castellani[3], and Karsten Held[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]ISC-CNR, Via dei Taurini 19, I-00185 Roma, Italy — [3]SMC, CNR-INFM and Dipartimento di Fisica, Università di Roma 'La Sapienza', Piazzale Aldo Moro 2, I-00185 Roma, Italy

A landmark of electronic correlations is the strong renormalization of the quasiparticle peak in the spectral function, and, as it has been recently demonstrated [1], the appearance of kinks in the self-energy at low frequency. As a consequence, strong renormalization of the Drude peak, of the temperature dependence of the optical sum rules and of the specific heat can be expected in the vicinity of the Mott-Hubbard transition. Indeed similar features have been observed in cuprates and, more generally, in transition metal oxides. DMFT calculations, using exact Diagonalization as an impurity solver and a large number of sites in the electronic bath, allow us to perform a detailed comparison with experiments. Our calculations unveil the existence of an anomalous deviation from Fermi-liquid-behavior at temperatures much lower than expected. Taking this deviation into account is important for a correct interpretation of the experimental data.

[1] K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I.A. Nekrasov, Th. Pruschke, and D. Vollhardt, Nature Physics **3**, 168 (2007).
[2] A. Toschi and M. Capone, cond-mat/0708.3475.
[3] A. Toschi, M. Capone, C. Castellani, and K. Held in preparation.

TT 28.4 Thu 10:15 H 2053

Mott-Hubbard transition in a two-band model: From three to two dimensions — •Philipp Hansmann, Xiaoping Yang, Alessandro Toschi, Giniyat Khaliullin, Ole Krogh Andersen, and Karsten Held — Max Planck Institute for Solid State Research, Stuttgart

The influence of dimensionality on the Mott-Hubbard transition in a two-band model is studied. More specifically we consider a two e_g-band Hubbard model at quarter filling which is analyzed within dynamical mean field theory. Nearest neighbor hopping and hybridization are taken into account as well as a small crystal-field splitting of the two e_g-bands. Starting from the three dimensional cubic symmetry the hopping in the crystallographic z-direction is tuned to zero where results for the two dimensional system are recovered. Although electronic correlations on surfaces and in two dimensions are expected to be stronger than in the three dimensional case, our results show that this effect is weakened as a result of the hybridization between the two e_g-orbitals.

TT 28.5 Thu 10:30 H 2053

Orbital-selective Mott transitions in a doped two-band Hub-

bard model — •Eberhard Jakobi, Nils Blümer, and Peter van Dongen — Institute of Physics, KOMET 337, Johannes Gutenberg University Mainz

Within the last few years, it has been established within dynamical mean-field theory (DMFT) that orbital-selective Mott transitions occur in half-filled degenerate two-band Hubbard with different bandwidths under quite general circumstances. We extend extend these studies to the general doped case, using a high-precision quantum Monte Carlo DMFT solver. For sufficiently strong interactions, orbital-selective Mott transitions as a function of total band filling are clearly visible in the band-specific fillings, quasi-particle weights and double occupancies.

TT 28.6 Thu 10:45 H 2053

Quantum phase transition in the two-band Hubbard model — •Theodoulos Costi and Ansgar Liebsch — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The interaction between itinerant and Mott localized electronic states in strongly correlated transition metal oxide materials with anisotropic Hund's exchange is studied within dynamical mean field theory in combination with the numerical renormalization group method . For values of the Hund's exchange and Coulomb interactions typical of many transition metal oxides, a novel nonmagnetic zero temperature quantum phase transition is found in the bad-metallic orbital-selective Mott phase of the two-band Hubbard model [1]. We describe the critical properties of this quantum phase transition and relate the critical exponents to those of an exactly solvable model.

[1] T. A. Costi and A. Liebsch, Phys. Rev. Lett. (2007); arXiv:0707.4535

15 min. break

TT 28.7 Thu 11:15 H 2053

Static Screening and Delocalization Effects in the Hubbard-Anderson Model — •Peter Henseler[1], Johann Kroha[1], and Boris Shapiro[2] — [1]Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Department of Physics, Technion-Israel Institute of Technology, Haifa 32000, Israel

We study the suppression of electron localization due to the screening of the disorder potential in a Hubbard-Anderson model within a static picture, where interactions are absorbed into the redefinition of the random on-site energies, leading to an interaction-induced renormalization of the random distribution of onsite energies.

First the one-dimensional case is discussed, where we focus on the change of the electron localization length at the Fermi level. Two different approximations are presented, either one yielding a non-monotonic dependence of the localization length on the interaction strength, with a pronounced maximum at an intermediate interaction strength. We then investigate the higher-dimensional case, applying the selfconsistent theory of Anderson localization to the present problem, and a comparison with recent numerical results is presented.

TT 28.8 Thu 11:30 H 2053

Real-space DMFT for inhomogeneous strongly correlated fermionic systems — •Michiel Snoek[1], Csaba Toke[1], Irakli Titvinidze[1], Krzysztof Byczuk[2], and Walter Hofstetter[1] — [1]J. W. Goethe-Universität, Frankfurt am Main, Deutschland — [2]Universität Augsburg, Augsburg, Deutschland

We introduce the real-space dynamical mean-field theory (R-DMFT) method to describe strongly interacting lattice fermions in the presence of an external, space dependent potential. This method relies only on the assumption that the self-energy is a local quantity and is exact in infinite dimensions. The power of the method is demonstrated by calculating Friedel oscillations in an ultracold Fermi gas in an optical lattice. Using the numerical renormalization group (NRG) and exact diagonalization as impurity solvers, we study the Mott transition in a harmonically confined Fermi gas in an optical lattice. In particular, the emergence of antiferromagnetic structures in the Fermi gas is analyzed in detail.

TT 28.9 Thu 11:45 H 2053

Micro-domain formation near the first-order Mott-Hubbard transition — •Qinyong Liu and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Near the first order Mott-Hubbard transition of the Hubbard model there is a region where metallic and insulating states can coexist in a finite range of temperatures. We study the formation of insulating or metallic micro-domains embedded in the metallic or insulating phase, respectively, within this coexistence region. In order to calculate the behavior of the density of states across a domain wall, the dynamical mean field theory (DMFT) is generalized to a layer-DMFT, where the selfenergy remains local, but the effective impurity is coupled to different dynamical baths, depending on its distance from the domain wall. We use the non-crossing approximation (NCA) as the impurity solver. Our results allow to compute the free energy of a micro-domain in dependence on its size and, hence, the thermal distribution of domain sizes in depencence of temperature. These results may be relevant for understanding the anomalous temperature dependence of the conductivity near the Mott-Hubbard transition.

TT 28.10 Thu 12:00 H 2053

Crossover behavior in the metallic state of the one-dimensional Holstein model — •Steffen Sykora, Arnd Hübsch, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The Holstein model is perhaps the simplest realization of a coupled electron-phonon system with a local interaction between dispersionless phonons of frequency ω_0 and electrons with hopping matrix element t. By applying the projective renormalization method (PRM), the physical properties of the one-dimensional model in the metallic state are investigated for the adiabatic case ($\omega_0/t \ll 1$), for the antiadiabatic case ($\omega_0/t \gg 1$), as well as for the intermediate case ($\omega_0/t \approx 1$). As a result we find that in the adiabatic case a phonon softening is observed at the Brillouin zone boundary whereas for the opposite case a hardening is found.

TT 28.11 Thu 12:15 H 2053

Spectral properties of locally correlated electrons in a BCS superconductor — •Johannes Bauer[1], Alex Hewson[1], and Akira Oguri[2] — [1]Department of Mathematics, Imperial College, London SW7 2AZ, UK — [2]Department of Material Science, Osaka City University, Sumiyoshi-ku, Osaka

We present a detailed study of the spectral properties of a locally correlated site embedded in a BCS superconducting medium. To this end the Anderson impurity model with superconducting bath is analysed by numerical renormalisation group (NRG) calculations. We calculate one and two-particle dynamic response function to elucidate the spectral excitation and the nature of the ground state for different parameter regimes with and without particle-hole symmetry. The position and weight of the Andreev bound states is given for all relevant parameters. We also present phase diagrams for the different ground state parameter regimes. This work is also relevant for dynamical mean field theory extensions with superconducting symmetry breaking.

TT 28.12 Thu 12:30 H 2053

Quantum critical scaling behavior of deconfined spinons — •Flavio Nogueira —

The talk has been moved to TT 19.16.

TT 29: Superconductivity: Mechanisms, Phase Diagram, Competing Order

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

TT 29.1 Thu 9:30 H 3010

Evidence for bulk s and d wave superconductivity and important c-axis involvement in cuprates — Rustem Khasanov[1], Alexander Shengelaya[2], •Annette Bussmann-Holder[3], Hugo Keller[1], and K. Alex Müller[1] — [1]Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Physics Institute of Tbilisi State University, Chavchavadze 3, GE-0128 Tbilisi, Georgia — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

To clarify the order parameter symmetry of cuprates, the magnetic penetration depth was measured along the crystallographic directions a, b, and c in single crystals of $YBa_2Cu_4O_8$ via muon spin rotation. This method is direct, bulk sensitive, and unambiguous. The temperature dependences of the penetration depth along the crystallographic a- and b-directions were found to exhibit an inflection point at low temperatures as is typical and provides evidence for two-gap superconductivity (TGS) with s + d wave character in the planes. In contrast, the penetration depth along the c-axis shows almost pure s wave character which never met the awareness of the community thereby highlighting the important role of c-axis effects. We conclude that TGS is a generic and universal feature in the bulk of cuprates.

TT 29.2 Thu 9:45 H 3010

Optimal lokalisierte Wannier Funktionen bestimmter Symmetrie als Voraussetzung für Supraleitung bzw. Magnetismus — •Ekkehard Krüger — Elfenstraße 107, 70567 Stuttgart

Beobachtungen an den Bandstrukturen elementarer Metalle sowie von Hochtemperatur-Supraleitern lassen stark vermuten, dass sowohl für stabile Cooper-Paare als auch für stabile magnetische Strukturen optimal lokalisierte Wannier Zustände bestimmter Symmetrie im Leitungsband eines Materials verantwortlich sind. Diese Beobachtungen können im Rahmen eines gruppentheoretischen verallgemeinerten Heisenberg-Modells verstanden werden, in dem die Symmetrie atomähnlicher Zustände im Leitungsband durch die Orbitale der Elektronen *und* durch die Mitbewegung der Atomrümpfe bestimmt wird. Die Auswirkungen auf das theoretische Verständnis von (Hoch-T_c-)Supraleitung und Magnetismus werden kurz diskutiert. Ergebnisse für den Antiferromagnet $YBa_2Cu_3O_6$ und den Hochtemperatur-Supraleiter $YBa_2Cu_3O_7$ werden vorgestellt.

TT 29.3 Thu 10:00 H 3010

Charge-carrier dynamics of high-T_c superconductors — •Martin Scheuch, Luca Perfetti, Tobias Kampfrath, Christian Frischkorn, and Martin Wolf — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

By using transient time-resolved THz spectroscopy, we get the full information of the complex conductivity of $Bi_2Sr_2CaCu_2O_{8+\delta}$ in the range from 8 to 30 THz. In addition to static measurements, we also performed femtosecond pump-probe experiments, where a visible pump pulse excites the sample and after variable time delay, the THz pulse measures the pump-induced change in the conductivity. This paves the way to observe the non-equilibrium states. Experiments are performed temperature-dependent from 5 to 300 K. Our results show the breaking of Cooper-pairs and their recovery. This will be discussed including electron cooling and phonon heating.

TT 29.4 Thu 10:15 H 3010

Variational cluster calculation of the magnetic resonance mode in high-T_c superconductors — •Sascha Brehm[1], Enrico Arrigoni[2], Michael Potthoff[3], Markus Aichhorn[1], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Graz, Austria — [3]Institut für Theoretische Physik, Universität Hamburg, Germany

We present a new quantum-cluster scheme for calculating two-particle correlation functions within symmetry-broken, e.g. antiferromagnetic (AF) and d-wave superconducting (dSC) phases. This scheme, which we apply to the 2-D Hubbard model, is based on the variational cluster approach (VCA) from which we obtain the normal and anomalous one-particle Green's functions in the thermodynamic limit from variationally optimized self-energies computed on finite clusters. In the spirit of this embedded cluster calculation, we also obtain the frequency and momentum dependent two-particle vertex from a calculation on an isolated cluster. It is specifically demonstrated that the new approach reproduces the magnetic resonance mode, which has been found in inelastic neutron scattering experiments in various underdoped high-T_c superconductors. Confirming a general belief, this resonance is indeed intimately related to the microscopic mechanism of superconductivity, i.e. it is a (S=1) magnetic exciton lying in the SC gap. In contrast to previous calculations, which are weak-coupling schemes (e.g. RPA), our scheme takes into account the strongly correlated physics of the high-T_c superconductors.

TT 29.5 Thu 10:30 H 3010

Single-particle vs. two-particle properties in LSCO — •Wolfgang Prestel, Bernhard Muschler, Leonardo Tassini, Michael Lambacher, Andreas Erb, and Rudi Hackl — Walther-Meißner-Institute, Garching

On the overdoped side, high-T_c superconductors can be described as normal, though strongly correlated, metals. In order to explore the doping range in which the correlations become dominant, we compare single-particle properties as seen by ARPES and two-particle properties as measured by, e.g., Raman, dc and optical transport. To this end, we implement a phenomenological model for the electronic spectral function resembling ARPES data and calculate two-particle quantities using a generalized Kubo formula. On the overdoped side, the results of the model calculations agree to within 20 % with the experimental data including spectral and temperature dependences. Towards optimal doping the experimental B_{1g} Raman response is strongly suppressed in an energy range below 1000 cm^{-1} in comparison to the spectra obtained from the model. This suppression is belived to originate from strong electronic correlations since it precedes the loss of spectral weight in the anti-nodal region found in ARPES experiments.

The project has been supported by the DFG under grant number Ha2071/3-2 via the Research Unit FOR538.

TT 29.6 Thu 10:45 H 3010

Phonon anomalies in detwinned $YBa_2Cu_3O_{6+x}$: Evidence for in-plane anisotropy in the electronic system — •Mohammed Bakr, Clemens Ulrich, Chengtian Lin, Manuel Cardona, and Bernhard Keimer — Max Planck Institute, Stuttgart, Germany

The pairing symmetry of high T_c superconductors is predominantly of d-wave character with a probable small s-wave component. In detwinned YBCO, this results in an ***ab***-anisotropy of the 2Δ gaps. Different experiments have revealed controversial ***ab***- discrepancies in the 2Δ gaps and therefore the s-wave contribution. Raman light scattering (RLS) allows us to probe the electronic signals directly and also anisotropies in the phonon lineshapes. We have performed RLS experiments on detwinned $YBa_2Cu_3O_{6.95}$ single crystals using different laser lights. Within the experimental error of 4 meV, the electronic gaps along ***a***- and ***b***- axes show no differences. Phonons are quite sensitive to changes in the electronic system. Therefore, some phonons show a pronounced Fano-type line shape which implies a strong electron-phonon coupling. In the normal state, the Fano asymmetry parameter q^{-1} shows a sizable ***ab***-anisotropy which can be understood by basic band structure calculations. Below T_c, q^{-1} changes drastically and in a distinguishable behavior for the ***a***- and ***b***-axes. For instance the B_{1g}-like mode at 340 cm^{-1} shows a substantial ***ab***-dissimilarity whereas the apical oxygen phonon at 501 cm^{-1} shows the largest anisotropy. Furthermore, we have found that the anisotropy in the q^{-1} is highly dependent on the exciting laser energy. Our results shed more light on the strong electronic correlations in high-T_c superconductors.

TT 29.7 Thu 11:00 H 3010

Modelling the normal-state properties of the heavily overdoped cuprate $La_{1.7}Sr_{0.3}CuO_4$ — •Alessandro Narduzzo[1,2], Guillaume Albert[1], Matthew M.J. French[1], Nikorn Mangkorntong[3], Makoto Nohara[3], Hidenori Takagi[3], and Nigel E. Hussey[1] — [1]University of Bristol, UK; — [2]IFW Dresden, Germany; — [3]University of Tokyo, Japan.

The metallic properties of high-T_c superconductors still represent a major unresolved issue. Fermi-liquid based interpretative approaches require the existence of a single quasiparticle scattering rate with an in-plane anisotropy that is temperature dependent. Here we model the temperature dependence of resistivity ρ, Hall coefficient R_H and magnetoresistance MR in the heavily overdoped non-superconducting cuprate $La_{1.7}Sr_{0.3}CuO_4$. Empirically, $\rho \sim T^2$ up to 50K, $MR \sim T^{-4}$ while R_H shows a strong temperature dependence, changing sign and becoming negative above $T \approx 170$K. The positive Hall coefficient at low temperatures appears inconsistent with the electron-like Fermi surface reported by ARPES measurements at this doping. By introducing a Fermi surface with large regions of negative curvature centred on the zone-diagonals and an anisotropic and temperature dependent scattering path length we manage to achieve a satisfactory explanation and fitting of the experimental results. Our analysis implies a striking breakdown of the isotropic-ℓ approximation at low temperatures in this heavily overdoped cuprate, a result that may have important implications for our understanding of the low-T Hall coefficient across the entire phase diagram [1]. [1] http://arxiv.org/abs/0707.4601.

15 min. break

Invited Talk TT 29.8 Thu 11:30 H 3010

Charge redistribution at YBCO-metal interfaces — •Udo Schwingenschlögl and Cosima Schuster — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Charge redistribution at YBCO-metal interfaces is crucial for technological applications of YBCO superconductors, since the band structure is modified on a local scale. In particular, the superconducting CuO_2 planes are intrinsically electron doped (underdoped) due to the metallic contact. In order to obtain quantitative insight into this intrinsic doping mechanism, the normal-state YBCO electronic structure close to YBCO-metal interfaces is studied by means of first-principles band calculations, based on density functional theory. Because of a strong lattice relaxation, it is essential to carry out a detailed structure optimization, which is done for prototypical interface geometries. Additional defects or substitution of the cations may support or compensate the charge transfer. Oxygen vacancies, for instance, tend to locally underdope the superconductor. Intentional overdoping by substituting Y by Ca, on the other hand, compensates this effect and therefore can be used to enhance the critical current density. In addition, effects of electronegative impurities, like F or Cl, are of interest, particularly as concerns the re-extraction of charge from an underdoped YBCO-metal interface.

TT 29.9 Thu 12:00 H 3010

Dynamical magnetic susceptibility in the lamellar cobaltate superconductor $Na_xCoO_2{\cdot}yH_2O$ — •Maxim Korshunov[1,2] and Ilya Eremin[1,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]L.V. Kirensky Institute of Physics, Siberian Branch of RAS, Krasnoyarsk, Russia — [3]Institute für Math. und Theor. Physik, TU Braunschweig, Braunschweig, Germany

We systematically analyze the influence of the superconducting gap symmetry and the electronic structure on the dynamical spin susceptibility in superconducting $Na_xCoO_2{\cdot}yH_2O$ within a three different models: the single a_{1g}-band model with nearest-neighbor hoppings, the realistic three-band t_{2g}-model with, and without e'_g pockets present at the Fermi surface. We show that the magnetic response in the normal state is dominated by the incommensurate antiferromagnetic spin density wave fluctuations at large momenta in agreement with experimental temperature dependence of the spin-lattice relaxation rate. Also, we demonstrate that the presence or the absence of the e'_g-pockets at the Fermi surface does not affect significantly this conclusion. In the superconducting state our results for $d_{x^2-y^2}$- or d_{xy}-wave symmetries of the superconducting order parameter are consistent with experimental data and exclude nodeless $d_{x^2-y^2}+id_{xy}$-wave symmetry. We further point out that the spin-resonance peak proposed earlier is improbable for the realistic band structure of $Na_xCoO_2{\cdot}yH_2O$. Moreover, even if present the resonance peak is confined to the antiferromagnetic wave vector and disappears away from it.

M.K. acknowledges support form INTAS YS Grant 05-109-4891 and RFBR Grant 06-02-90537-BNTS.

TT 29.10 Thu 12:15 H 3010

Mesoscopic effects in small superconducting grains: a semiclassical approach to BCS theory — Antonio M Garcia-Garcia[2], •Juan Diego Urbina[1], Emil Yuzbashyan[3], Klaus Richter[1], and Boris Altshuler[4] — [1]nstitut für Theoretische Physik, Universität Regensburg, 93053 Regensburg — [2]Physics Department, Princeton University, Princeton, New Jersey 08544, USA — [3]Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08544, USA — [4]Physics Department, Columbia University, 538 West 120th Street, New York, NY 10027, USA

We present a novel approach to mesoscopic superconductivity based on a semiclassical approximation for *both* the density of states and the interaction matrix elements [1] entering the BCS gap equation. In this way, the discretness of the single-particle spectra and the inhomogeneity of the single particle eigenfunctions are included consistenly as mesoscopic fluctuations around the bulk values. We apply the theory to 3D cubic grains, finding good agreement with exact numerical calculations. For grains with irregular shape we predict a novel dependence of the gap with the excitation energy, present in an experimentally relevant region of parameters [2].

[1] J. D. Urbina and K. Richter *Phys. Rev. Lett.* **97**, 214101 (2006).
[2] A. M. Garcia-Garcia, J. D. Urbina, Emil Yuzbashyan, K. Richter and B.L Altshuler cond-mat/0710.2286 (2006).

TT 29.11 Thu 12:30 H 3010

Magnetic Flux Periodicity of h/e in Superconducting Loops — •Florian Loder[1], Thilo Kopp[1], Arno Kampf[1], Jochen Mannhart[1], Christof Schneider[1], and Yuri Barash[2] — [1]EKM, Institut für Physik, Universität Augsburg, 86135 Augsburg — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

We apply the BCS theory to superconducting rings with unconventional order parameter symmetries. An external magnetic flux changes the character of the states in the condensate; as a consequence the energy of the superconducting ground state varies with a flux period of h/e. This h/e periodicity is caused by the flux-induced reconstruction of the supercurrent carrying condensate.

To be published in Nature Physics (2008)

TT 29.12 Thu 12:45 H 3010

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]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [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, 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. 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.

TT 30: Correlated Electrons: Spin Systems and Itinerant Magnets 2

Time: Thursday 10:30–11:30 Location: EB 202

TT 30.1 Thu 10:30 EB 202

Quantum phases of the anisotropic Shastry-Sutherland model — •Zi Yang Meng and Stefan Wessel — Institute for Theoretical Physics III, Stuttgart University, Germany

We present results from quantum Monte Carlo simulations of the anisotropic spin-1/2 XXZ model on the orthogonal dimer lattice of the Shastry-Sutherland model, in the sign-problem free parameter region with ferromagnetic transverse spin exchange. In this regime, the model also corresponds to a system of repulsive hard-core bosons. In the absence of a magnetic field, we find solid, superfluid and a dimer triplet phase, and study the various quantum phase transitions between these phases. We also study the magnetization process out of the dimer triplet phase and explore the possibility of triplon supersolidity in this system. Implications of our results for the Heisenberg antiferromagnet on the Shastry-Sutherland model and the compound $SrCu_2(BO_3)_2$ are discussed.

TT 30.2 Thu 10:45 EB 202

Topological excitations of correlated spinless fermions: slave boson approach — •Sebastien Burdin and Mukul Laad — Max-Planck-Institut PKS, Nöthnitzer Strasse 38, 01187 Dresden, Germany

We study the general problem of spinless electrons on a periodic lattice, with a nearest neighbor exchange t and a nearest neighbor Coulomb repulsion V. Following the approach of the slave boson approximation,

we introduce auxiliary bosons and fermions; a site with one electron corresponds to a site occupied by an auxiliary fermion, and an empty site is represented by a boson. The fermionic degrees of freedom are then formally integrated, providing an effective action for the bosonic field. This effective action is solved analytically in the specific case of a square lattice at half filling in the regime $t \ll V$. The ground state is a charge ordered insulator. We show analytically that in the continuum limit the low energy excitations are collective solitonic excitations. Our results confirm some results which have been previously obtained from numerical simulations [1]. They also provide a systematic analytical scheme which might allow us to describe fractional charge excitations of frustrated electronic systems [2].

[1] P.M.R. Brydon, J.X. Zhu, and A.R. Bishop, cond-mat/0509764
[2] P. Fulde, K. Penc, and N. Shannon, Ann. Phys. (Berlin) 11, 892 (2002)

TT 30.3 Thu 11:00 EB 202

Heisenberg Spin-1 Chains and Ladders with Bilinear-Biquadratic Interactions in a Magnetic Field — •Salvatore R. Manmana[1], Tamás A. Toth[1], Andreas Läuchli[2], and Frédéric Mila[1] — [1]Institute of Theoretical Physics (CTMC), EPF Lausanne, CH-1015 Lausanne, Switzerland — [2]IRRMA, PPH-Ecublens, CH-1015 Lausanne, Switzerland

We investigate the magnetic properties of Heisenberg spin-1 chain and ladder systems with bilinear-biquadratic interactions in a magnetic field by applying the density matrix renormalization group method (DMRG) and a variational wavefunction ansatz. For the chains, the magnetization and the dominating spin and quadrupolar correlation functions are computed in the various regions of the zero-field phase diagram. In the critical quadrupolar phase ($\pi/4 < \theta < \pi/2$), the magnetization curve is dominated by a pronounced kink at finite values of the field and the magnetization. After giving a sketch of the zero-field phase diagram of the ladder systems, we present results for various sets of parameters, aiming to gain insight into magnetization properties in the presence of frustration.

TT 30.4 Thu 11:15 EB 202

Quantum fluctuations in high field magnetisation of 2D squarelattice J_1-J_2 antiferromagnets (exchanged with TT 8.8) — Peter Thalmeier[1], Michael Zhitomirsky[2], •Burkhard Schmidt[1], and Nic Shannon[3] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Commisariat à l'Energie Atomique, DSM/DRFCM/SPSMS, Grenoble, France — [3]H H Wills Physics Laboratory, Bristol, United Kingdom

The square lattice J_1–J_2 Heisenberg model with spin $S = 1/2$ has three magnetic and two nonmagnetic phases. It describes a number of recently found layered vanadium oxide perovskites. We discuss the magnetisation curve and high-field susceptibility using spin-wave theory and exact diagonalisation in the whole J_1–J_2 plane. We compare both results and find good overall agreement in the sectors of the phase diagram with magnetic order. Close to the nonmagnetic regions the magnetisation curve shows strong deviations from the classical linear behaviour caused by large quantum fluctuations and spin-wave approximation breaks down. On the FM side ($J_1 < 0$) where one approaches the quantum gapless spin nematic ground state this region is surprisingly large. We find that inclusion of second order spin-wave corrections does not lead to fundamental improvement. Quantum corrections to the tilting angle of the ordered moments are also calculated. They may have both signs, contrary to the always negative first order quantum corrections to the magnetisation. Finally we investigate the effect of the interlayer coupling and find that the quasi-2D picture remains valid up to $|J_\perp/J_1| \sim 0.3$.

TT 31: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 2

Time: Thursday 11:45–13:00 Location: EB 202

TT 31.1 Thu 11:45 EB 202

Time-Dependent Transport Phenomena and the History Dependence of the Time-Dependent Current — •Elham Khosravi[1], Stefan Kurth[1], Gianluca Stefanucci[2], and Eberhard Gross[1] — [1]Institut für Theoretische Physik, Freie Universität Berlin,Berlin, Germany — [2]Department of Physics, University of Rome Tor Vergata, Rome, Italy

We propose a time-dependent approach to investigate transport phenomena within open boundary time-dependent density functional theory which is based on a numerical algorithm for the time propagation of the non-interacting time-dependent Schrödinger or Kohn-Sham equation. The algorithm is used to study time-dependent transport phenomena such as bound state oscillations, transients, AC effects, electron pumps. It has been shown [Phys. Rev. B 75, 195115 (2007)] that the presence of at least two bound states in the biased electrode-device-electrode system of non interacting electrons, leads to persistent oscillations in the total current. Here we study how the amplitude of oscillations depends on the applied bias or gate voltage and on the initial state.

TT 31.2 Thu 12:00 EB 202

Correlation effects in charge and spin transport properties of quantum impurity models — •Thomas Schmidt[1], Andrei Komnik[1], and Alexander Gogolin[2] — [1]Physikalisches Institut, Universität Freiburg — [2]Imperial College, London, UK

We have investigated the spin and charge transport properties of the Anderson impurity model (AIM) under non-equilibrium conditions. While in the non-interacting case the spin-resolved full counting statistics (FCS) is described by a purely binomial distribution, a small Coulomb interaction U induces correlated electron-pair transport which changes the FCS profoundly. In order to address the complementary large-U domain, we analysed the strong-coupling Kondo fixed point and derived an exact result for a special choice of parameters. The results agree for all regimes. Finally, we propose an experimental setup based on a Hanbury Brown and Twiss interferometer in which these effects can be observed.

Invited Talk TT 31.3 Thu 12:15 EB 202

Electronic transport through nanostructures — •Peter Schmitteckert — Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Karlsruhe Institute of Technology

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 various approaches within the DMRG method to obtain the conductance of strongly interacting nanostructures attached to non-interacting leads. First I discuss the embedding method where the transmission amplitude is calculated from the ground state stiffness, which is then used to obtain the conductance. Next I review the Kubo approach within DMRG. By switching to a momentum space representation of the leads, this approach allows the study of systems with very small energy scales, including Kondo physics. These calculations can also be used to extract exact functionals to be used within the framework of Density Functional Theory (DFT). Then I present the approach of calculating the nonequilibrium differential conductance from real-time simulations within DMRG with special emphasis on the Interacting Resonant Level model. Finally I discuss the Lippmann-Schwinger approach to obtain multi-particle scattering states.

TT 31.4 Thu 12:45 EB 202

Is spin-charge separation observable in transport experiments? — •Tobias Ulbricht[1] and Peter Schmitteckert[2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Insitute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Insitute of Technology, Germany

We consider a one-dimensional chain consisting of an interacting area coupled to non-interacting leads. Within the area, interaction is mediated by a local onsite repulsion. Using real time evolution within the Density Matrix Renormalization Group (DMRG) scheme, we study the dynamics of wave packets in a two-terminal transport setup. In contrast to previous works, where excitations were created by adding potentials to the Hamiltonian, we explicitely create right moving single particle excitations in the left lead as the starting condition.

TT 32: Correlated Electrons: Poster Session

Time: Thursday 14:00–18:00 Location: Poster B

TT 32.1 Thu 14:00 Poster B

Matrix product state approach for a two-lead, multi-level Anderson impurity model — •Andreas Holzner[1,2], Andreas Weichselbaum[2], and Jan von Delft[2] — [1]Institute for Theoretical Physics C, RWTH Aachen, D-52056 Aachen, Germany — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany

We exploit the common mathematical structure of the numerical renormalization group and the density matrix renormalization group, namely matrix product states, to implement an efficient numerical treatment of a two-lead Anderson impurity model. By adopting a star-like geometry, where each species (spin and lead) of conduction electrons is described by its own Wilson chain, instead of using a single Wilson chain for all species together, we achieve a very significant reduction in the numerical resources required to obtain reliable results. We illustrate the power of this approach by calculating some ground state properties of a four-level quantum dot coupled to two leads. The success of this proof-of-principle calculation suggests that the star geometry constitutes a promising strategy for future treatments of multi-band quantum impurity models.

TT 32.2 Thu 14:00 Poster B

Deconvolution procedures for dynamical DMRG spectra — •Martin Paech and Eric Jeckelmann — Leibniz Universitaet Hannover, Germany

The dynamical density-matrix renormalization group (DDMRG) method provides the frequency-dependent correlation functions of finite-size low-dimensional systems with great accuracy. The spectrum in the thermodynamic limit can often be obtained by a deconvolution of the finite-system DDMRG data under some regularity assumptions for the spectrum. We discuss deconvolution procedures for general spectra and illustrate them with a study of the density of states in one-dimensional correlated electron systems.

TT 32.3 Thu 14:00 Poster B

Quantum Phase Transitions in the Bosonic Single-Impurity Anderson Model — •Hyun-Jung Lee and Ralf Bulla — Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, D-86135 Augsburg,*Germany

We consider a quantum impurity model in which a bosonic impurity level is coupled to a non-interacting bosonic bath, with the bosons at the impurity site subject to a local Coulomb repulsion U. Numerical renormalization group calculations for this bosonic single-impurity Anderson model reveal a zero-temperature phase diagram where Mott phases with reduced charge fluctuations are seperated from a Bose-Einstein condensed phase by lines of quantum critical points. We investigate the dynamics of the impurity model in various circumstances and prepare the ground for the dynamical mean-field theory of the Bose-Hubbard model.

TT 32.4 Thu 14:00 Poster B

Entanglement entropy dynamics in quantum impurity systems — •David Roosen[1], Karyn Le Hur[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Studying entanglement entropy in quantum many body systems has become interesting for quantum information science, where entanglement is the main source of speed-up in quantum computers, and for condensed matter theory, due to its role as a non-classical correlation in quantum phase transitions (for a recent review, see [1]).

In earlier publications the entanglement between a localized spin and a bosonic bath has been studied [2,3]. Here we investigate characteristic time-scales where the quantum impurity system becomes entangled, as well as universality of the short-time dynamics. Specifically we analyze the real-time dynamics of entanglement entropy in the anisotropic Kondo model, applying a time-dependent Numerical Renormalization Group (NRG) algorithm [4].

[1] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, quant-phys/0703044.
[2] K. Le Hur, P. Doucet-Beaupré, and W. Hofstetter, Phys. Rev. Lett. **99**, 126801 (2007).
[3] A. Kopp, and K. Le Hur, Phys. Rev. Lett. **98**, 220401 (2007).
[4] F. Anders, and A. Schiller, Phys. Rev. Lett. **95**, 196801 (2005).

TT 32.5 Thu 14:00 Poster B

Properties of a molecular 3-level impurity coupled to a fermionic bath — •Jon-Olaf Krisponeit, Frithjof B. Anders, and Gerd Czycholl — Institut für Theoretische Physik, Universität Bremen

We examine a molecular impurity, consisting of three local orbitals coupled to a fermionic bath. The Coulomb repulsion U and a ferromagnetic Hund's exchange coupling $J > 0$ between the local electrons are taken into account.

Thermodynamic as well as transport properties are calculated using the numerical renormalization group (NRG). We analyze their dependencies on the level positions, the temperature T and the strength of Hund's coupling J. We identify the fixed points, the corresponding quantum phase transitions and the scaling laws involved. The parameter dependence of the low temperature crossover scale T_0 is given. Furthermore the influence of an asymmetric coupling strength between bath and impurity is discussed.

TT 32.6 Thu 14:00 Poster B

The Kondo box: a mean-field approach — Rainer Bedrich, •Sebastien Burdin, and Martina Hentschel — Max-Planck-Institut PKS, Nöthnitzer Strasse 38, 01187 Dresden, Germany

We study the Kondo effect induced by a magnetic impurity interacting with a small metallic grain or a quantum dot. 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 chemical potential. The latter can be experimentally tuned by varying a gate voltage applied to the metallic grain. 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 [1], suggesting that the mean-field approximation is valid. A more realistic situation is then considered, for which the energy levels and wave function amplitudes are distributed following random matrix theory in order to model chaotic mesoscopic systems.

[1] W.B. Thimm, J. Kroha, and J. von Delft, Phys. Rev. Lett. **82**, 2143 (1999); R.K. Kaul, G. Zarand, S. Chandrasekharan, D. Ullmo, and H.U. Baranger, Phys. Rev. Lett. **96**, 176802 (2006); S. Kettemann, and E.R. Mucciolo, Phys. Rev. B **75**, 184407 (2007)

TT 32.7 Thu 14:00 Poster B

Functional Renormalization Group Approach to a Single-Level QuantumDot in Non-Equilibrium — •Andreas Dirks, Riccardo Gezzi, and Thomas Pruschke — Institut für Theoretische Physik der UniversitätGöttingen

Properties of a recently proposed [1] functional RG approach to non-equilibrium quantum many-particle systems are being discussed with respect to its suitability to describe transport through a single-level quantum dot beyond linear-response theory. Compared to previous calculations, the full energy-dependence of the irreducible vertex functions is preserved in the RG flow in order to obtain more accurate results for transport properties as function of applied bias, gate voltage and temperature. As nice side effect we avoid an analytical continuation procedure necessary for standard imaginary time approaches.

[1] R. Gezzi, Th. Pruschke, and V. Meden, Phys. Rev. B **75**, 045324 (2007)

TT 32.8 Thu 14:00 Poster B

Scattering of heavy fermions and slow spin waves off fast phonons — •David Rasch and Achim Rosch — Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany

While in ordinary metals and antiferromagnets the velocity of sound is much smaller than the velocity of the electrons or spin waves, this

is not the case in heavy fermion compounds or magnetic systems with small exchange couplings. The latter systems have recently been studied extensively in the context of field tuned quantum phase transitions and the Bose Einstein condensation of magnons. We investigate the scattering of fast phonons from slow electronic and spin excitations and study its influence on heat transport. Here we focus on the transport properties of spin chains and spin ladders coupled to three dimensional phonons.

TT 32.9 Thu 14:00 Poster B

Kondo volume collapse and the Kondo breakdown transition in Heavy Fermions — •Andreas Hackl and Matthias Vojta — Institut für theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln

The unconventional critical behavior near magnetic quantum phase transitions in various heavy-fermion metals, apparently inconsistent with the standard spin-density-wave scenario, has triggered proposals on the breakdown of the Kondo effect at the critical point. Here we investigate the fate of such a zero-temperature transition upon coupling of the electronic to lattice degrees of freedom. Specifically, we study a Kondo-Heisenberg model with volume-dependent Kondo coupling – this model displays both Kondo volume collapse and Kondo-breakdown transitions, as well as a Lifshitz transition associated with a change of the Fermi-surface topology. Within a large-N treatment, we find that the Lifshitz transition tends to merge with the Kondo volume collapse and hence becomes first order, whereas the Kondo breakdown transition remains of second order except for very soft lattices. Interesting physics emerges at the quantum critical endpoint of the Kondo volume collapse: In two space dimensions, this endpoint is located at the Lifshitz line for a large range of parameters, thus two critical phenomena coincide without fine tuning. We briefly analyze the critical theory for such a situation, and finally relate our findings to current heavy-fermion experiments.

TT 32.10 Thu 14:00 Poster B

Heavy-fermion metals with hybridization nodes: Unconventional Fermi liquids and competing phases — •Matthias Vojta and Heidrun Weber — Institut für Theoretische Physik, Universität Köln, 50937 Köln, Germany

Microscopic models for heavy-fermion materials often assume a local, i.e., momentum-independent, hybridization between the conduction band and the local-moment f electrons. Motivated by recent experiments, we consider situations where this neglect of momentum dependence is inappropriate, namely when the hybridization function has nodes in momentum space. We explore the thermodynamic and optical properties of the highly anisotropic heavy Fermi liquid, resulting from Kondo screening in a higher angular-momentum channel. The dichotomy in momentum space has interesting consequences: While e.g. the low-temperature specific heat is dominated by heavy quasiparticles, the electrical conductivity at intermediate temperatures is carried by unhybridized light electrons. We then discuss aspects of the competition between Kondo effect and ordering phenomena induced by inter-moment exchange: We propose that the strong momentum-space anisotropy plays a vital role in selecting competing phases. Explicit results are obtained for the interplay of unconventional hybridization with unconventional, magnetically mediated, superconductivity, utilizing variants of large-N mean-field theory. We make connections to recent experiments on CeCoIn5 and other heavy-fermion materials.

TT 32.11 Thu 14:00 Poster B

Ambient-pressure thermodynamic measurements on UGe_2 — •Frédéric Hardy[1,2], Christoph Meingast[1], Hilbert v. Löhneysen[1,2], Jacques Flouquet[3], Andrew Huxley[3], Jason Lashley[4], Robert A. Fisher[5], and Norman E. Phillips[5] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]SPSMS-DRFMC, CEA-Grenoble, 38054 Grenoble cedex, France — [4]Materials Science Division and Technology Division, LANL, Los Alamos, New Mexico 87545, USA — [5]Materials Science Division, LBNL, Berkeley, California 94720, USA

The pairing interaction leading to the formation of the Cooper pairs remains unidentified in the ferromagnetic superconductor UGe_2. Nevertheless, there is strong experimental evidence that superconductivity is not mediated by the magnetic fluctuations that drive $T_{\mathrm{Curie}}(p)$ to zero; it rather appears closely related to another phase boundary $T_x(p)$ that occurs at lower pressure. Theoretical works suggested that this additional phase boundary could arise either from a coupling between SDW and CDW orderings or from a peak in the electronic density of states. Although the existence of this anomaly is experimentally incontestable between 0.6 and 1.2 GPa, the situation at ambient pressure remains ambiguous. We discuss the aforementioned scenarios in the light of recent high-resolution thermal expansion and calorimetric measurements realized under high magnetic fields at ambient pressure.

TT 32.12 Thu 14:00 Poster B

Dynamic magnetic order in $CeCu_2Si_2$ — •O. Stockert[1], J. Arndt[1], E. Faulhaber[2], H.S. Jeevan[1], C. Geibel[1], P. Fouquet[3], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Institut Laue-Langevin, Grenoble, France

The heavy-fermion compound $CeCu_2Si_2$ attracts still considerable interest due to the competition between antiferromagnetic order and superconductivity. The nature of the magnetic order is an incommensurate spin-density wave below $T_N \approx 800\,\mathrm{mK}$ determined by the nesting properties of the Fermi surface. Recently we observed that the magnetic Bragg peaks in only magnetically ordered $CeCu_2Si_2$ are broadened in q space. Starting from long-range order the magnetic Bragg peaks broaden below $T \approx 550\,\mathrm{mK}$. At $T = 100\,\mathrm{mK}$ a correlation length $\xi \approx 130\,\text{Å}$ has been estimated. From this finite correlation length/domain size at lowest temperature a finite lifetime of the magnetic peaks was expected. However, in neutron scattering experiments using a triple-axis spectrometer no broadening in energy was observed. Hence, the neutron spin-echo technique was chosen for this investigation due to the higher energy resolution. Data were recorded at different temperatures below T_N. From the spin-echo spectra some dynamic nature of the magnetic order in only magnetically ordered $CeCu_2Si_2$ can be inferred. The fluctuation rate of the antiferromagnetic order is estimated to be in the order of 50 MHz at lowest temperatures. Our results will be discussed in comparison to other measurements.

TT 32.13 Thu 14:00 Poster B

Magnetic excitations in $CeCu_2Ge_2$ — •Astrid Schneidewind[1], Oliver Stockert[2], Karin Schmalzl[3], Micha Deppe[2], Julia Arndt[2], Christoph Geibel[2], Frank Steglich[2], and Michael Loewenhaupt[1] — [1]Inst. f. Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [2]Max-Planck-Institut-CPfS, D-01178 Dresden, Germany — [3]Jülich Centre of Neutron Science, D-52425 Jülich, Germany, and Institut Laue-Langevin, F-38042 Grenoble, France

$CeCu_2Ge_2$ is a heavy-fermion compound showing incommensurate antiferromagnetic order with Kondo-compensated moments below $T_N = 4.15$ K [1,2]. Calculations of the Fermi surface show that a local character of the Ce 4f moments is not able to explain the incommensurate nesting vector as observed [3]. Involving an also itinerant component of the Ce 4f moments results in a nesting vector $\mathbf{q}$ which agrees well with the experimental values of $\mathbf{q}$ [3]. Since magnetic excitations are sensitive on the localization of the magnetic moments, we started to study the magnetic excitation spectrum to understand the magnetic order in $CeCu_2Ge_2$. In a first neutron scattering experiment on a $CeCu_2Ge_2$ single crystal the magnetic propagation vector was confirmed to be incommensurate and temperature dependent as reported by Krimmel et al. [2]. Furthermore, magnetic excitations have clearly been detected at low energies ($\hbar\omega \leq 2$ meV) below T_N displaying different temperature and $\mathbf{q}$-dependences.

[1] A. Krimmel et al., Physica B 234-236 (1997) 877.
[2] A. Krimmel et al., Phys. Rev. B 55 (1997) 6416.
[3] G. Zwicknagl, J. of Low Temp. Phys. 147 (2007) 123.

TT 32.14 Thu 14:00 Poster B

μSR-studies on the Heavy-Fermion-Superconductor $CeCoIn_5$ — •Johannes Spehling[1], Jeff Sonier[2], Eric Bauer[3], Robert Heffner[3], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU-Dresden, D-01069 Dresden, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, BC, Canada V5A 156 — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

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 Ovchinikov in 1964/1965. We have carried out transverse field μSR-measurements between 2T and 5T ($\hat{c}$-axis 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 should occur. The data clearly evidence the fielddriven change from second to first order transition at about 4.8T. On the other hand no additional line broadening is observed at very low temperatures below Tc in this orientation ($\hat{c} \parallel$ H), which disagrees with the assumption of the possible FFLO state.

[1] A. Bianchi,R. Movshovich,C. Capan,P.G. Pagliuso,and J. L. Sarrao, PRL, Vol.91, Number 18, 2003

TT 32.15 Thu 14:00 Poster B

Scanning Tunneling Spectroscopy studies on heavy fermion superconductors — •Stefan Ernst[1], Steffen Wirth[1], Hirale Jeevan[1], Christoph Geibel[1], Zachary Fisk[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics and Astronomy, UC Irvine

Scanning Tunneling Spectroscopy (STS) is a powerful tool for mapping the local electronic density of states of conducting 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 is expected to make a valuable contribution to the understanding of this class of materials. Fundamental properties such as the symmetry of the SC order parameter or, possibly, excitations due to the SC pairing interaction might be revealed.
This work reports on STM measurements carried out at low temperatures (320 mK) and under UHV conditions. A magnetic field of up to 12 T could be applied to confirm superconductivity of clean samples. For the materials investigated here, spectroscopic features in the order of a few hundred μeV are expected, calling for an excellent energy resolution during STS. The sufficiently high resolution of our STM has been verified by resolving the sub-meV SC energy gap of aluminum. Clean sample surfaces were prepared by *in situ* cleaving of the single crystals. Preliminary STS measurements were conducted on single crystalline samples of the HF superconductors $CeCoIn_5$ and $CeCu_2Si_2$.

TT 32.16 Thu 14:00 Poster B

Magnetic linear dichroism as new tool to determinecrystal fields in cubic Ce, Yb and Pr compounds — •Peter Koerner, Maurits Haverkort, Thomas Willers, Zhiwei Hu, Andrea Severing, and Liu Hao Tjeng — Institute of Physics II, University of Cologne

We have recently shown that polarization dependent soft-x-ray absorption spectroscopy (using linearly polarized light) is a powerful tool to probe the charge distribution of the crystal-field ground state of Ce Heavy-Fermion and Kondo intermetallics with tetragonal site symmetry [1]. The so-called linear dichroic signal at the Ce $M_{4,5}$ edges can be very large and is easily measured, thereby providing accurate quantitative information. For cubic systems, however, this dichroic effect vanishes. We now explore theoretically the feasibility to generate a dichroic signal by applying a strong magnetic field to the cubic system, thereby still using linearly polarized light. In this poster we will present under which conditions the lifting of the degeneracy by the Zeeman splitting will give rise to a detectable linear dichroic effect which can provide information about the charge distribution of the crystal-field ground state in cubic Ce, Yb compounds and the Pr skuterudites.. We note that this type of magnetic linear dichroism is different from that observed in e.g. Fe_2O_3 [2].

[1] P. Hansmann, A. Severing, Z. Hu, M.W. Haverkort, C.F. Chang, S. Klein, A. Tanaka, H.H. Hsieh, H.J. Lin, C.T. Chen, B. Fak, P. Lejay, L.H. Tjeng , Cond-Mat 0710.2778v1

[2] e.g. P. Kuiper et al., Phys. Rev. Lett. 70, 1549 (1993).

TT 32.17 Thu 14:00 Poster B

New correlated materials with phosphorus: A challenge for the crystal grower — •Anton Jesche, Cornelius Krellner, Nubia Caroca-Canales, Arpana Prasad, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The f-shell of Ce, Eu, Yb, and U can adopt different configurations, magnetic or non-magnetic, depending on the chemical surrounding. In the past decades, a large variety of systems were intensively studied due to the occurrence of many unusual features, like e.g. the formation of heavy-fermions, of unconventional superconductivity, and of unconventional metallic and magnetic states. Most of these systems contain Al, Si, Ge, In, and Sn beside the f-element and transition metals (T). On the way to look for new correlated materials, we have started the synthesis of several P-containing compounds. The crystal growth is rather challenging because of the high reactivity of elemental P. We succeeded in preparing CeTPO, CeT_2P_2, and $EuNi_2P_2$ using a Sn-flux method. For the CeTPO, CeT_2P_2 series the chemical structures are already known; however, no physical properties were reported. In this contribution we will present the details of the synthesis and discuss the physical properties determined by means of magnetic susceptibility, specific heat, and electrical resistivity measurements.

TT 32.18 Thu 14:00 Poster B

Preparation of $Sr_{1-x}Ca_xRuO_3$ thin films — •Melanie Schneider, Vasile Mosneaga, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universitaet Goettingen, Friedrich-Hund Platz 1, 37077 Goettingen

The series $Sr_{1-x}Ca_xRuO_3$ displays a continuous evolution from itinerant electron magnetism with $T_c = 160$ K ($x = 0$) towards a paramagnetic metallic state at $x = 1$. Previous studies on polycrystalline bulk samples raise the question whether the series shows a quantum critical point [1] or phase separation near $x = 0.7$ [2].
Here, we report first results on thin films which have been grown epitaxially on $SrTiO_3$ substrates by the metalorganic aerosol deposition technique. This technique is based on the use of a solution containing acetylacetonates of Sr^{2+}, Ca^{2+} and Ru^{3+}. Growth conditions have been optimized by the variation of the $(Sr_{1-x}Ca_x)$ to Ru ratio, deposition rate, molarity of the solution and deposition temperature. X-ray diffraction as well as STM, electrical resistivity and magnetization measurements are reported.

[1] K. Yoshimura *et al.*, *Phys. Rev. Lett.* **83**, 4397 (1999).
[2] Y.J. Uemura *et al.*, *Nature Physics* **3**, 29 (2007).

TT 32.19 Thu 14:00 Poster B

Structural studies on transition metal oxides with only one or two electrons in the 3d shell — •A. C. Komarek[1], T. Möller[1], M. Isobe[2], M. Gottschlich[1], M. Meven[3], M. Hölzel[3,4], A. Senyshyn[3,4], W. Morgenroth[5], D. Trots[5,4], M. Grüninger[1], and M. Braden[1] — [1]Institute of Physics II, University of Cologne — [2]Institute for Solid State Physics, The University of Tokyo — [3]TU Munich, FRM-II, Garching — [4]Institute for Materials Science, TU Darmstadt, Darmstadt — [5]Hasylab/DESY, Hamburg

Transition metal oxides with only one or two electrons in the 3d-shell are particularly interesting, as diffraction may more easily isolate the impact of the active electrons. A) The vanadate AV_2O_5 shows a variety of low-dimensional phenomena. We confirm the persistence of charge ordering of LiV_2O_5 down to 2 K by single crystal neutron diffraction and present an electron density study. B) We were able to solve the complex, distorted tetragonal hollandite ($K_2V_8O_{16}$) structure below the MI-transition at 175 K revealing a dimerization of the vanadium ions in one of two vanadium chains and a zig-zag-chain formation in the neighbouring chain. C) $CaCrO_3$ is a d^2 system with the unusual Cr oxidation state 4^+. It appears to be a bad metal, as found in optical spectroscopy, but in contrast to most metallic transition metal oxides $CaCrO_3$ orders antiferromagnetically with a pronounced structural anomaly occuring just at the Néel temperature. D) Cubic spinels AM_2O_4 with magnetic M ions have attracted strong attention due to intrinsic frustration. We determined the electron density of ZnV_2O_4.

TT 32.20 Thu 14:00 Poster B

Magnetic order of $CeNi_xGa_{4-x}$ — •Veronika Fritsch[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 investigate the ternary Ce-Ni-Ga system with samples prepared by flux-growth method in Ga-flux. The series $CeNi_xGa_{1-x}$ crystallizes in the tetragonal $BaAl_4$-structure. The homogeneity range of this structure is restricted to a narrow region around $x = 1$. The Ga-rich compounds have previously been reported to exhibit ferromagnetism [1]. Our systematic study shows that with increasing Ni content the lattice parameters shrink. However, they do not obey Vegard's law. The magnetic transition temperature, as identified from the sharp maximum in the magnetic susceptibility, increases slightly with increasing Ni content. On the other hand the absolute value of the magnetization at the transition drops around one order of magnitude. We did not find any difference between field-cooled and zero-field cooled magnetization measurements nor a hysteresis in the magnetization versus field curves. This leads us to the conclusion that our samples order antiferromagnetically.

[1] E. V. Sampathkumaran et al., Phys. Rev. B **47**(13), 8349, (1993).

TT 32.21 Thu 14:00 Poster B

Uniaxial pressure and strain dependences of the characteristic energies in $CeCu_{6-x}Au_x$ — •Kai Grube[1], Stefanie Drobnik[1,2], Roland Schäfer[1], Frédéric Hardy[1], Christoph Meingast[1], Oliver Stockert[3], and Hilbert von Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]MPI für chemische Physik fester Stoffe, 01187 Dresden, Germany

If paramagnetic compounds are driven into a magnetically ordered state by a nonthermal control parameter, the spontaneous symmetry breaking in the ordered state, as well as the interplay of characteristic energies inevitably lead to a change of the anisotropy of the compound at low temperatures. This can be used to identify the dominant energy scales and to study in more detail continuous phase transitions at zero temperature, i.e. so-called quantum critical points (QCP). The archetypical heavy-fermion system $CeCu_{6-x}Au_x$ is one of the best investigated examples of a magnetic QCP. It can easily be tuned across the onset of antiferromagnetic order by changing its volume either by alloying with Au or applying pressure. For several distinct Au contents we have determined the uniaxial pressure and strain dependences of the Kondo and the magnetic interaction energies, with the Grüneisen parameter obtained through thermal expansion, specific heat, and compressibility measurements. The results show a strongly anisotropic antiferromagnetic phase which develops from a nearly isotropic Kondo-lattice state.

TT 32.22 Thu 14:00 Poster B

High-pressure magnetization measurements on single-crystalline CoS_2 — •Sandra Drotziger[1], Kai Grube[2], Marc Uhlarz[1], Christian Pfleiderer[3], John Wilson[4], and Hilbert von Löhneysen[1,2] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe — [3]Physik Department E21, Technische Universität München, 85748 Garching — [4]H.H. Wills Physics Laboratory, University of Bristol, UK

Suppression of magnetic order in weak itinerant magnets has recently attracted scientific interest due to novel phases emerging in the vicinity of a quantum phase transition. Among these systems, the pyrite compound CoS_2 is a promising candidate for general considerations as it has a simple cubic structure with high magnetic isotropy. At $T_C \approx 122\,K$ CoS_2 develops ferromagnetic order with a spontaneous moment of $\mu_s = 0.84\,\mu_B$/Co. With increasing pressure the ferromagnetism is suppressed to lower temperatures and the order of the phase transition changes from second to first order at the tricritical point $p^* \approx 0.1\,GPa$ [1]. For $p > p^*$ a first order field-induced phase transition is observed. We report pressure studies of the DC magnetization measurements on CoS_2 single crystals as a function of temperature down to 2.3 K and magnetic field up to 12 T. The measurements were performed in a miniaturized diamond anvil cell made of a non-magnetic CuBe alloy. The temperature of the metamagnetic transition increases linearly, with a slope almost independent of p.

[1] S. Barakat, PhD Thesis, University of Cambridge (2001).

TT 32.23 Thu 14:00 Poster B

$CeRu_2Si_2$ and Quantum Critical Metamagnetism? — •Franziska Weickert[1,2], Philipp Gegenwart[3,1], Markus Garst[4], and Frank Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]Hochfeld-Magnetlabor Dresden, 01328 Dresden — [3]I. Physikalisches Institut, Universität Göttingen, 37077 Göttingen — [4]Institut für Theoretische Physik, Universität Köln, 50938 Köln

$CeRu_2Si_2$ is a well-known prototypical heavy fermion system and shows a sudden strong increase in the magnetization M and the sample length ΔL for magnetic fields parallel to the crystallographic c-direction at around 7.8 T. These anomalies occur below 4 K and sharpen with decreasing temperatures, but no features for a first order phase transition are observed down to 15 mK.

We report new thermal expansion α, magnetostriction λ and specific heat C/T measurements, which have been made in mT magnetic field steps around the metamagnetic crossover down to 15 mK on very pure single crystals.

The results show hints for the existence of a quantum critical endpoint in $CeRu_2Si_2$ and were compared with an extended model of metamagnetic quantum criticality, which was first introduced by *Millis et al.* in 2002.

TT 32.24 Thu 14:00 Poster B

Development of the magnetic order in $Yb(Rh_{1-x}Co_x)_2Si_2$ — •Christoph Klingner, Cornelius Krellner, Tanja Westerkamp, Niels Oeschler, Manuel Brando, Christoph Geibel, and Frank Steglich — Max Planck Institute for Chemical Physics of Solids, D-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) can be shifted to higher temperature by applying pressure. Doping with Cobalt results in positive chemical pressure, allowing therefore the investigation of the magnetic phase diagram and the behavior while stabilizing the antiferromagnetic ordered state. The advantage of less complex measurements compared to high pressure experiments leads to more detailed and precise results than in pressure studies. 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 between 0 and 1. The low temperature properties studied by resistivity, specific heat and magnetization measurements for different concentrations will be presented. Further on the behaviour of the transitions under an applied magnetic field will be discussed. Finally, a phase diagram of $Yb(Rh_{1-x}Co_x)_2Si_2$ will be presented and compared with the pressure phase diagram of $YbRh_2Si_2$.

TT 32.25 Thu 14:00 Poster B

Thermodynamics of Spin-Ladder and Spin-Chain Systems close to Quantum Criticality — •J. Rohrkamp[1], T. Lorenz[1], A. V. Sologubenko[1], O. Heyer[1], M. Garst[2], F. Anfuso[2], A. Rosch[2], K. Krämer[3], and M. M. 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 32.26 Thu 14:00 Poster B

Search for coupled S=1/2 dimer systems in a new class of nitronyl nitroxides biradicals — •K. Remović-Langer1[1], U. Tutsch[1], C. T. Pham[1], M. Baumgarten[2], E. A. Mostovich[2], B. Wolf[1], and M. Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, Max-von-Laue-Str. 1, SFB/TR 49, D-60438 Frankfurt(M), Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, SFB/TR 49, D-55128 Mainz, Germany

Recently, quantum magnets such as coupled-dimer systems and easy-plane antiferromagnets have emerged as interesting objects for studying the properties of magnetic field-induced Bose-Einstein condensation (BEC). Up until the present day, most of the studies have been focused on the magnetic field-induced BEC. Some recent experiments, however, give evidence for a transition which could be interpreted as pressure-induced BEC. So far, TlCuCl3, is the only quantum magnet on which field- and pressure-induced transitions have been studied. Biradical-based coupled-dimer systems, yielding moderate intradimer and tunable dimer-dimer interactions, are promising target materials for studying the properties of those field- and pressure-induced quantum phase transitions. We report here on the results of magnetic measurement on a group of metal-organic nitronyl nitroxides dimer systems which are proving to be a promising class of material for realization of systems to study field- and pressure-induced quantum phase transitions and their critical phenomena.

TT 32.27 Thu 14:00 Poster B

Structural and magnetic properties of a betaine-bridged trimer Cu^{2+} spin system — •K. Remović-Langer[1], B. Wolf[1], L. Wiehl[2], E. Haussühl[2], B. Winkler[2], N. Hasselmann[3], F. Sauli[3],

P. Kopietz[3], and M. Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, Max-von-Laue-Str. 1, SFB/TR 49, D-60438 Frankfurt(M). — [2]Institut für Mineralogie/Kristallographie, J.W. Goethe-Universität, Altenhöferallee 1, D-60438 Frankfurt(M). — [3]Institut für Theoretische Physik, J.W. Goethe-Universität, Max-von-Laue-Str. 1, SFB/TR 49, D-60438 Frankfurt(M).

A new betaine complex of Cu(II) ($S = 1/2$), with the general formula 2b*3$CuCl_2$*2H_2O with b = betaine ($C_5H_{11}NO_2$), has been synthesized and characterized magnetically. The structure of this metal-organic compound consists of centrosymmetric trimer units in which the neighboring Cu(II) atoms are bridged by the carboxylate groups of two betaine molecules. All Cu(II) ions show a nearly planar quadratic environment. In the ab-plane, a two-dimensional network of hydrogen bonds connects each trimer with four other trimers in a nearly quadratic arrangement. The obtained magnetic properties of Cu-betaine complex can be satisfactorily explained by using a magnetic model of coupled spin $S = 1/2$ trimers sitting on a quadratic lattice with an intra-trimer antiferromagnetic (AF) Cu-Cu coupling of J/k_B = 14 K and weak inter-trimer AF interaction J'/k_B= 4 K.

TT 32.28 Thu 14:00 Poster B

An effective dimer-monomer model for the distorted diamond chain azurite ($Cu_3(CO_3)_2(OH)_2$) — •Sebastian Köhler[1], Bernd Wolf[1], Andreas Brühl[1], Mariano de Souza[1], Katarina Remović-Langer[1], Yeekin Tsui[1], Ulrich Tutsch[1], Jürgen Schreuer[2], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, D-60438 Frankfurt(M) — [2]Institut für Mineralogie, Ruhr-Universität Bochum, 44780 Universitätsstraße 150

The S=1/2 spins in the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) are connected to one-dimensional structures called distorted diamond chains. Given that all three exchange constants are antiferromagnetic, the distorted diamond chain is a simple realization of a one-dimensional frustrated spin system. The theoretically examined phase diagram at $T = 0$ shows a ferrimagnetic, a dimerized and a spin-fluid phase. We present measurements of the specific heat as a function of temperature and magnetic field together with magnetic susceptibility data under hydrostatic pressure, which can be well interpreted using a simple model, where two of three spins in Azurite are connected to dimers in the singlet state ($J_{intra-dimer} \approx 50$ K), while the remaining monomer spins effectively form uniform, linear spin chains ($J_{eff} = 7$ K). Our experimental data support the description of Azurite for moderate magnetic fields in terms of the dimer-monomer model. In addition, the pressure dependence of the susceptibility directly indicates the large spin-phonon interaction in this low-dimensinal spin system.

TT 32.29 Thu 14:00 Poster B

Phase diagram close to a conductance plateau transition in a quantum wire — •Matthias Sitte[1], Julia S. Meyer[2], Achim Rosch[1], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — [2]Department of Physics, The Ohio State University, Ohio 43210, USA

We consider a quantum wire of spin-polarized (spinless) electrons close to the quantum phase transition where a second sub-band becomes activated as a function of gate voltage resulting in a jump of the zero temperature conductance. The filled first sub-band is treated as a Luttinger liquid, and it exchanges pairs of electrons with the second sub-band. It was shown in Ref. [1] that the conductance plateau transition is preempted by the formation of an inter-band pairing state. In the limit of infinitely strong inter-band density-density coupling, the latter transition is of Ising type. We perform a perturbative analysis around this strong coupling limit and determine the phase diagram. We find that the critical Ising mode induces superconducting fluctuations in the Luttinger liquid of the filled band, that are reflected in a logarithmically strong attractive interaction and a corresponding reduction of its plasmon velocity. We discuss possible consequences of this strong renormalization like a fluctuation-induced first order transition to a phase separated state preempting Ising criticality.

[1] J. S. Meyer, K. A. Matveev, and A. I. Larkin, Phys. Rev. Lett. **98**, 126404 (2007).

TT 32.30 Thu 14:00 Poster B

Electric and magnetic Properties of the Kagomé Systems $YBaCo_4O_{7+\delta}$ and $YBaCo_3MO_7$ (M=Fe,Al) — •Nils Hollmann[1], Martin Valldor[1], Zhiwei Hu[1], Antoine Maignan[2], Joachim Hemberger[1], Arata Tanaka[3], Liu Hao Tjeng[1], Thomas Lorenz[1], and John Mydosh[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Labaratoire CRISMAT, Caen — [3]Department of Quantum Matter, Hiroshima University

$YBaCo_4O_{7+\delta}$, $YBaCo_3FeO_7$ and $YBaCo_3AlO_7$ are closely related systems with cobalt ions in kagomé layers. In these kagomé layers, the triangular arrangement of the cobalt ions gives rise to a high degree of magnetic frustration. $YBaCo_4O_7$ reversibly changes the oxygen content depending on temperature and oxygen pressure. We present a study of magnetization, electrical transport and X-ray absorption of these materials. The systems are insulators and the electrical resistivity shows an anisotropy. The temperature dependence of the magnetization shows signs of strong frustration and spin-glass-like behaviour. This is studied with both DC and AC magnetization measurements. With the help of polarization dependent X-ray absorption, we deduce the valency and the orbital occupation of the cobalt ions. The valencies found can be used to prove the oxygen stochiometry.

TT 32.31 Thu 14:00 Poster B

Preparation and Characterization of $BaCoO_2$ and Sr-doped $EuCoO_3$ — •Marco Reuther, Kerstin Dönecke, John Mydosh, Thomas Lorenz, and Martin Valldor — II. Physikalisches Institut, Universität zu Köln, Germany

We have prepared polycrystals of $BaCoO_2$ and (Eu,Sr)CoO_3. $BaCoO_2$ is an air sensitive material whose physical properties are hardly explored. The structure of $BaCoO_2$ is trigonal with Co^{2+} ions in tetrahedral coordination [1]. Our magnetization measurements suggest a canted antiferromagnetic order with $T_N \approx 370$ K.

$EuCoO_3$ is insulating with Co^{3+} ions in the nonmagnetic low spin state up to about 400K [2]. Already small amounts of Sr induce a ferromagnetic order with $T_C \approx 160$ K due to the presence of Co^{4+} ions. Because of Co^{3+} remains in the low spin state we can observe the pure magnetic moment of Co^{4+} by Sr-doping. The electrical resistivity decreases with Sr but remains insulating.

[1] U. Spitsbergen et al., Acta Cryst. **13**, 197 (1960).
[2] J. Baier et al., PRB **71**, 014443 (2005)

TT 32.32 Thu 14:00 Poster B

Resonant diffraction from charge and spin ordering in $La_{1.5}Sr_{0.5}CoO_4$ — •Christian Schüssler-Langeheine[1], Matthias Cwik[1], Chun Fu Chang[1], Hsueh-Hung Wu[1,2], Marcel Buchholz[1], Zhiwei Hu[1], Thomas Willers[1], Enrico Schierle[3], Ralf Feyerherm[3], Detlef Schmitz[3], Mohammed Benomar[1], Markus Braden[1], and L. Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]NSRRC, Taiwan — [3]HMI c/o BESSY

Cobalt oxides are particularly interesting materials because of the different possible spin states of the Co^{3+} ion, which can occur in the low-spin, intermediate-spin or high-spin state. This adds another degree of freedom to charge, spin and orbital occupation of other transition metal ions. For $La_{1.5}Sr_{0.5}CoO_4$ commensurate charge and spin order was reported with a very unusual suppression of static magnetic ordering.

We studied this system using resonant diffraction at the Co K and $L_{2,3}$ resonance in order to obtain information about both charge and spin ordering. We find a pronounced pattern of incommensurate charge ordering not observed by neutron diffraction. From the magnetic scattering data we are able to determine the ordered orbital momentum and find indications for a more complex magnetic ordering than discussed so far.

Supported by the DFG through SFB 608 and by the BMBF.

TT 32.33 Thu 14:00 Poster B

Orbital degree of freedom in $La_{7/8}Sr_{1/8}MnO_3$: Temperature-dependent rearrangement of orbital states — •Michael Merz[1,2], Christian Pinta[1,3], Sebastian Prinz[2], Peter Nagel[1], Andrei Samartsev[3,1], Stefan Schuppler[1], Pascal Reutler[4], and Bernd Büchner[4] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Institut für Kristallographie, Jägerstraße 17-19, RWTH Aachen, 52066 Aachen — [3]Fakultät für Physik, Universität Karlsruhe, 76128 Karlsruhe — [4]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01171 Dresden

One of the most unusual phases found among charge and orbital ordered systems appears for $La_{7/8}Sr_{1/8}MnO_3$ below 150 K: a *ferromagnetic insulating* (FMI) state. With O1s near-edge x-ray absorption fine structure and single-crystal x-ray diffraction we studied the temperature-dependent evolution of this FMI phase. Our results give the following picture: Above $T_{JT} \approx 275$ K, strong fluctuations prevent the orbitals from ordering. Upon cooling below T_{JT}, a first-order phase transition to a cooperative Jahn-Teller distorted phase takes

place. When decreasing the temperature below 180 K, more and more O and Mn^{3+} atoms arrange their orbitals to the orbital polaron state, and this process leads to a continuous phase transition towards the FMI state. Once established, the local orbital polarons remain stable objects upon further cooling and may well form the orbital polaron lattice below T_{CO} as suggested by resonant x-ray scattering [1].

[1] J. Geck et al. Phys. Rev. Lett. 95, 236401 (2005).

TT 32.34 Thu 14:00 Poster B

Surface topographic and spectroscopic studies of charge ordering $La_{0.5}Sr_{1.5}MnO_4$ using Scanning Tunneling Microscopy — •Paul Sass[1], Grzegorz Urbanik[1,2], Christian Hess[1], Torben Hänke[1], Bernd Büchner[1], Antoni Ciszewski[2], Pascal Reutler[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institute of Experimental Physics, University of Wroclaw, 50-204 Wroclaw, Poland — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, Bâtiment 414, 91405 Orsay, France

We have studied the compound $La_{0.5}Sr_{1.5}MnO_4$ which can be considered as a textbook example of charge and orbital ordering by means of Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). We were able to cleave the material in-situ under Ultra High Vacuum conditions prior to the STM/STS studies. Topographic scans routinely reveal atomically resolved surfaces both above and below the charge ordering temperature $T_{CO} \approx 225$ K (down to $T \approx 205$ K). The step height analysis suggests cleaving between the (Sr,La)O-layers. We have studied the temperature dependence of the electronic structure both for $T > T_{CO}$ and $T < T_{CO}$. The STS clearly reveals finite DOS at the Fermi level for $T > T_{CO}$ and the opening of a gap $\Delta \approx 0.5$ eV just below T_{CO}. In the topographic studies we find nanometer scale modulations with various periodicity. We discuss these modulations in view of the inherent charge and orbital ordered state of this material. We compare our results with STS studies on other transition metal oxides exhibiting inhomogeneous charge distributions.

TT 32.35 Thu 14:00 Poster B

Magnetic 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 present measurements of the magnetization M, specific heat c_p and resistance ρ of EuC_{2+x} (x=0, 0.1) compounds. The magnetization data show a ferromagnetic ordering at $T_C \simeq 14$K with a saturation moment of $\simeq 7\frac{\mu_B}{FE}$. This suggests an oxidation state of Eu^{2+}. 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 resistance ρ over a couple of orders of magnitude indicating a metal-insulator transition (MIT). Moreover, an applied magnetic field shifts 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 magnetorsistance of the better known system of 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 32.36 Thu 14:00 Poster B

Electronic properties of transition metal impurities in MgO thin films — •Rainald Gierth[1], Tim Haupricht[1], Chun-Fu Chang[1], Zhiwei Hu[1], Thomas Koethe[1], H. H. Hsieh[2], H.-J. Lin[3], C. T. Chen[3], and Liu Hao Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

We have studied the electronic structure of transition metal impurities in MgO. These systems 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 spectra can change significantly e.g. due to the influence of non-local screening effects. We present our core level and valence band photoemission data of Ni and Mn impurities in MgO thin films epitaxially grown on Ag(001) *in-situ*, taken at different photon energies. Changes in the shape as well as in the width of the spectra are observed. The experimental results are compared to various theoretical approaches.

TT 32.37 Thu 14:00 Poster B

Correlated band structure of $3d^2$ vanadates — •David Heilmann and Eva Pavarini — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

We study the correlated band structure and the momentum-resolved spectra for $3d^2$ vanadates, like $LaVO_3$ and YVO_3, using a combination of a first-principles technique and Dynamical Mean-Field Theory with a Monte Carlo impurity solver.

The self-energy for the effective $3d$ bands is calculated using Maximum-Entropy spectral analysis of the Monte Carlo results and a self-consistent procedure. We use this self-energy to calculate the full momentum-resolved spectrum and the correlated band structure, which we compare to available spectroscopy experimental results. We also discuss the effects of the lattice distortions and chemistry.

TT 32.38 Thu 14:00 Poster B

Quantum Monte Carlo Simulations in Continuous Time: An Application to the Hubbard Model — •Sebastian Fuchs and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We perform quantum Monte Carlo simulations of the Hubbard model using the Dynamical Cluster Approximation (DCA) [1]. Hereby the complexity of the full lattice problem is reduced by mapping it to a finite size cluster self-consistently embedded in a mean-field. The resulting cluster problem is solved by a Monte Carlo procedure using a weak coupling expansion in continuous imaginary time [2]. Compared to the traditional Hirsch-Fye algorithm simulations can be much more efficient and systematical errors due to a discretization of the imaginary time axis are avoided.

Our main focus is the investigation of the single-particle properties of the Hubbard model in the antiferromagnetic phase. Using analytic continuation of the Monte Carlo data the DCA permits us to calculate spectral functions with explicit k-dependence.

Our implementation of the algorithm 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] Th. Maier *et. al.*, Rev. Mod. Phys. **77**, 1027 (2005)
[2] A. N. Rubstov *et. al.*, Phys. Rev. B **72**, 035122 (2005)
[3] `http://alps.comp-phys.org`

TT 32.39 Thu 14:00 Poster B

Mott transition in one dimension: Benchmarking dynamical cluster approaches — •Matthias Balzer[1], Werner Hanke[1], and Michael Potthoff[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]I. Institut für Theoretische Physik, Universität Hamburg

The variational cluster approach (VCA) is applied to the 1D Hubbard model at $T = 0$ using clusters (chains) of up to ten sites with full diagonalization and the Lanczos method as cluster solver. Within the framework of the self-energy-functional theory (SFT), different cluster reference systems with and without bath degrees of freedom, in different topologies and with different sets of variational parameters are considered. Static and one-particle dynamical quantities are calculated for half-filling as a function of U as well as for fixed U as a function of the chemical potential to study the interaction- and filling-dependent metal-insulator (Mott) transition. We compare the VCA results with exact results available from the Bethe ansatz, with essentially exact dynamical DMRG data, with (cellular) dynamical mean-field theory and full diagonalization of isolated Hubbard chains. Several issues are discussed including convergence of the results with cluster size, the ability of cluster approaches to access the critical regime of the Mott transition and efficiency in the optimization of correlated-site vs. bath-site parameters. We also study the role of bath sites for the description of excitation properties and as charge reservoirs for the description of filling dependencies. The VCA turns out to be a computationally cheap method which is competitive with established cluster approaches.

TT 32.40 Thu 14:00 Poster B

A new DCA scheme for calculating two-particle correlation functions of the 2D Hubbard model — •Stephan Hochkeppel, Fakher Assaad, and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Based on the Dynamical Cluster Approximation (DCA), we present a new approach to calculate two-particle Green's functions for Hubbard-

type models. In a first step, the DCA together with quantum Monte-Carlo as a cluster solver is used to compute the single-particle spectral functions ($A(\mathbf{k},\omega)$) of the hole-doped Hubbard model. U(1) as well as SU(2) symmetry breaking is allowed so as to access superconducting states (dSC) as well as antiferromagnetic (AF) order. The temperature dependence of $A(\mathbf{k},\omega)$ from the paramagnetic to the dSC phase is studied in detail, the aim being a detailed study of the evolution of the pseudogap.

Two-particle quantities are computed within a quantum cluster approach, where the dynamical vertex is extracted from the cluster and the DCA dressed Green functions are used to calculate the bubble. The quality of the new approach is tested by comparing the resulting Neel temperature to that obtained by allowing for symmetry breaking within the DCA. Signatures of spin- and charge-correlation functions in the corresponding single-particle spectral functions are studied and resolved in detail.

TT 32.41 Thu 14:00 Poster B

Pseudogap and magnetic incommensurability in the Hubbard model — •Michael Schreiber[1] and Alexei Sherman[2] — [1]Institut für Physik, Technische Universität, Chemnitz, Germany — [2]Institute of Physics, University of Tartu, Tartu, Estonia

The energy spectrum and the magnetic susceptibility of the two-dimensional repulsive Hubbard model are investigated with the use of a diagram technique for the case of strong correlations in which an expansion in powers of the hopping constant is used. For small lattices and high temperatures obtained results are in agreement with data of Monte Carlo simulations. It is shown that with departure from half-filling an additional narrow band arises near the Fermi level. By the dispersion, bandwidth and the variation with the electron concentration $\bar{n}$ this band is close to the spin-polaron band of the t-J model. For moderate doping a pseudogap appears near the Fermi level. The magnitude of the pseudogap and its change with $\bar{n}$ are similar to the pseudogap in hole-doped cuprate perovskites. With the departure from half-filling the low-frequency magnetic susceptibility becomes incommensurate and the incommensurability parameter grows with $1-\bar{n}$. The incommensurability, its dependence on the frequency and electron concentration resemble experimental results in lanthanum cuprates.

TT 32.42 Thu 14:00 Poster B

Direct calculation of self-energies of the infinite-dimensional Hubbard model by D-DMRG — •Patrick Grete, Carsten Raas, and Götz S. Uhrig — Theoretische Physik I, Technische Universität Dortmund, 44221 Dortmund

We treat the infinite-dimensional Hubbard model within a DMFT-framework by solving the local impurity-problem (SIAM) within dynamic density-matrix-renormalisation (D-DMRG). Instead of extracting the self-energies in a numerically unstable way via the Dyson equation, we use a modified Green function to calculate the self-energies directly. In addition to sharp excitation peaks at the inner edges of the Hubbard bands, we find trough-like features in the imaginary part of the self-energy. They correspond to kinks in the real part of the self-energy. Their relation to collective modes is discussed.

TT 32.43 Thu 14:00 Poster B

Electronic transitions in a Mott-Hubbard insulator under external perturbations — •Luis Craco and Helge Rosner — Max-Planck-Institut fuer Chemische Physik fester Stoffe, 01187 Dresden, Germany

The general problem of perturbation induced electronic transitions is addressed using extensions of the LDA+DMFT scheme. It is shown how the Mott-Hubbard insulating state of YTiO3 is affected by external pressure [1] and magnetic-field [2]. The correlated spectra fond at ambient conditions is shown to be in good agreement with experiments (PES and optics) [3]. Under pressure [1] we found a continuous reduction of the Mott-Hubbard gap at small pressures which is consistent with indications from recent mid-infrared optical absorption studies. We also consider the problem of magnetic-field induced orbital switching and reverse orbital polarization and its possible implications to experiments for YTiO3 [2] and correlated materials of great interest.

[1] L. Craco, M.S. Laad, S. Leoni and H. Rosner, submited to PRB-RC.

[2] L. Craco and H. Rosner, in preparation.

[3] L. Craco, S. Leoni, M.S. Laad, and H. Rosner, Phys. Rev. B 76, 115128 (2007).

TT 32.44 Thu 14:00 Poster B

Boson-controlled quantum transport — •Holger Fehske[1], Andreas Alvermann[1], Gerhard Wellein[2], and David M. Edwards[3] — [1]Ernst Moritz Arndt Universität Greifswald, Greifswald, Germany — [2]Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Imperial College London, London, United Kingdom

We investigate transport within some background medium by means of an effective lattice model with a novel form of fermion-boson coupling. The bosons correspond to local fluctuations of the background. The model captures the principal transport mechanisms that apply to a great variety of physical systems, and can be applied to describe the motion of lattice and spin polarons, or the dynamics of a particle coupled to a bath. Performing large-scale numerical simulations based on highly efficient variational Lanczos and Chebyshev moment expansion techniques, we analyse the newly proposed model by exactly calculating the single quasiparticle effective mass, ground-state dispersion and spectral function, as well as the Drude weight and the optical conductivity for an infinite one-dimensional system. For the half-filled band case, we establish a metal-insulator quantum phase transition by analysing the particle-particle and particle-boson correlations and photoemission spectra.

TT 32.45 Thu 14:00 Poster B

Time evolution in 2D quantum percolation — •Gerald Schubert and Holger Fehske — Ernst-Moritz-Arndt-Universität Greifswald, Germany

The quantum percolation problem of finding extended or localised wave functions on the spanning cluster shows a strong dependence on the dimension and connectivity of the underlying lattice. For cubic lattices in three dimensions (3D), the existence of a quantum percolation threshold, p_q, only above which extended states exist, is well documented in the literature. Although the exact determination of the actual value of p_q is difficult, the results agree on $p_c < p_q < 1$, where p_c is the classical percolation threshold. The situation is less clear for the 2D hypercubic lattice with estimates for p_q ranging from 0.7 to 1. Here we investigate the time evolution of a wave packet initially localised on the spanning cluster by means of a Chebyshev expansion technique. Depending on the concentration of accessible lattice sites p, we find qualitatively different behaviour: The wave packet stays localised in a finite region for $p < p_q$ or spreads over the whole spanning for $p_q < p$ cluster. This gives evidence of $p_q < 1$. Of course our calculations have to be complemented by a careful finite-size analysis. Due to the high efficiency of the Chebyshev method, at present, we are able to increase the treatable system sizes up to 5000×5000, which enables us to rule out some of previous estimates for p_q.

TT 32.46 Thu 14:00 Poster B

Projective renormalization approach (PRM) to the one-dimensional Hubbard model — •Christian Köhler, Steffen Sykora, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The usual method for the investigation of the low-energy properties of the one-dimensional Hubbard model with linear electron dispersion is based on the bosonization approach for the densities of the two electron branches. Instead of using a Bogoliubov transformation to diagonalize the bosonized Tomonaga-Luttinger Hamiltonian, in the PRM the interaction between the densities on the two branches is eliminated successively. As a result, one achieves a renormalized Hamiltonian with no coupling between the two branches. In this way, an improved evaluation for the Luttinger parameters can be obtained.

TT 32.47 Thu 14:00 Poster B

Dynamical properties of the one-dimensional Holstein model — •Peter Pippan and Hans Gerd Evertz — TU Graz, Austria

We study the phonon dynamics of the one-dimensional Holstein model of spinless fermions. Using cluster loop updates in spin space and a phonon integration in Fourier space, we employ a QMC method with hardly any auto correlations even at temperatures close to zero. We present precise data for the phonon spectral function in both the metallic luttinger liquid and the insulating charge density wave phase for a wide range of phonon frequencies.

TT 32.48 Thu 14:00 Poster B

Dispersion renormalization in quasi-1d interacting electron systems — •Jutta Ortloff and Carsten Honerkamp — Theoretische Physik Universität Würzburg

We investigate the interaction-induced change of the dispersion in

coupled onedimensional chains of interacting fermions. We use a functional renormalization group method with flat cutoff and high wavevector-resolution beyond the standard g-ology treatment. In general, the flow of the Fermi points is rather mild and does not change the main characteristics of the flows to strong coupling. We furthermore analyze how the renormalization of the dispersion correlates with the dominant interaction channel.

TT 32.49 Thu 14:00 Poster B

Approaching experimental setups: 1D quantum wire coupled to 2D leads — •Peter Wächter[1], Volker Meden[2], and Kurt Schönhammer[1] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, Germany

A major experimental challenge in low-dimensional physics is the clear confirmation of Luttinger-Liquid(LL)-behavior in one-dimensional correlated electron systems. A prominent characteristic property of LL-physics is the scaling of a variety of observables as functions of external parameters with exponents controlled by a single parameter, the LL-parameter K. In this work we focus on the scaling of the conductance G as function of the temperature. In particular, we extend the investigation of the LL scaling of G from the mostly considered case of 1d leads connected to the end of a 1d quantum wire to 2d leads coupled arbitrarily to a 1d quantum wire, a geometry often used in experiments. We present numerical results for a variety of configurations and discuss the underlying physical mechanisms.

TT 32.50 Thu 14:00 Poster B

Entanglement entropy and quantum phase transition — •Alex Cojuhovschi and Eric Jeckelmann — Leibniz Universitaet Hannover, Germany

We study the bipartite entanglement entropy in the one-dimensional half-filled extended Hubbard model with nearest neighbor repulsion. The entropy is calculated in finite open chains using the density-matrix renormalization group method and in infinite systems using the matrix-product state proposed by Vidal. We discuss the phase diagram of this model, in particular the possible existence of a spontaneous long-range order of the bond-order wave type (dimerization), the behavior of the bipartite entropy at the quantum phase boundaries, and the performance of Vidal's infinite-system method.

TT 32.51 Thu 14:00 Poster B

Quasistatic spin correlations in the frustrated spin-chain cuprate Li_2ZrCuO_4 above T_N — •Yulieth Arango[1], Evgeniya Vavilova[2], Vladik Kataev[1,2], Olga Volkova[3], Aleksandr Vasilyev[3], and Bernd Buechner[1] — [1]Institute for Solid State and Material Research IFW Dresden, D-01171 Dresden, Germany — [2]Kazan Physical Technical Institute, 420029 Kazan Russia — [3]Moscow State University 119992 Moscow Russia

Li_2ZrCuO_4 is a new frustrated quasi-1D spin system with unusual thermodynamic properties due to its proximity to the ferromagnetic critical point. This material contains CuO_2 chains along the crystallographic c-axis, with frustrated exchange interactions between the Cu spins S = 1/2. We carried out high field Cu^{2+} ESR and ^{7}Li-NMR measurements on an oriented powder, in a broad temperature range. The ESR data reveal temperature and orientation dependent anisotropy of the g-factor, as well as a progressive broadening of the linewidth below T $\approx$ 80 K. Two antiferromagnetic resonance modes were observed below $T_N \approx 8$ K in long range magnetically ordered state. Surprisingly these modes can be seen also in an extended T-range above T_N. This is in an agreement with the unusual ^{7}Li-NMR linewidth and relaxation rates behaviour above T_N . The data analysis suggests the occurrence of quasi-static spin correlations in the chain planes (bc-plane) and anisotropic T-dependent internal field below 80 K. The presence of these features far above T_N indicates a substantial frustration of spin-spin interactions in Li_2ZrCuO_4.

TT 32.52 Thu 14:00 Poster B

High-field magnetization studies of the quasi-1D quantum spin systems $(Y,Nd)_2BaNiO_5$ and Li_2ZrCuO_4 — •Florian Kretzschmar[1], Rüdiger Klingeler[1], Natalia Tristan[1], Yulieth Arango[1], Stefan-Ludwig Drechsler[1], Elena Popova[3], Olga Volkova[3], Alexander Vasiliev[3], Harison Rakoto[2], and Bernd Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, 01171 Dresden, Germany — [2]Laboratoire National des Champs Magnétiques Pulsés, 31432 Toulouse, France — [3]Low Temperature Physics Department, Moscow State University, 119991 Moscow, Russia

Quasi-one-dimensional quantum spin systems show fascinating ground states which low-energy excitations can often nicely investigated by high field magnetisation studies. Here, we report on static (up to 17T) and pulsed (up to 60T) magnetic field studies on the highly frustrated S=1/2 spin chains in Li_2ZrCuO_4 and on the interplay of S=1 chains and classical 4f-moments in $(Y_{1-x}Nd_x)_2BaNiO_5$. For the latter system, a Haldane gap is observed even for $x = 1$ where long antiferromagnetic order is realized. For $x = 1$, we find two field induced metamagnetic transitions which field dependence qualitatively changes for smaller x. We discuss this change in terms of the distance between Nd ions vs. the correlation length along the Haldane chains. In Li_2ZrCuO_4, our measurements on oriented powders show an unusual anisotropy. In addition, the saturation field of $\sim$20T implies that the inter-chain coupling plays a crucial role in such highly frustrated systems.

TT 32.53 Thu 14:00 Poster B

Optical Excitations of the Spin-Ladder $Sr_{14-x}Ca_xCu_{24}O_{41}$ from FIR to UV — •C. Hilgers[1], M. Grüninger[1], M. Reuther[1], U. Ammerahl[2], P. Ribeiro[3], B. Büchner[3], and A. Revcolevschi[2] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire de Physico-Chimie de L'Etat Solide, Université Paris-Sud, France — [3]IFW Dresden

We present low-temperature optical conductivity data of the hole-doped spin-ladder compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ between 10 meV and 6 eV for x = 0, 5, and 8. The investigation aims at the understanding of the electronic structure, charge carrier distribution and low-temperature anomalies in the phonon excitation spectra. The optical conductivity along the rung and leg directions was derived by analyzing a combination of ellipsometry and reflectivity data. The temperature and doping dependence of the charge-transfer excitations is investigated with focus on excitonic effects. Moreover, the transfer of spectral weight from low to high energy is studied as a function of temperature.

TT 32.54 Thu 14:00 Poster B

Magnetic excitations in S=1/2 chains and five-leg ladders: an optical study — •Eva Benckiser[1], Markus Grüninger[1], Marco Reuther[1], Thomas Lorenz[1], Pascal Ribeiro[2], Christian Hess[2], and Alexandre Revcolevschi[3] — [1]Institute of Physics II, University of Cologne, Germany — [2]IFW Dresden, Germany — [3]Laboratoire de Chimie des Solides, University Paris-Sud, France

The crossover from 1D chains via n-leg ladders to 2D planes is very interesting. However, hardly any experimental data exist for $n > 2$. We have grown single crystals of the 5-leg ladder $La_8Cu_7O_{19}$ in an image furnace. A contribution of the magnetic excitations to the optical conductivity arises due to the simultaneous excitation of a phonon. Our optical data represent the first experimental result on the magnetic excitations of n-leg ladders ($n > 2$) at high energies. We find a surprising resemblance with the well-understood spectrum of a two-leg ladder. In particular, our data strongly suggest the existence of bound states of magnetic excitations also in the 5-leg ladder.

In the zig-zag double chain (Sr,Ca)CuO_2, the observation of two-spinon excitations for polarization parallel to the chains enables us to determine the exchange coupling $J = 227 \pm 4$ meV very accurately, which resolves an old controversy. We report the dependence of J on temperature and Ca substitution. Moreover, we discuss a new mechanism (without invoking a phonon) which explains the observation of magnetic excitations for polarization *perpendicular* to the chains ($E \parallel b$). The relevance of this contribution to the optical conductivity for other quantum spin systems is pointed out.

TT 32.55 Thu 14:00 Poster B

Unusual increase of the hole mobility in the quasi-1D $Sr_{14}Cu_{24}O_{41}$ upon Zn doping — •M. Yehia[1], P. Ribeiro[1], F. Kretzschmar[1], V. Kataev[1], C. Hess[1], R. Klingeler[1], B. Büchner[1], H. ElHaes[2], G. Roth[2], U. Ammerahl[3], and A. Revcolevschi[3] — [1]Leibniz-Institute for Solide State and Materials Research, IFW-Dresden, 01171 Dresden, Germany — [2]RWTH-Aachen, 52056 Aachen, Germany — [3]Laboratoire de Physico-Chimie de l'État Solide, Université Paris-Sud, 91405 Orsay, France

Single crystals of $Sr_{14}Cu_{24-x}Zn_xO_{41}$ ($0 \le x \le 0.75$) were studied using ESR, static magnetization and conductivity measurements. ESR measurements reveal a remarkable influence of the hole dynamics on the Cu-spin relaxation for all values of x and suggest an increase of

the hole mobility and a decrease of the charge ordering temperature. This is consistent with the conductivity measurements $\sigma(T)$ which imply a significant increase of σ with increasing Zn content reflecting the enhancement of the hole mobility. Static magnetization shows that a spin-gap like feature is preserved for all Zn concentrations. We discuss possible scenarios for the remarkable impact of the Zn doping on the spin relaxation and conductivity.

TT 32.56 Thu 14:00 Poster B

Electrical transport measurements in the Ca-doped ladders $Sr_{14-x}Ca_xCu_{24}O_{41}$ — •M. E. Navarro Fuentes[1], A. Narduzzo[1], H. ElHaes[2], P. Ribeiro[1], C. Hess[1], B. Büchner[1], U. Ammerahl[3], and A. Revcolevschi[3] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Université Paris-Sud, Orsay, France.

We report on measurements of electrical resistivity in the Ca-doped spin ladders $Sr_{14-x}Ca_xCu_{24}O_{41}$ ($0< x <12$) in the temperature range $6K< T <300K$. The resistivities along the ladders (ρ_c) and perpendicular to them (ρ_a) decrease by two and one order of magnitude respectively upon Ca-doping; ρ_c in particular displays a crossover from insulating to metallic behavior for $x >11$. While this insulator to metal crossover represents an interesting and as yet unresolved issue in its own right (as both the spin and the itinerant hole systems are arguably in a state of intermediate dimensionality between 2 and 3) its understanding may ultimately shed light on the conundrum the physics of high-temperature superconductors represents. We present an interpretation of the observed results in the light of existing theoretical frameworks.

TT 32.57 Thu 14:00 Poster B

Electrochemical doping of Vanadium Oxide Nanotubes — •A. Popa[1], I. Hellmann[1], R. Klingeler[1], V. Kataev[1], E. Vavilova[1,2], Y. Arango[1], C. Täschner[1], M. Knupfer[1], H.-H. Klauss[3], C. Masquelier[4], and B. Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, Kazan, Russia — [3]Technical University-Dresden,Germany — [4]Laboratoire de Réactivité et de Chimie des Solides, Amiens, France

A new class of nanoscale low-dimensional magnets, mixed valent vanadium oxide multiwall nanotubes (VOx-NTs), show up diverse novel properties ranging from spin frustration and semiconductivity to ferromagnetism by doping with either electrons or holes. The structural low dimensionality and mixed valency of vanadium ions yield a complex temperature dependence of the static magnetization and the nuclear relaxation rates. Upon electron doping of VOx-NTs, our spectroscopic data confirm an increased number of magnetic $V^{4.4+}$ sites. Interestingly, a considerable superparamagnetic moment of $0.1\mu_B$ is found at room temperature after electrochemical intercalation of 10% of Li while no strong effect on the magnetization occurs for other doping levels. Recent μSR studies on $Li_{0.1}$VOx-NT indeed confirm that more than 40% of the sample is magnetic. This result is corroborated by Li^7-NMR measurements which confirm the increase of $V^{4.4+}$ sites upon Li doping and imply an additional internal magnetic field only for the doping level 0.1.

TT 32.58 Thu 14:00 Poster B

Investigations on oxide nanocompounds — •Ingo Hellmann[1], Andreia Popa[1], Yulieth Arango[1], Evgenia Vavilova[1,2], Anupama Parameswaran[1], Rüdiger Klingeler[1], Vladislav Kataev[1], Galina Zakharova[3], Christine Täschner[1], Martin Knupfer[1], and Bernd Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Kazan Physical Technical Institute, Kazan, Russia — [3]Institute of Solid State Chemistry, Yekaterinburg, Russia

In transition metal oxide nanocompounds the small size of these structures as well as charge, spin and orbital degrees of freedom of the 3*d*-ions lead to properties which can be quite different from the respective bulk materials. We applied optical spectroscopy, PES and EELS as well as static magnetization, ESR and NMR studies in order to obtain insight into the rich physics of these materials. Vanadium oxide nanotubes exhibit diverse properties ranging from spin frustration and semiconductivity to superparamagnetism or even ferromagnetism by Li-doping. The intercalation of a small amount of other ions, such as Co, Fe, Mn, Cr, strongly affects the magnetic and electronic characteristics. As an example, $Co_{0.18}V_2O_5$ nanotubes show antiferromagnetic ordering at 15 K. Interestingly, a ferromagnetic hysteresis is observed at still lower temperatures. A similar magnetic response was obtained for α-MnO_2 nanorods which consist of edge coupled octahedra forming tunnel-like structures. The Mn-ion is present in a 4+ oxidation state with spin S = 3/2. By electron doping via an electrochemical reaction or in-situ evaporation using lithium, the manganese valency can be tuned in order to obtain Mn^{3+} sites having spin S = 2.

TT 32.59 Thu 14:00 Poster B

Magnetic ordering in organic transition-metal compounds — •L. Huang[1], R. Beyer[1], T. Papageorgiou[1], O. Ignatchik[1], T. Herrmannsdörfer[1], J. Wosnitza[1], S. Gemming[2], J. Manson[3], and J. Schlueter[4] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf (FZD), D-01314 Dresden, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung (FZD) — [3]Department of Chemistry and Biochemistry, Eastern Washington Univ., Cheney, USA — [4]Materials Science Division, Argonne National Laboratory, Argonne, USA

The magnetic properties of metalorganic compounds attract much attention as their structural and electronic exchange dimensionality can vary between one and three. Here, we present data of representatives which exhibit magnetic ordering and have been recently investigated by means of magnetometry and calorimetry. In the quasi-cubic compound $[Cu(HF_2)(pyz)_2]BF_4$, we have observed an antiferromagnetic (AF) ordered phase occurring at $T_N = 1.6K$ and a rich magnetic phase diagram up to $14\,T$ as well. Above T_N, the specific heat of that compound is in reasonable agreement with the predictions of the model for a $s = \frac{1}{2}$ 2D square lattice quantum Heisenberg AF describing the in-plane exchange via the $Cu-F-H-F-Cu$ bonds. In the quasi-1D compound $Mn(glycine)(H_2O)_2Cl_2$ which is structurally arranged in helical chains, we have observed an unexpected 3D AF ordering at $T_N = 0.84\,K$, both in the results of the heat capacity and ac susceptibility. Probably, the 3D exchange is mediated by hydrogen bonds between the chains in addition to $Mn–O–Mn$ bonds along the chains.

TT 32.60 Thu 14:00 Poster B

Magnetostriction and thermal expansion of the spin-ladder compound $(C_5H_{12}N)_2CuBr_4$ — Thomas Lorenz[1], •Fabrizio Anfuso[2], Markus Garst[2], Achim Rosch[2], Oliver Heyer[1], Christian Rüegg[3], and Karl Krämer[4] — [1]Institute of Physics II, University of Cologne, Germany — [2]Institute of Theoretical Physics, University of Cologne, Germany — [3]Centre for Nanotechnology and Dep. of Phys. and Astronomy, University College London, UK — [4]Department of Chemistry and Biochemistry, University of Bern, Switzerland

We present high-resolution measurements of the thermal expansion and magnetostriction of piperidinium copper bromide $(C_5H_{12}N)_2CuBr_4$. The experimental data at low and intermediate temperatures are very well described by a two-leg spin-ladder Hamiltonian with rung and nearest neighbor leg couplings. The thermal expansion shows a complex behavior with various sign changes and approaches a "one-dimensional" $1/\sqrt{T}$ divergence at the critical fields. As a consequence of a *two-coupling constants* model, the magnetostriction and thermal expansion along arbitrary spatial directions are always representable as linear combination of two simple spin correlation functions. We compute these functions with numerical and analytical methods and we find remarkable quantitative agreement along the three crystallographic directions for all the temperatures measured (from 400mK up to 8K !).

Supported by the DFG by through SFB 608.

TT 32.61 Thu 14:00 Poster B

Thermal conductivity of spin-1/2 chain compound $LiCu_2O_2$ — •Agnieszka Kondrat[1], Patrick Ribeiro[1], Nikolai Hlubek[1], Christian Hess[1], Bernd Büchner[1], and Sang-Wook Cheong[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]Rutgers Center for Emergent Materials & Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey, USA

We report on heat conductivity measurements of Heisenberg spin-1/2 chain compound $LiCu_2O_2$. κ(T) along the chains reveals a double-peak structure, where the minimum on the curve (T=24K) corresponds to a magnetic phase transition from paramagnetic to a spirally ordered state. Thermal conductivity is slightly dependent on magnetic field. A comparison is made to another spin-chain compound $SrCuO_2$, where excess thermal conductivity of magnetic origin was found along the chain direction.

TT 32.62 Thu 14:00 Poster B

Mott-Hubbard vs. charge-transfer type: optical conductivity of $LaSrMnO_4$ — •A. Gössling, M.W. Haverkort, M. Benomar,

H. Wu, D. Senff, T. Möller, M. Braden, J.A. Mydosh, and M. Grüninger — Institute of Physics II, University of Cologne, Germany

Using ellipsometry we study the optical conductivity of insulating $LaSrMnO_4$ between 0.75 and 5.8 eV from 15 to 330 K. The layered structure gives rise to a pronounced anisotropy. Based on a local multiplet calculation we obtain (i) an excellent description of our data, (ii) a detailed peak assignment in terms of the multiplet splitting of Mott-Hubbard and charge-transfer (CT) bands, and (iii) *effective* electronic parameters, e.g. the on-site Coulomb repulsion $U_{\rm eff}$=2.2 eV, the in-plane CT energy Δ_a=4.5 eV, and the crystal-field parameters ($10\,Dq$=1.2 eV, Δ_{eg}=1.4 eV, and Δ_{t2g}=0.2 eV). The spectral weight of the lowest peak (at 1-2 eV) changes by a factor of 2 as a function of temperature, which can be attributed to the change of the nearest-neighbor spin-spin correlation function. Interpreting $LaSrMnO_4$ effectively as a Mott-Hubbard insulator naturally explains this strong T dependence, the relative weight of the different peaks, and the pronounced anisotropy. From the transmittance we determine the onset of the optical gap $\Delta^a_{\rm opt}$ = 0.4-0.45 eV at 15 K and 0.1-0.2 eV at 300 K. Our data show that the crystal-field splitting is too large to explain the anomalous T dependence of the c-axis lattice parameter by thermal occupation of excited crystal-field levels. Alternatively, we propose that a thermal population of the upper Hubbard band gives rise to the shrinkage of the c-axis lattice parameter.

TT 32.63 Thu 14:00 Poster B

$1/f^\alpha$–noise studies of quasi–2D organic charge–transfer salts — •Jens Brandenburg[1], Jens Müller[1], and John Schlueter[2] — [1]Max–Planck–Institut for Chemical Physics of Solids, Dresden, Germany — [2]Argonne National Laboratory, Argonne, USA

Organic charge–transfer salts (κ–$(ET)_2X$; X=$Cu[N(CN)_2]Cl$, $Cu[N(CN)_2]Br$) exhibit various ground states whereas strong (el–el)- and (el–ph)-interactions as well as the quasi–2D Fermi–surface play an important role. Especially the anomalous normal state and the possibly unconventional superconducting phase evolving from an antiferromagnetic Mott–insulating state are in the focus of current investigations. For instance there is an ongoing controversy about the origin of the unusual normal state — characterised by the so called T^*–anomaly — in which a pseudogap behaviour, a crossover from a "bad metal" to a Fermi–liquid and a phase transition of density–wave type is discussed [1]. To understand the exceptional properties of the normal state in more detail, $1/f^\alpha$–noise was studied systematically since the intrinsic carrier dynamics is of particular interest. At different temperatures spectra have been measured and analysed with respect to changes of the frequency exponent α and the temperature progression of the normalised spectral weight S_R/R^2. The behaviour of these quantities is evaluated using a simple mathematical model which allows the extraction of excitation energies causing the excess noise in these materials. The implications of disorder on the ground state properties are discussed.

[1] N. Toyota, M. Lang, J. Müller; *Low Dimensional Molecular Metals*; Springer (Berlin Heidelberg), 2007

TT 32.64 Thu 14:00 Poster B

Magnetic Field Effects on a Quasi-2D Organic Compound Close to the Mott Transition — •Mariano de Souza[1], Andreas Bruehl[1], Christian Strack[1], Bernd Wolf[1], Dieter Schweitzer[2], and Michael Lang[2] — [1]Physikalisches Institut, J.W. Goethe-Universität, Max-von-Laue Str. 1, SFB/TRR49, D-60438 Frankfurt am Main, Germany — [2]3.Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany

Organic charge-transfer salts of the κ-phase$(BEDT\text{-}TTF)_2X$ family have been the subject of intensive research in the field of strongly correlated electron systems over the last few years. In this contribution, we present high-resolution directional dependent dilatometry studies under magnetic fields on the fully deuterated X=$Cu[N(CN)_2]Br$ salt, recognized to be situated close to the Mott metal-insulator (MI) transition [1]. Our findings reveal the insensitivity of the Mott MI transition temperature under fields up to 10 T, which is in accordance with the proposal of a Mott insulating state with a hole localized on a dimer. For fields along the interlayer b-axis, a field-induced (FI) phase transition at T_{FI}=9.5 K is observed. The latter is discussed in terms of a spin-flop transition with strong magneto-elastic coupling accompanied by a suppression of percolative superconductivity for magnetic fields above 1 T. [1] M. de Souza, A. Brühl, Ch. Strack, B. Wolf, D. Schweitzer, and M. Lang, Phys. Rev. Lett. **99**, 037003 (2007).

TT 32.65 Thu 14:00 Poster B

Two-channel conductivity in a layered organic metal characterized by a weakly incoherent interlayer transport regime. — •Mark V. Kartsovnik[1], Werner Biberacher[1], and Natalia D. Kushch[2] — [1]Walther–Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Institute for Problems of Chemical Physics, Russian Acadedmy of Sciences, Chernogolovka, Russia

We report on detailed studies of the interlayer MR of the layered organic metal alpha-(BEDT-TTF)2KHg(SCN)4 performed on several crystals characterized by different crystal quality. The angular dependence of MR is found to undergo a crossover from the conventional classical behaviour at low magnetic fields to the anomalous one at high fields. The crossover cannnot be explained by the field-induced confinement model proposed earlier for (TMTSF)2PF6 [1]. We propose an alternative phenomenological model based on parallel coherent and incoherent contributions to the interlayer conductivity. The model is able to explain not only the observed crossover but also anomalous features found in a number of other layered metals situated in the transient region between the fully coherent and incoherent transport regimes.

[1] D. G. Clarke and S. P. Strong, Adv. Phys. 46 (1997) 545.

TT 32.66 Thu 14:00 Poster B

Magnetic and superconducting properties of metal and oxide nanoclusters on biological templates — •C. Walter[1], M. Bartkowiak[1], O. Ignatchik[1], T. Herrmannsdörfer[1], J. Wosnitza[1], M. Merroun[2], K. Pollmann[2], J. Raff[2], and S. Selenska-Pobell[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf (FZD), D-01314 Dresden, Germany — [2]Institut für Radiochemie, FZD, Dresden, Germany

Nanogranular materials will play an important role in future technologies due to their exciting magnetic and superconducting properties that differ strongly from their bulk counterparts. In this study, we have focused on metal and oxide nanoclusters that have been deposited on a biological template, a self-assembling surface layer (S-layer) of *Bacillus sphaericus* JG-A12 which is composed of identical monomers. We present data of Pd, Pb, and Fe_3O_4 nanograins with sizes of 2, 19, and 13 nm respectively. The magnetization data obtained for the palladium clusters demonstrate that the Stoner enhancement factor of the d conduction-electron susceptibility is clearly reduced compared to the one of bulk Pd. For the Pb nanograins we have investigated the superconducting B-T phase diagram and encountered a superconducting critical field of the size of several Tesla which is strongly enhanced in comparison to the corresponding critical magnetic field of 0.09 T for bulk Pb. Last but not least we investigated the superparamagnetic properties of Fe_3O_4 nanograins and have found a magnetic anomaly at 30 K. Here, we present magnetization data taken by SQUID magnetometry as well as experimental results of dielectric measurements.

TT 32.67 Thu 14:00 Poster B

The ground state phase diagram of the Kondo-lattice model — •Sören Henning and Wolfgang Nolting — Humboldt Universität zu Berlin, Deutschland

We present the ground state (T=0) phase diagram of the 3D Kondo-lattice model. By using a moment conserving decoupling approach for the electronic self-energy we have calculated the inner energies of different phases explicitly. The phase diagram is then constructed by comparing the energies for the different phases. For low coupling J we find that depending on the band filling different anti-ferromagnetic configurations are favored. For larger J ferromagnetism is favored except for the half-filled band case. Furthermore, regions of phase-separation are determined by an explicit Maxwell construction.

TT 32.68 Thu 14:00 Poster B

Calculation of Magnetic Phases and Resistivity in an Extended Two-band Kondo Lattice Model — •Martin Stier and Wolfgang Nolting — Festkörpertheorie, Institut für Physik, Humboldt-Universität,12489 Berlin, Germany

We use an extended two-band Kondo lattice model (KLM) to investigate the occurrence of different (anti-)ferromagnetic phases depending on several model parameters. With regard to real CMR-materials like the manganites we have added a Jahn-Teller term, direct antiferromagnetic coupling and Coulomb interaction to the basic KLM. The use of an interpolating self-energy approach and a modified RKKY treatment allows us to calculate the model's electronic and magnetic properties self-consistently. Thereby we are not restricted to classi-

cal spins. We present zero-temperature phase diagrams which show a strong influence on the important parameters (Hund's coupling, direct antiferromagnetic exchange, Jahn-Teller distortion, different Coulomb interactions). Some of those calculations can be extended to finite temperatures. Our theoretical results are in good agreement with experimental measurements.

TT 32.69 Thu 14:00 Poster B

Effective Models for Undoped and Doped Spin Ladders from Self-Similar Continuous Unitary Transformations — •Sebastian Duffe and Götz Uhrig — Technische Universität Dortmund

Spin ladder systems, occuring e.g. in $Sr_{14}Cu_{24}O_{41}$ or $La_6Ca_8Cu_{24}O_{41}$, are important as model systems for 2D high-Tc superconductors. We are generating effective Hamiltonians for these systems systematically by using continuous unitary transformations (CUT). The CUT is performed self-similarly in real space for the coefficients of operator monomials in second quantization. The finite correlation length allows us to omit farther reaching processes.

The triplet excitations on the rungs with their dressing are our quasiparticles called "triplons". The CUT yields a block-diagonal Hamiltonian conserving the quasiparticle number. This effective Hamilton is used to calculate the dispersion for one triplon and the multi-triplon continua. The CUT has been improved decisively by using a new basis for the triplet states that takes advantage of the spin symmetry of the Hamiltonian. Furthermore, the generator is adapted such that it is possible to achieve convergence for much higher values of the coupling constant parallel to the ladder. In this way, the treatment of doping has become also possible.

TT 32.70 Thu 14:00 Poster B

Does There Exist a Baym-Kadanoff Construction for the Heisenberg Model? — •Stephan Filor and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen

A powerful tool for treating fermionic systems in a cluster approximation is the self-energy functional approach developed by Potthoff [1]. Our goal is to generalize this idea to the general (anisotropic) Spin-Heisenberg model.

To that end an analogue of a Baym-Kadanoff construction for the free energy as a functional of dynamical quantities such as green functions respectively self-energies is needed. Due to the structure of the spin operator algebra, which differs essentially from the usual one for fermions or bosons, this is not possible to achieve in a straightforward way.

To solve the problem we resort to the spin diagram technique proposed by Izyumov et. al. [2] which we use to develop a suitable variational approach to a Heisenberg lattice.

[1] M. Potthoff, Eur. Phys. J. B **32**, 429 (2003)
[2] Y.A. Izyumov, Y.N. Skryabin, Statistical Mechanics of Magnetically Ordered Systems, Plenum, New York (1988)

TT 32.71 Thu 14:00 Poster B

The phase diagram of the J_1-J_2-Heisenberg model using auxiliary fermions — •Johannes Reuther, Jan Brinckmann, and Peter Woelfle — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe

We consider the two-dimensional spin-1/2 J_1-J_2-Heisenberg model: In addition to the nearest neighbor coupling $J_1 > 0$ we introduce frustration by a next nearest neighbor coupling $J_2 > 0$. It is well known that for $J_2 = 0$, $J_1 \neq 0$ the model features a Néel-like ground state, while for very large J_2 the system shows antiferromagnetic order on both sublattices. This is called collinear order. In between, i.e., in the vicinity of the ratio $J_1/J_2 = 1/2$ a state without magnetic order is expected.

We use the auxiliary fermion-formulation of spin operators in conjunction with a method proposed by Popov and Fedotov. The latter enables us to take exactly into account the auxiliary-particle constraint (i.e. the projection onto the physical Hilbert space).

The ground state phase diagram of the model is calculated using a simple diagrammatic approximation for the fermion's self energy. We find a Néel state at small J_1 and a continuous transition into a non-magnetic state if J_1 is increased beyond a critical value. On the other hand for large J_2 we find the expected collinear state. The magnetic excitation spectrum and correlation length are studied in detail, in particular for the non-magnetic phase around $J_1/J_2 = 1/2$.

TT 32.72 Thu 14:00 Poster B

Raman Scattering from the $S = 1/2$ Heisenberg Antiferromagnet on the Triangular Lattice — Natalia Perkins[1,2] and •Wolfram Brenig[3] — [1]Physics Department, University of Wisconsin-Madison, Madison, WI 53706-1390, U.S.A. — [2]Bogoliubov Laboratory of Theoretical Physics, JINR, Dubna, Russia — [3]Institute for Theoretical Physics, Technical University of Braunschweig, 38106 Braunschweig

Magnetic Raman scattering provides for an effective tool to investigate the spectrum of singlet excitations at small momenta in quantum magnets. In this context the two-magnon Raman spectrum (2M-RS) has been studies extensively in two- and three-dimensional collinear antiferromagnets. Here we present results from a calculation of the 2M-RS of the two-dimensional triangular $S = 1/2$ antiferromagnet, which orders in a non-collinear 120°-structure. First, and using spin-wave theory to $O(1/S)$, we show that the bare 2M-RS has its maximum strongly shifted off from the upper bound of the two-magnon continuum. This is due to significant $1/S$-corrections of the one-magnon dispersion and is in sharp contrast to the 2M-RS of the square-lattice AFM. Second, we study the impact of 2M interactions on the 2M-RS by solving the corresponding Bethe-Salpeter equation numerically to leading order in $1/S$. Finally the dependence of the 2M-RS on the scattering geometry will be clarified.

TT 32.73 Thu 14:00 Poster B

Ground state phases of the spin-1/2 J_1–J_2 frustrated Heisenberg model on the square lattice: a coupled cluster study — •Rachid Darradi[1], Jörg Schulenburg[2], Sven Krüger[3], Ronald Zinke[1], and Johannes Richter[1] — [1]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg, 39016 Magdeburg, Germany — [2]Universitätsrechenzentrum, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany — [3]IESK, Kognitive Systeme, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany

We investigate the ground state phases of spin-1/2 frustrated Heisenberg antiferromagnet on the square lattice (J_1–J_2 model) using the coupled cluster method (CCM) in high orders of approximation. We have calculated the ground state energy, the sublattice magnetization, the spin stiffness and generalized susceptibilities. We determine the quantum critical points for both the semiclassical Néel and collinear phase as $J_2^{c1} \approx 0.43 J_1$ and $J_2^{c2} \approx 0.62 J_1$ respectively, which is in good agreement with the results obtained by other approximations. Based on susceptibilities which are related to valence-bond crystal order parameters we also discuss the nature of the quantum disordered phase separating the two semiclassical phases.

TT 32.74 Thu 14:00 Poster B

The influence of the inter-chain coupling on the spiral ground state of the frustrated quasi-one-dimensional spin-half Heisenberg magnet — •ronald zinke[1], stefan-ludwig drechsler[2], and johannes richter[1] — [1]Institut für theoretische Physik, Universität Magdeburg, PO Box 4120 — [2]Leibnitz-Institut für Festkörper- und Werkstoffforschung (IWF) D-01171 Dresden, P.O. Box 270116

Recent investigations on edge-shared chain cuprates such as $LiCuVO_4$, $NaCu_2O_2$ or Li_2ZrCuO_4 have identified these materials as quasi-one-dimensional frustrated quantum helimagnets with an incommensurate spiral ground state. While strictly one-dimensional frustrated quantum magnets have been widely studied theoretically, the role of the experimentally relevant inter-chain couling $J_\perp$ on the spiral ground state has not been discussed so far.

We perform coupled cluster method (CCM) calculations for coupled frustrated spin-$\frac{1}{2}$ J_1-J_2-chains. We consider different signs for the exchange interactions J_1 and $J_\perp$ this way realizing frustrated ferro- as well as antiferromgnets. We study the influence of quantum fluctuations and of the interchain coupling $J_\perp$ on the position of the transition from the commensurate collinear to the incommensurate spiral ground state and on the pitch angle θ. We find that not only the transition point but also the nature of the transition (first order/second order) depends on the strength of quantum fluctuations.

TT 32.75 Thu 14:00 Poster B

Optical spectroscopy on multiferroic $MnWO_4$ — •Thomas Möller[1], Joachim Hemberger[1], Markus Grüninger[1], Andrei Pimenov[2], Alexey Shuvaev[2], Petra Becker-Bohatý[3], and Ladislav Bohatý[3] — [1]2. Physikalisches Institut, Universität zu Köln — [2]Experimentelle Physik 4, Universität Würzburg — [3]Institut für Kristallographie, Universität zu Köln

$MnWO_4$ (Huebnerite) crystallizes in a monoclinic crystal structure composed of alternating layers of Mn^{2+} and W^{6+} ions which are octahedrally coordinated by oxygen ions. The partially frustrated spin system exhibits a negative Curie-Weiss temperature $T_{CW} \approx -75$ K in the paramagnetic regime and undergoes a sequence of transitions into complex antiferromagnetic phases below $T_N \approx 13.5$ K, including transitions from commensurate to incommensurate and collinear to non-collinear magnetic order, which are connected to the onset or decay of ferroelectric polarization [1]. Thus $MnWO_4$ belongs to the class of multiferroics. We present a detailed study of the phonon modes of this compound based on polarized reflectivity measurements in the FIR and MIR regime. In addition, polarized transmission measurements in the sub-mm regime below the phonon frequencies have been carried out in order to investigate the low-energy magnetoelectric excitations, so-called electro-magnons [2,3].

[1] A.H. Arkenbout et al., Phys. Rev. B **74**, 184431 (2006);
[2] A. Pimenov et al., Nature Phys. **2**, 97 (2006);
[3] D. Senff et al., Phys. Rev. Lett. **98**, 137206 (2007).

TT 32.76 Thu 14:00 Poster B

High-field Gd^{3+}–ESR on the spin-antiferromagnet $GdNi_2B_2C$ — •Uwe Schaufuss[1], Ferenc Murányi[1], Vladislav Kataev[1], Mathias Dörr[2], Martin Rotter[3], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research — [2]Institut für Festkörperphysik, Technische Universität Dresden — [3]Institute for Physical Chemistry, University of Vienna, Austria

The layered metalic compounds RNi_2B_2C (R = rare earth ions) attracted attention in the last years for its rich TH–phase diagrams. superconductivity and antiferromagnetic (afm) ordering with commensurate or incomensurate spin structure can be found in this material family. In order to obtain a deeper insight in the magnetic interactions in the spin-only antiferromagnet $GdNi_2B_2C$ we have performed Gd^{3+}–electron spin resonance study in a frequency range $10 - 350$ GHz on a single crystal of this material. The main crystalographic axes were successively set parallel to the magnetic field. We found that the Korringa relaxation rate was surprisingly anisotropic implying anisotropic interactions between the localized Gd^{3+}-spins and the conduction electrons. In the afm state we observed a large isotropic afm-gap of 76 GHz which is much larger than expected from the dipole-dipole interaction. This gap is field dependent and vanishes in strong fields. We will discuss possible reason for the unusual magnetic anisotropy in $GdNi_2B_2C$.

The work was supported by the DFG through SFB 463.

TT 32.77 Thu 14:00 Poster B

Heat capacity, thermal expansion and magnetic properties of the itinerant ferromagnet MnSi — •Qin Zhang[1], William Knafo[1,2], Frédéric Hardy[1,2], Kai Grube[1], Peter Schweiss[1], Hilbert v. Löhneysen[1,2], Christoph Meingast[1], and Thomas Wolf[1] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

MnSi, which is one of the most studied weak itinerant ferromagnetic systems, has recently attracted considerable attention due to its novel magnetic phase diagram under pressure and associated non-Fermi-liquid like resistivity [1,2]. Here, we present heat capacity, thermal expansion, magnetostriction and magnetization data on several different MnSi crystals, which were grown either from Mn, Si or Sn flux using the Bridgman method. Our results show that the details of the magnetic ordering transition depend strongly on whether the crystal is grown from Mn or Si enriched flux, although single-crystal x-ray refinements of these crystals show no difference of the Mn and Si site occupation within an error of $\pm 0.5\%$.

[1] C. Pfleiderer, D. Reznik, L. Pintschovius, H. v. Löhneysen, M. Garst, A. Rosch, Nature 427 (2004) 227
[2] C. Pfleiderer, S.R. Julian, G.G. Lonzarich, Nature 414 (2001) 427

TT 32.78 Thu 14:00 Poster B

Electronic Quasiparticles on the Spin-Wave Energy Scale in Ferromagnets — •Andreas Hofmann[1], Xiaoyu Cui[1], Jörg Schäfer[1], Eli Rotenberg[2], Luc Patthey[3], and Ralph Claessen[1] — [1]Universität Würzburg, D-97074 Würzburg — [2]Lawrence Berkeley Laboratory, Berkeley, CA 94720, USA — [3]Paul-Scherrer-Institut, CH-5232 Villigen

Angle-resolved photoemission (ARPES) is excellently suited to resolve energy renormalization of electronic quasiparticles dressed with an excitation. Beyond electron-phonon coupling, one must expect the fingerprint of magnetic excitations. Significant mass enhancement due to spin excitations has been identified for the first time in metallic surface states of Fe(110) [1]. The energy window exceeds that of phonons by far and is in striking coincidence with the spin wave spectrum. Bulk bands of magnetic materials are also subject to strong mass enhancement, as reflected e.g. in the Fermi velocity. In most recent experiments on Ni(110) using ARPES, the question has been addressed whether such electronic self-energy effects can be resolved in the spectral function. In taking ARPES data at symmetry planes of the Ni Fermi surface, structure is indeed observed in the real and imaginary parts of the self-energy. The energy scale of 200-300 meV coincides with characteristic spin wave energies. Moreover, the bulk bands show indication of two simultaneous kinks, on both the phonon and spin wave energy scale. The consequences of such experiments will be analyzed.

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

TT 32.79 Thu 14:00 Poster B

Magnetic ordering in striped nickelates — •Udo Schwingenschlögl[1], Cosima Schuster[1], and Raymond Frésard[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, 6 Bld. du Maréchal Juin, F-14050 Caen

Stripe phases are observed in a large variety of materials, including layered copper and nickel oxides. It is expected that the electronic properties of these doped Mott insulators can be described using suitably chosen Hubbard models, care being taken of the orbital degeneracy for the nickelates. However, the ground state of the microscopic models depends crucially on the choice of parameters. Hence, an estimate from ab initio calculations is desirable. We report on the electronic and magnetic structure of the striped nickelate $Sr_xLa_{2-x}NiO_4$ with x=1/3, where diagonal filled stripes are formed, using DFT (GGA) calculations. In contrast to experimental findings, the LDA+U approach results in A-type diagonal filled antiferromagnetic stripes, while in the pure GGA scheme C-type diagonal filled stripes are favored. A further determination of the structural parameters is therefore required.

TT 32.80 Thu 14:00 Poster B

Ferromagnetism in the multi-orbital periodic Anderson model — •Unjong Yu, Krzysztof Byczuk, and Dieter Vollhardt — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

At less than half-filling the localized f-electrons of the periodic Anderson model (PAM) can order ferromagnetically already at moderate values of the Coulomb repulsion U [1]. In the case of disorder in the f-level the corresponding critical temperature T_C always decreases [2,3]. By contrast, disorder in the conduction electrons can give rise to a surprisingly rich non-monotonic dependence of T_C [3]. Here we present results of the first investigation of the influence of *band-degeneracy* of the conduction- and/or f-electrons on the stability of the ferromagnetic phase of the PAM. In particular, a remarkable increase of T_C with the degeneracy in the localized levels is found. The origin of this increase and other features will be discussed.

[1] A. N. Tahvildar-Zadeh, M. Jarrell, and J. K. Freericks, Phys. Rev. B **55**, R3332 (1997).
[2] D. Meyer, Solid State Commun. **121**, 565 (2002).
[3] U. Yu, K. Byczuk, and D. Vollhardt, "Effect of Disorder on Ferromagnetism in the Periodic Anderson Model", in preparation.

TT 32.81 Thu 14:00 Poster B

Valence transition in the periodic Anderson model — •Alexander Mai, Nham Phan Van, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The origin of a possible quantum valence transition in the periodic Anderson model has been discussed controversially over the last years. Using an extension of the Projector-based Renormalization Method (PRM) to a continuous renormalization technique (CPRM) we try to merge the different points of view into one. We show that for fixed particle density the transition is smooth with a small slope in systems with small orbital degeneracy, whereas it becomes rather steep for large degeneracies. In contrast, for fixed chemical potential we find a rather abrupt change as function of the f-electron energy. The discussion is completed by an outlook on a possible superconducting phase in the PAM.

TT 32.82 Thu 14:00 Poster B

Valence transition in the periodic Anderson model in the

presence of a Coulomb repulsion between f- and conduction electrons — •Nham Phan Van, Alexander Mai, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The extended periodic Anderson model with a Coulomb repulsion U_{fc} between localized f and conduction electrons has been investigated by use of the Projector-based renormalization method (PRM). As function of the f-level energy ε_f a transition from an integer f-valence at low ε_f to a mixed valent behavior at higher ε_f is found. For fixed total electron number the transition becomes sharper if U_{fc} is increased. According to literature a sharp valence transition should be accompanied by the occurence of a superconducting phase.

TT 32.83 Thu 14:00 Poster B

Phase transition in the Hubbard-Holstein model with infinitely large Coulomb repulsion — •Andreas Eberlein, Steffen Sykora, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The one-dimensional Hubbard-Holstein model is studied in the limit of infinitely large on-site Coulomb repulsion. By using the projector-based renormalization method (PRM), the electron-phonon interaction ($\sim g$) is successively eliminated and an uncoupled system of renormalized correlated electrons and phonons is obtained. As a result, for the case of quarter filling a phase transition from a Luttinger liquid at small g to a charge-ordered state (CDW) at large g is expected.

TT 32.84 Thu 14:00 Poster B

Coexistence of superconductivity and charge-density waves in a two-dimensional Holstein model at half-filling — •Steffen Sykora, Arnd Hübsch, and Klaus W. Becker — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The competition of charge-density waves (CDW) and superconductivity (SC) is studied in a two-dimensional half-filled Holstein model by use of the projector-based renormalization method (PRM). As is well known, in one dimension the coupling of electrons to phonons leads to a transition from a metallic to a Peierls distorted insulated state when the coupling exceeds a critical value. On the other hand, in two dimensions the electron-phonon interaction may also be responsible for the formation of Cooper pairs. In this paper, the competing influence of superconductivity and charge order will be discussed for two dimensions. The PRM not only allows to study SC and CDW correlation functions but gives direct access to the order parameters.

TT 32.85 Thu 14:00 Poster B

Mapping of parent Hamiltonians: spin chains and the fractional quantum Hall effect — •Ronny Thomale and Martin Greiter — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D 76128 Karlsruhe

Motivated by the striking similarities of the Gutzwiller wave function for $S = 1/2$ spin chains and the Laughlin wave function for bosons at Landau level filling fraction $\nu = 1/2$, we establish a general mapping between the corresponding Hilbert spaces. We then employ this mapping to obtain a parent Hamiltonian for the spin systems starting from a parent Hamiltonian for the bosonic quantum Hall liquid.

TT 32.86 Thu 14:00 Poster B

Lifetime of spinless fermions on a square lattice — •Mehmet Kadiroglu and Jochen Gemmer — Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

We investigate the dynamics of spinless fermions on a square lattice which may hop to nearest neighbor sites, and also experience a hard-core repulsion at the nearest neighbor sites. We are especially interested in the dynamics of an excited state where one spinless fermion is put additionally into the system and occupies a momentum mode. We try to determine the lifetime of this excitation by perturbation theoretical methods, such as Green's functions techniques and/or Projection operator techniques.

TT 32.87 Thu 14:00 Poster B

Quantum Monte Carlo Study of SSH and breathing type Hamiltonians — •Hans Gerd Evertz and Peter Pippan — TU Graz, Austria

Using a QMC method based on the loop algorithm we study fermionic systems coupled to dynamical phonons in one dimension. Within this method it is possible to study SSH type models as well as Holstein type models with momentum dependent couplings (e.g. breathing phonons) and arbitrary phonon dispersions. We access the dynamical properties of the systems via the phonon spectral function and the one particle dynamical correlation function.

TT 32.88 Thu 14:00 Poster B

A Multi-Scale Many-Body Approach for Strongly Correlated Electrons — •Shuxiang Yang[1,2], Thomas Pruschke[1], and Mark Jarrell[2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Dept. of Physics, University of Cincinnati, Cincinnati, OH, USA

We present the parquet formalism which is based on the exact Feynman diagrammatical relationships of the vertex functions with different two-particle reducibilities. Within this formalism, five methods with different levels of approximation can be devised. One of them is the so-called Multi-Scale Many-body (MSMB) approach which separates the problem into short length scales treated explicitly with quantum Monte Carlo (QMC) methods, intermediate length scales treated diagrammatically using fully irreducible vertices obtained from QMC, and long length scales treated in the mean field. This approach will be used to develop a better understanding of materials such as lanthanides, actinides, and complex transition metal oxides where correlations over many length scales are central to the phase diagram, or to aid in material design to improve and search for new correlated materials.

TT 33: Symposium: High-Temperature Superconductivity

Time: Thursday 14:00–19:10 Location: H 0104

Invited Talk TT 33.1 Thu 14:00 H 0104

Transport Evidence for Quantum Criticality in Electron-doped Cuprates — •Richard Greene — University of Maryland, College Park, USA

Over the past few years, strong evidence for quantum critical behavior in electron-doped cuprates has been observed in transport [1], optical conductivity [2], ARPES [3], and neutron scattering [4] experiments. More recent work on $Pr_{2-x}Ce_xCuO_4$ films, using high-field resistivity and Hall Effect up to 60 T [6], low temperature thermopower [5] in the normal state, and in-plane angular magnetoresistance (AMR) [7], are consistent with the view that a quantum phase transition occurs under the superconducting dome near x =0.16 doping. These measurements can be interpreted with a spin-density-wave induced reconstruction of the Fermi surface, which leads to both electron and hole-like pockets. In this talk, I will review some of this work and compare it to recent high-field transport experiments in hole-doped cuprates, where evidence of electron-like Fermi surface pockets has been found [8].

1) Dagan et al. PRL 92, 167001 (2004) ;
2) Zimmers et al. Europhys. Lett. 70, 225 (2005);
3) Matsui et al., PRB 75, 224514 (2007) and references therein;
4) Motoyama et al., Nature 445, 912 (2007) and references therein;
5) Li et al. PRB 75, 020506R (2007) ;
6) Li et al. PRL 99, 047003 (2007) ;
7) W. Yu et al. PRB 76, 020503R (2007) ;
8) LeBoeuf et al. Nature 450, 533 (2007)

TT 33.2 Thu 14:30 H 0104

Signatures of non-monotonic d-wave gap in electron-doped cuprates — •Ilya Eremin[1,2], Evelina Tsoncheva[3], and Andrey Chubukov[3] — [1]Max-Planck Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Institute für Mathematische und Theoretische Physik, TU-Braunschweig, D-38106 Braunschweig, Germany — [3]Department of Physics, University of Wisconsin, Madison, WI 53706, USA

We address the issue whether the data on optical conductivity and Raman scattering in electron-doped cuprates below T_c support the idea that the $d-$wave gap in these materials is non-monotonic along the Fermi surface. We calculate the conductivity and Raman intensity

for elastic scattering, and find that a non-monotonic gap gives rise to several specific features in optical and Raman response functions. We argue that all these features are present in the experimental data on $Nd_{2-x}Ce_xCuO_4$ and $Pr_{2-x}Ce_xCuO_4$ compounds.

Invited Talk TT 33.3 Thu 14:45 H 0104

Superconductivity in the Hubbard model and the two gap energy scales in high-temperature superconductors — •Markus Aichhorn[1], Enrico Arrigoni[2], Michael Potthoff[3], Zhong Bing Huang[4], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Institut für Theoretische Physik und Computational Physics, Technische Universität Graz — [3]I. Institut für Theoretische Physik, Universität Hamburg — [4]Department of Physics, Hubei University, Wuhan, China

Quite after the discovery of high-temperature superconductivity in the cuprate compounds, it has been proposed that the essential physics of these materials is captured by the Hubbard model. Although this model is conceptually very simple, an exact solution is not known for more than one spatial dimension. Thus, approximate or numerical evaluations are needed for these quasi 2D materials. Our understanding of the ground-state properties of the 2D Hubbard model has improved a lot due to the development of the dynamical mean-field theory and its cluster extension. We will discuss recent results obtained by the variational cluster approach (VCA), focusing on the symmetry-broken phases at zero temperature. Besides the discussion of the competition between antiferromagnetism and d-wave superconductivity at low hole doping, we will focus on the doping evolution of the superconducting gap. We show that the Hubbard model is indeed able to describe the experimentally found two energy scales in the underdoped cuprates, and give a possible explanation of this feature in terms of a spin-fluctuation-mediated pairing mechanism.

15 min. break

TT 33.4 Thu 15:30 H 0104

Momentum-resolved electron-phonon coupling and self-energy effects in $YBa_2Cu_3O_7$: an LDA study — •Rolf Heid[1], Klaus-Peter Bohnen[1], Roland Zeyher[2], and Dirk Manske[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

The observation of kinks in the electronic dispersion of high-T_c cuprates by angle resolved photoemission experiments has revived the discussion about the importance of electron-phonon interaction in the cuprates. Here we determine the effect of the electron-phonon coupling on the electronic self-energy in the normal state within the local-density approximation. Using a realistic phonon spectrum we determine the momentum and frequency dependence of $\alpha^2F(\mathbf{k},\omega)$ in $YBa_2Cu_3O_7$ for the bonding, antibonding, and chain band. We find that the maximum in the real part of the self-energy at low frequencies is about a factor 5 too small compared to the experiment. The renormalization factor $Z(\mathbf{k},\omega)$, which determines the change in the slope of the electronic dispersion due to the interaction, varies smoothly as a function of frequency and momentum. These findings show that, at least within the LDA, phonons cannot produce well-pronounced kinks in $YBa_2Cu_3O_7$.

TT 33.5 Thu 15:55 H 0104

The phonon buckling mode in $YBa_2Cu_3O_{6+x}$ measured by inelastic neutron scattering — •Markus Raichle[1], Dmitry Reznik[2], Mohammed Bakr[1], Vladimir Hinkov[1], Klaudia Hradil[3], Daniel Lamago[2], Clemens Ulrich[1], Markus Bröll[1], Philippe Bourges[2], Yvan Sidis[2], Chengtian Lin[1], and Bernhard Keimer[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Laboratoire Léon Brillouin, Paris, France — [3]Universität Göttingen, Göttingen, Germany

Cuk et al. [Phys. Rev. Lett. 93, 117003 (2004)] and Devereaux et al. [Phys. Rev. Lett. 93, 117004 (2004)] relate the antinoidal kink in ARPES measurements with the B1g phonon buckling mode. However, this assumption is controversial as this kink has also been related to the magnetic resonance mode by Kaminski et al. [Phys. Rev. Lett. 86, 1070 (2001)] and Kim et al. [Phys. Rev. Lett. 91, 167002 (2003)]. Until now inelastic neutron scattering measurements on this phonon mode on $YBa_2Cu_3O_{6+x}$ by Reznik et al. [Phys. Rev. Lett. 75, 2396 (1995)] has only been done on twinned samples for x=1. Here we present high resolution neutron measurements on the buckling mode on YBCO for x=0.6 and x=1.0. These measurements performed at Puma and 1T1 at Saclay have been made on fully detwinned samples. Thus we could show that this phonon mode performes an anisotropic superconductivity-induced interaction with a neighboring phonon mode. Hence these measurements enrich the experimental evidence for superconductivity induced phonon effects in high temperature superconductors.

TT 33.6 Thu 16:10 H 0104

d-wave stripes in cuprates: Valence bond order coexisting with nodal quasiparticles — •Matthias Vojta — Institut für Theoretische Physik, Universität Köln, 50937 Köln, Germany

We point out that unidirectional bond-centered charge-density-wave states in cuprates involve electronic order in both s- and d-wave channels, with non-local Coulomb repulsion suppressing the s-wave component. The resulting bond-charge-density wave, coexisting with superconductivity, is compatible with momentum-space features seen in recent photoemission and tunneling data and as well as in neutron-scattering measurements, once long-range order is destroyed by slow fluctuations or glassy disorder.

TT 33.7 Thu 16:35 H 0104

Charge order in $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ studied by resonant soft X-ray diffraction — •J. Fink[1,2], E. Weschke[3], E. Schierle[3], J. Geck[4], H. Hawthorn[4], H. Widati[4], H.-H. Hu[5], H. Dürr[1], B. Büchner[2], and G. A. Sawatzky[4] — [1]BESSY, Albert-Einstein-Strasse 15, 12489 Berlin — [2]IFW Dresden — [3]Hahn-Meitner-Institut Berlin — [4]UBC Vancouver, Canada — [5]II. Physikalisches Institut, Universität Köln

Stripe-like phases in hole-doped cuprates, in which antiferromagnetic domains are separated by periodically spaced domain walls to which the charge carriers are segregated, are caused by a complex interplay between lattice defects and charge and spin degrees of freedom. In $La_{1.8-x}Eu_{0.2}Sr_xCuO_4$ a stripe-like phase replaces almost the entire superconducting phase because in this system stripes are stabilized by the existence of a low-temperature tetragonal phase in a large concentration range. In order to directly prove the existence of charge ordering in these compounds we have used resonant soft X-ray scattering at the O1s and Cu2p edges. Long-range charge order exists at low temperatures and x close to 1/8. At higher temperatures and for x = 0.15 the coherence length is reduced due to fluctuations and/or a reduced order.

TT 33.8 Thu 16:50 H 0104

q-dependence of the giant bond-stretching phonon anomaly in the stripe compound $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ measured by IXS — •Daniel Lamago[1,2], Dmitry Reznik[2], T. Fukuda[3], K. Yamada[4], and A.Q.R. Baron[4] — [1]CEA Saclay, 91191 Gif Sur Yvette, France — [2]Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [3]Synchrotron Radiation Research Unit, Japan Atomic Energy Agency (Spring 8), Sayo, Hyogo 679-5148, Japan — [4]Materials Dynamics Laboratory, Harima RIKEN, 1-1-1 Kouto, Sayo, Hyogo, 679-5148 Japan

Inelastic x-ray scattering (IXS) was used to study the Cu-O bond-stretching vibrations in the static stripe phase compound $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$. It was found that the intrinsic width in Q-space of the previously reported huge anomalous phonon softening and broadening is approximately 0.08 r.l.u. HWHM. A detailed comparison was also made to inelastic neutron scattering (INS) studies, which reported a two-peak lineshape with a "normal" and an "anomalous" phonon peaks. The "normal" branch in the neutron data seems to be mostly suppressed in the high resolution IXS data. Otherwise the agreement between the INS and the IXS was excellent.

TT 33.9 Thu 17:05 H 0104

Charge ordering phenomena and superconductivity in cuprates — •Leonardo Tassini, Bernhard Muschler, Wolfgang Prestel, Rudi Hackl, Michael Lambacher, and Andreas Erb — Walther-Meissner-Institut, 85748 Garching, Germany

The relationship between charge ordering phenomena and superconductivity was investigated with electronic Raman scattering in $La_{2-x}Sr_xCuO_4$ (LSCO) and $Y_{1-y}Ca_yBa_2Cu_3O_{6+x}$ (Y-123) single crystals. New low-energy excitations were found that are interpreted in terms of dynamical stripes. Below the onset point of superconductivity p_{sc1} the stripes are oriented along the diagonal of the CuO_2 planes for both LSCO and Y-123. The Raman data indicate that diagonal stripes compete with superconductivity. Apparently, stripes along the

Cu − O direction lead to a relatively low-T_c such as in LSCO, while two-dimensional ordering such as observed by neutron scattering in Y-123 leads to high-T_c of the order of 100 K.

The project has been supported by the DFG under grant number Ha2071/3-1 via the Research Unit FOR 538.

15 min. break

TT 33.10 Thu 17:45 H 0104

Electronic liquid crystal state in a strongly underdoped high-temperature superconductor — •V. Hinkov[1], D. Haug[1], B. Fauque[2], Y. Sidis[2], P. Bourges[2], A. Ivanov[3], C. Bernhard[4], CT. Lin[1], and B. Keimer[1] — [1]MPI-FKF, Stuttgart — [2]LLB, Saclay, France — [3]ILL, Grenoble, France — [4]Univ. of Fribourg, Switzerland

Liquid crystals are states of matter without static crystalline order that break the rotational symmetry of free space while at least partially preserving its translational symmetry. Highly correlated electronic phases with symmetry properties analogous to those of conventional liquid crystals have been theoretically predicted (Kivelson et al., Nature 393, 550) and recently discovered in the layered bulk transition metal oxide $Sr_3Ru_2O_7$ (Borzi et al., Science 315, 214). In both cases, however, these phases are stable only at milli-Kelvin temperatures and in high magnetic fields, and have thus far only been probed by transport measurements. After briefly summarizing our work on $YBCO_{6.6}$ (Hinkov et al., Nature Physics 3, 780), we report the spontaneous onset of a strong one-dimensional, incommensurate modulation of the spin system in the underdoped high-temperature superconductor $YBa_2Cu_3O_{6.45}$ upon cooling below 150 K, while muon-spin-relaxation experiments on the same sample demonstrate that static magnetic order is absent down to temperatures of at least 2 K. The symmetry properties of the spin system thus match those of a nematic liquid crystal over a wide temperature range. Soft spin fluctuations are thus a microscopic route towards the formation of electronic nematic phases, which can coexist with high-T_c superconductivity.

TT 33.11 Thu 18:10 H 0104

ARPES of Bi-cuprates: Did we mix up apples and oranges? — •Lenart Dudy, Olaf Lübben, Beate Müller, Alica Krapf, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr.15, D-12489 Berlin, Germany

In the two decades of research on the pairing mechanism of the hole-doped high temperature superconductors, angular resolved photoemission (ARPES) has shown to be a good tool to study its microscopic origin [1]. But although two dimensional patterns in scanning tunneling microscopy(STM) have been discovered for a long time [2], the impact of these modulations on the photoemission signal is still widely ignored. Therefore we argue that features extracted out of photoemission experiments like the self energy and its temperature dependence have to be handled more critically. This will be demonstrated in context to an experimental motivated simple model [3], where the photoemission signal is decisively influenced by the modulations found by STM.

[1] A. Damascelli et al., Rev. Mod. Phys. 75, 473 (2003) and reference therein; M.R. Norman and C. Pepin, Rep. Prog. Phys. 66, 1547 (2003) and reference therein

[2] Ø. Fischer et al., Rev. Mod. Phys. 79, 353 (2007) and reference therein

[3] L. Dudy et al., Solid State Comm. 143, 422 (2007)

TT 33.12 Thu 18:25 H 0104

Effects of out-of-plane disorder on the superconductivity of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ — •Jürgen Röhler[1], Christoph Trabant[1], Johanna Frielingsdorf[1], Rabia Djemour[1], Victor Martovitsky[2], Lenart Dudy[3], Helmut Dwelk[3], and Alica Krapf[3] — [1]Universität zu Köln, 50937 Köln — [2]Lebedev-Institute, 119991 Moscow — [3]Humboldt Universität zu Berlin, 12489 Berlin

The effects of out-of-plane substitutional order/disorder on cuprate superconductivity remains to a large extent an unresolved issue. We have investigated the connection between superconductivity and the lattice effects arising from the heterovalent doping of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$, $x = 0.8 - 0.1$. Decreasing lanthanum content tunes the compound through the entire underdoped and overdoped regimes. Cu-K and La-K EXAFS served as local structural probes, and single crystal x-ray diffraction for the determination of the basic unit cell, and the symmetry of the supercell. The oxygen atoms in the CuO_2 planes were found significantly disordered, dependent on doping, and to exhibit minimum disorder around $x_{opt} = 0.33$. But the degree of substitutional disorder in the out-of-plane La environment turned out independent on the concentration of the La dopants, the superstructure symmetry, and the crystal growth parameters, whereas T_c depends sensitively on them. No evidence was found for possible concentration dependent site changes of the La dopant from the nominal Sr to the Bi sites. We discuss the probably crucial role of the interstitial oxygen atoms for the superconducting properties of the $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ system.

Supported by the ESRF through projects HE2473 and HE2644.

TT 33.13 Thu 18:40 H 0104

Indications on fluctuation origin of the recently observed giant Nernst effect in superconductors above T_c — •A.A. Varlamov — COHERENTIA-INFM, CNR, Rome, Italy

There are two types of fluctuation corrections: the first, like conductivity, have to be compared with the corresponding value of the normal state, the second, like fluctuation magnetization, reflect appearance of principally new quality and have to be compare with the anomalous diamagnetism of superconducting phase. I will show that the Nernst signal belongs to the effects of the second type. Both GL phenomenology and microscopic analysis indicate that Nernst effect, negligible in normal metal manifests itself by giant fluctuations along the line $T_c(H)$.

TT 34: Correlated Electrons: Metal-Insulator Transition 2

Time: Thursday 14:00–19:00 Location: H 2053

TT 34.1 Thu 14:00 H 2053

Phase transitions and orbital fluctuations in $3d^2$ vanadates — •Eva Pavarini[1], Molly De Raychaudhury[2], and Ole K. Andersen[3] — [1]Institut für Festkörperforschung, Forschungzentrum Jülich, Jülich, Germany — [2]S.N. Bose National Centre for Basic Sciences, Kolkata, India — [3]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany

We investigate [1] the importance of quantum orbital fluctuations in the orthorhombic and monoclinic phases of the Mott insulators $LaVO_3$ and YVO_3. First, we construct *ab-initio* material-specific t_{2g} Hubbard models. Then, by using dynamical mean-field theory, we calculate the spectral matrix as a function of temperature. Our Hubbard bands and Mott gaps are in very good agreement with spectroscopy. We show that in orthorhombic $LaVO_3$, quantum orbital fluctuations are strong and that they are suppressed *only* in the monoclinic 140 K phase. In YVO_3 the suppression happens already at 300 K. We show that Jahn-Teller *and* $GdFeO_3$-type distortions are both crucial in determining the type of orbital and magnetic order in the low temperature phases.

[1] M. De Raychahudhury, E. Pavarini, O.K. Andersen, Phys. Rev. Lett. **99**, 126402 (2007).

TT 34.2 Thu 14:15 H 2053

Magnetic Moment Collapse-Driven Mott Transition in MnO — •Jan Kunes[1], Alexey V. Lukoyanov[2], Vladimir I. Anisimov[3], Richard T. Scalettar[4], and Warren E. Pickett[4] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86135 — [2]Ural State Technical University-UPI, 620002 Yekaterinburg, Russia — [3]Insitute of Metal Physics, Russian Academy of Sciences, 620041 Yekaterinburg, Russia — [4]Department of Physics, University of California, Davis 95616, U.S.A.

We employ a combination of numerical density-functional bandstructure and dynamical mean-field theory to study the evolution of electronic properties of MnO under pressure. Motivated by recent high-pressure experiments we investigate the relationship between high-spin to low-spin transition (moment collapse), insulator-to-metal (Mott) transition and isostructural volume collapse. Our results, which closely resemble the experimental observations, demonstrate that the moment collapse and Mott transition happen simultaneously and that the

crystal-field splitting, not the band broadening, is the driving force behind the transition. The Mott transition turns out to be essentially a consequence of local atomic states, high-spin or low-spin, placing different constraints on the electron propagation resulting in insulating or metallic ground states respectively. Energy vs volume curve shows that the specific volume changes discontinuously at the transition. The study represents a significant progress over previous theories which did not provide a reliable picture of the Mott transition.

TT 34.3 Thu 14:30 H 2053

Birth and Death of Quasiparticles in the Mott-Hubbard Prototype V_2O_3 — Leonetta Baldassarre[1], Andrea Perucchi[1,2], Daniele Nicoletti[1], Alessandro Toschi[3], •Giorgio Sangiovanni[3], Karsten Held[3], Massimo Capone[4], and Stefano Lupi[1] — [1]CNR-INFM COHERENTIA and Dipartimento di Fisica, Università di Roma "La Sapienza" — [2]Sincrotrone Trieste S.C.p.A., in Area Science Park, Trieste — [3]Max-Planck Institut für Festkörperforschung, Stuttgart — [4]SMC, CNR-INFM and Dipartimento di Fisica, Università di Roma "La Sapienza" and ISC-CNR, Roma

The infrared conductivity of V_2O_3 is measured in the whole phase diagram to study the behavior of quasiparticles which appear above the Néel temperature T_N, and eventually disappear further enhancing the temperature. We present theoretical calculations demonstrating that this loss of coherence in the vicinity of the Mott transition is enhanced by small changes of the lattice parameters. This leads to a downturn in the optical conductivity at small frequencies, as our experimental data show above 450 K.

TT 34.4 Thu 14:45 H 2053

Interplay of electron-electron and electron-phonon interaction in the metal to insulator transition in vanadium oxides. — •Leonetta Baldassarre[1,2], Emanuele Arcangeletti[1], Andrea Perucchi[1], Daniele Nicoletti[1], Daniele Di Castro[1], Carlo Marini[1], Paolo Postorino[1], and Stefano Lupi[1] — [1]CNR-INFM COHERENTIA and Department of Physics, University of Rome "La Sapienza" , Rome, Italy — [2]Experimentalphysik II, Universität Augsburg, D-86135 Augsburg, Germany

Several families of vanadium oxides display metal to insulator transitions (MIT) often driven by both temperature (T) and pressure (P) with jumps of conductivity up to 7 orders of magnitude. While the transition in V_2O_3 is considered as induced mainly by electronic correlation (Mott-Hubbard transition), the MIT mechanism that drives the electronic transition in VO_2 is still unclear, probably determined by an interplay between electronic and lattice degrees of freedom.

Here we present a complete investigation of MIT as a function of T and P of V_2O_3 and VO_2. Infrared measurements have been performed in a wide range of T (10-600 K) and P (0-15 GPa) in order to cover the rich phase diagrams of those materials. P-dependent Raman measurements have also been performed on VO_2 so to follow also the lattice dynamics. Moreover, the high temperature incoherent phase is discussed in V_2O_3, the ideal playground to study the correlation effects on the low-energy electrodynamics.

TT 34.5 Thu 15:00 H 2053

Pressure-induced phase transitions in the oxyhalides TiOX — •Christine Kuntscher[1], Simone Frank[1], Alexej Pashkin[1], Helge Hoffmann[1], Matthias Klemm[1], Siegfried Horn[1], Andreas Schönleber[2], Sander van Smaalen[2], Sebastian Glawion[3], Michael Sing[3], and Ralph Claessen[3] — [1]Experimentalphysik 2, Universität Augsburg, D-86135 Augsburg, Germany — [2]Laboratory of Crystallography, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (X=Cl,Br) are spin-Peierls compounds with exotic properties. With the electronic configuration $3d^1$ they are Mott-Hubbard insulators with a charge gap of ≈2 eV. They were discussed to exhibit a resonating valence bond state and high-temperature superconductivity upon doping. However, up to now a metallization upon doping was not successful. Our recent pressure-dependent infrared spectroscopic investigations on TiOCl suggest that the application of external pressure is an alternative way to induce an insulator-to-metal transition in TiOX [1]. We have extended our spectroscopic investigations on TiOX to the far-infrared range, in order to verify the pressure-induced metallization. X-ray powder diffraction measurements under pressure show that the insulator-to-metal transition coincides with a structural phase transition.

We acknowledge the ANKA Angströmquelle Karlsruhe and the ESRF for the provision of beamtime and the DFG for financial support.

[1] C. A. Kuntscher et al., Phys. Rev. B **74**, 184402 (2006).

TT 34.6 Thu 15:15 H 2053

Spectral weight transfer upon doping in the low-dimensional Mott-Hubbard systems TiOCl and TiOBr — •Sebastian Glawion, Karin Goss, Markus Scholz, Michael Sing, and Ralph Claessen — Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg

Transition metal oxyhalides have seen increasing interest in the past few years due to their non-canonical phase transitions into incommensurate and commensurate spin-Peierls phases and their potential as prototypical $3d^1$ Mott insulators. For pristine TiOCl and TiOBr, a transition into a metallic phase under pressure has been reported which, however, seems to be structurally driven. Using XPS and ARPES we investigated the possibility of band-filling controlled metal-insulator transitions using n- and p-type doping. The layered crystal structure allows for easy intercalation of different dopant species into the van-der-Waals gaps between the Cl-separated Ti-O double layers. Indeed, XPS shows that the Ti valency is reduced through charge transfer from the dopant. While the new spectral weight in the charge gap, as observed by ARPES, nicely follows the expected behaviour for the correlated bands of a Mott insulator, no quasiparticle peak can be found at the chemical potential. The seeming abscence of a metallic QP can be reconciled in a picture where its coherent weight is transferred to higher binding energies due to coupling to polaronic or other degrees of freedom.

15 min. break

TT 34.7 Thu 15:45 H 2053

Spectral weight distribution of d^1 Mott insulators $LaTiO_3$ and $YTiO_3$ — H. Roth[1], •T.C. Koethe[1], Hua Wu[1], Z. Hu[1], A. Hendricks[1], J. Gegner[1], M.W. Haverkort[1], T. Lorenz[1], J.C. Cezar[2], N.B. Brookes[2], I.S. Elfimov[3], G.A. Sawatzky[3], and L.H. Tjeng[1] — [1]II.Physikalisches Institut Universität zu Köln — [2]European Synchrotron Radiation Facility (ESRF), BP 220, 38043 Grenoble Cedex, France — [3]Department of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, British Columbia, Canada, V6T 1Z1

We have utilized bulk-sensitive photoelectron spectroscopy to study the valence band spectral weight distribution of d^1 Mott insulators $LaTiO_3$ and $YTiO_3$. We observed appreciable differences in the spectra, reflecting the difference in the one-electron band width. We also found that the Ti $3d$ spectra of both materials are much broader than the occupied $3d$ bands calculated by band theories. The mean-field inclusion of the Hubbard U explains the band gap but produces even narrower bands, indicating the complete breakdown of standard mean-field theories in describing excitation spectra. We associate the observed spectra with the propagation of a hole in a system with surprisingly well suppressed charge fluctuations thereby showing characteristics of a t-J model.

TT 34.8 Thu 16:00 H 2053

Charge ordering in perovskite rare-earth titanate compounds — •A. C. Komarek[1], M. Reuther[1], N. Hollmann[1], A. Cousson[2], F. Bouree[2], M. Hölzel[3,4], A. Senyshyn[3,4], P. Link[3], D. Trots[5,4], C. Baehts[5,4], T. Lorenz[1], and M. Braden[1] — [1]Institute of Physics II, University of Cologne, Cologne — [2]LLB, CEA/CNRS, Saclay — [3]TU Munich, FRM-II, Garching — [4]Institute for Materials Science, TU Darmstadt, Darmstadt — [5]Hasylab/DESY, Hamburg

Having a single electron in the 3d shell, the rare-earth (RE) titanates $RETiO_3$ have attracted strong interest to study the complex interplay of charge, orbital and magnetic degrees of freedom. Substituting divalent earth-alkali for the RE, a metal-insulator transition is induced, which in case of $Y_{1-x}Ca_xTiO_3$ occurs only at rather high doping. We have studied the hole-doped system $(Y,Er,Lu)_{1-x}Ca_xTiO_3$ by various diffraction techniques, by resistivity and by magnetic susceptibility measurements. This system shows a complex phase diagram of structural distortions accompanied by a metal-insulator transition. We ascribe the complex behavior to the coexistence of an insulating monoclinic phase with a metallic low-temperature orthorhombic phase. Our neutron diffraction data show that charge ordering occurs in the monoclinic phase. Even away from half-doping, we find two distinct Ti sites in a checkerboard arrangement, with significantly different TiO_6

coordination.

TT 34.9 Thu 16:15 H 2053

Dynamic scaling at MIT in yttrium hydride switchable mirrors — •A. V. Pronin[1], I. G. Romijn[2], H. B. Brom[2], A. F. Th. Hoekstra[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZD, 01314 Dresden, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

Yttrium hydride demonstrates a remarkable transition of its electronic and optical properties upon change of hydrogen concentration: a thin YH_x film can be continuously and reversibly brought from a shiny metal at $x = 2$ to a transparent dielectric at $x = 3$, by changing pressure of the surrounding hydrogen gas [1]. It has been showed that the metal-insulator transition (MIT) could be neatly passed under constant hydrogen pressure by changing the carrier doping via ultraviolet illumination at low temperatures [2]. Pronounced electron-electron interactions are posited to lead to the opening of a large optical gap. The established scaling laws of the conductivity with temperature and doping [2] are strong indications for the quantum nature of the metal-insulator transition in YH_x. To shed more light on the quantum nature of the MIT, the frequency dependence of conductivity is very informative. In an extensive frequency range, frequency ω and temperature T will influence the conductivity in a similar way, which will lead to a so-called ω/T-scaling behaviour. In this talk results on the optical conductivity in the sub-terahertz regime will be presented.

[1] J. N. Huiberts, *et al.*, Nature (London) **380**, 231 (1996).
[2] A. F. Th. Hoekstra, *et al.*, Phys. Rev. Lett. **86**, 5349 (2001).

TT 34.10 Thu 16:30 H 2053

Bulk electronic structure of the layered cobaltate $La_{2-x}Sr_xCoO_4$ — •A. Hendricks, T.C. Koethe, Z. Hu, N. Hollmann, M. Benomar, M. Cwik, T. Lorenz, and L.H. Tjeng — II. Physikalisches Institut Universität zuKöln

The electronic and magnetic properties of the perovskite system $La_{1-x}Sr_xCoO_3$ has been investigated for many decades now and still is subject of active research. In the undoped compound $LaCoO_3$, the correlated nature of the cobalt 3+ ions leads to a temperature driven spin state transition from a $S = 0$ low spin (LS) ground state to a higher spin state, the nature of which has been discussed controversially as either $S = 1$ intermediate or $S = 2$ high spin (HS) state. Upon introducing Co^{2+} by doping with Sr, a metal insulator transition and long range ferromagnetic ordering have been observed. Very recently, the related system $La_{2-x}Sr_xCoO_4$ has been synthesized in order to investigate properties of Co 2+/3+ ions in a environment, which leads in the case of cuprates and nickelates to interesting charge and spin ordering phenomena. While the magnetism of the cobaltates appears to be dominated by Co^{2+} ions in HS, exhibiting short range magnetic order at low temperatures, the spin state of the Co^{3+} is still under debate. Using bulk sensitive soft-x-ray photoelectron spectroscopy, we investigated the valence band electronic structure of $La_{2-x}Sr_xCoO_4$, $0.3 \leq x \leq 0.8$, and its temperature dependence. Our results demonstrate a strong Co^{3+} LS contribution.

TT 34.11 Thu 16:45 H 2053

The spin state issue in the RBaCo$_2$O$_{5.5}$ cobaltates — •Hua Wu, Zhiwei Hu, Tobias Burnus, Daniel Khomskii, and Liu Hao Tjeng — II. Physikalisches Institut, Universität zu Köln

The double perovskites RBaCo$_2$O$_{5+\delta}$ (R=rare earth, $0 \leq \delta \leq 1$) display intriguing phenomena such as charge and orbital ordering, as well as antiferromagnetic to ferromagnetic transition, depending on the oxygen concentration. In particular, the δ=0.5 system shows a giant magnetoresistance effect, and its metal-insulator transition has been often interpreted in terms of a spin-state transition [1,2], which, however, is fiercely debated [3,4]. To address the spin-state issue, we performed density-functional theory calculations which include a mean-field correction for the correlation effects caused by the Co 3d electrons. We have investigated various scenarios with different combinations of the low-, intermediate- and high-spin (LS, IS, and HS) states. Our results show that the pyramidally coordinated Co^{3+} ions are exclusively in the HS state since [3], in disagreement with [1,2]. The octahedrally coordinated Co^{3+} can be stabilized into a LS-HS ordered state if we take into account the superstructure recently reported [4]. Our results put limits as to how much spin-state transition could accompany the metal-insulator transition.

[1] C. Frontera *et al.*, Phys. Rev. B **65**, 180405(R) (2002).
[2] A. A. Taskin *et al.*, Phys. Rev. Lett. **90**, 227201 (2003).
[3] Z. Hu *et al.*, Phys. Rev. Lett. **92**, 207402 (2004).
[4] D. D. Khalyavin *et al.*, Phys. Rev. B **75**, 134407 (2007).

TT 34.12 Thu 17:00 H 2053

X-ray absorption and x-ray magnetic dichroism study on Ca_3CoRhO_6 and Ca_3FeRhO_6 — •Tobias Burnus[1], Zhiwei Hu[1], Júlio C. Cezar[2], Seiji Niitaka[3], Hua Wu[1], Hidenori Takagi[3,4], Chun Fu Chang[1], Nicholas B. Brookes[2], Ling-Yun Jang[5], Keng S. Liang[5], and L. Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]RIKEN and CREST, Saitama, Japan — [4]University of Tokyo, Japan — [5]National Synchrotron Research Center, Hsinchu, Taiwan

The valence-state of the transition-metal ions in the chain-like compounds Ca_3CoRhO_6 and Ca_3FeRhO_6 is currently an issue under debate. Using numerical simulations and x-ray absorption spectroscopy at the Rh-$L_{2,3}$, the Co-$L_{2,3}$, and the Fe-$L_{2,3}$ edges we reveal a Co^{2+}/Rh^{4+} configuration in Ca_3CoRhO_6 and Fe^{3+}/Rh^{3+} in Ca_3FeRhO_6. X-ray magnetic circular dichroism at the Co-$L_{2,3}$ edge shows that the Co^{2+} ions carry a giant orbital moment of about $1.7\mu_B$. We attribute this to a $d_0^1 d_2^1$ ground state for the high-spin Co $3d^7$ configuration in trigonal prismatic coordination. The intrachain-ferromagnetic coupling of two neighboring Co ions is mediated by a low-spin Rh^{4+} ion ($S = 1/2$) in between.

15 min. break

TT 34.13 Thu 17:30 H 2053

Crystal Structure of layered manganites — •Olaf Schumann[1], Stephen Price[1], Hua Wu[1], Theresa Fernandez-Diaz[2], Pascal Reutler[3], Alexandre Revcolevschi[3], and Markus Braden[1] — [1]II. Phys. Institut; Universität zu Köln, Zülpicher Straße 77, 50937 Köln — [2]ILL, Grenoble, France — [3]LPCES, Paris Orsay, France

Manganites in a perowskite structure have attracted strong attention during the past years, mainly because of the discovery of the colossal magneto resistivity effect (CMR) and complex charge, orbital and magnetic ordering phenomena. Because of the twining in the perowskites, precise structural investigations to determine the ordering pattern are hampered. Therefore we investigated the single-layer manganites, which show similar ordering phenomena but only small magneto-resistivity effects. Since these materials are not intrinsically twinned, structure determination can be performed with much higher precision. For the ordered phase of half-doped manganites, two models were proposed, the Zener polaron model with bond-centered charge ordering and the so called CE-type model with size centered charge and orbital order, leading to two different Mn-sites. We present the results of powder and single crystal diffraction studies on $La_{0.5}Sr_{1.5}MnO_4$. From a neutron diffraction study on the D10 diffractometer and several x-ray diffraction experiment on our home diffractometer we can unambigously distinct between the two proposed models. The Zener-polaron model does not yield a satisfying description of the observed intensities. Details of the the ordered structure in the CE-Type model will be discussed.

TT 34.14 Thu 17:45 H 2053

Nanometer-scale phase separation in colossal magnetoresistive manganite — •Sahana Roessler[1], Stefan Ernst[1], Steffen Wirth[1], Frank Steglich[1], B. Padmanabhan[2], Suja Elizabeth[2], and H. L. Bhat[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Department of Physics, Indian Institute of Science, Bangalore 560012, India

In strongly correlated electron systems an intrinsic instability of the electronic state and competing long-range interactions may result in the formation of nanometer-sized regions of different phases. We have carried out scanning tunneling microscopy/spectroscopy on single crystals of a colossal magnetoresistive manganite $Pr_{0.68}Pb_{0.32}MnO_3$ at different temperatures in order to probe their spatial homogeneity across the metal-insulator transition temperature T_{M-I}. In this compound, the Curie temperature T_C is lower than T_{M-I} [1]. Spectroscopic studies revealed inhomogeneous maps of the zero-bias conductance with small patches of metallic clusters on a length scale of 2-3 nm only within a narrow temperature range close to the metal-insulator transition. A detailed analysis of conductance histograms based on these maps gave direct evidence for phase separation into insulating and metallic regions in the paramagnetic metallic state, i.e. for $T_C \lesssim T \lesssim T_{M-I}$, and homogeneous states otherwise, i.e. for $T < T_C$ as well as $T > T_{M-I}$ [2].

[1] B. Padmanabhan *et al.* J. Magn. Magn. Mat. **307** 288 (2006).
[2] S. Rößler *et al.* IEEE Trans. Magn. **43** 3064 (2007).

TT 34.15 Thu 18:00 H 2053

Scanning tunneling microscopy and spectroscopy study of charge and orbital ordering transition in $La_{0.5}Sr_{1.5}MnO_4$ — •Grzegorz Urbanik[1,2], Paul Sass[1], Christian Hess[1], Torben Hänke[1], Bernd Büchner[1], Antoni Ciszewski[2], Pascal Reutler[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institute of Experimental Physics, University of Wroclaw, 50-204 Wroclaw, Poland — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, Bâtiment 414, 91405 Orsay, France

The charge and orbital ordering compound $La_{0.5}Sr_{1.5}MnO_4$ has been studied by Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). Cleaving of the crystal exposes flat surfaces on which atomically resolved topographic images are routinely achieved above the charge ordering temperature $T_{CO} \approx 225$ K and below (down to $T \approx 205$ K). We have studied the temperature dependence of the electronic structure both for $T > T_{CO}$ and $T < T_{CO}$. The temperature dependent STS clearly reveals finite DOS at the Fermi level for $T > T_{CO}$ and the opening of a gap $\Delta \approx 0.5$ eV just below T_{CO}. In the topographic studies we find nanometer scale modulations with various periodicity and orientations. We compare these modulations with the inherent charge and orbital ordered state of this material.

TT 34.16 Thu 18:15 H 2053

$Hg_2Ru_2O_7$, a New Magnetic Pyrochlore Showing a Metal-Insulator Transition — •Reinhard K. Kremer, Jun Sung Kim, Wilhelm Klein, and Martin Jansen — Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The new pyrochlore compound $Hg_2Ru_2O_7$ was prepared under elevated oxygen pressure and characterized by x-ray diffraction, magnetic susceptibility, heat capacity, electrical resistivity and Hall effect measurements. $Hg_2Ru_2O_7$ undergoes a simultaneous metal-insulator and antiferromagnetic ordering transition at ∼108 K with the critical temperature decreasing under hydrostatic pressure.[1] $Hg_2Ru_2O_7$ is compared with other *p*-block metal oxoruthenates with pyrochlore structure which qualitatively show a very similar behavior. General trends are discussed.

[1] W. Klein, R. K. Kremer and M. Jansen, J. Mater. Chem. **17**, 1356 (2007).

TT 34.17 Thu 18:30 H 2053

Frustrated metallicity in the quasi-one-dimensional metal $PrBa_2Cu_4O_8$ — •Alessandro Narduzzo[1,2], Araz Enayati-Rad[1], Florence Rullier-Albenque[3], Shigeru Horii[4], and Nigel E. Hussey[1] — [1]University of Bristol, UK; — [2]IFW Dresden, Germany; — [3]Saclay, Paris, France; — [4]University of Tokyo, Japan.

We have investigated the metallic ground state of the extremely anisotropic quasi-one-dimensional metal $PrBa_2Cu_4O_8$ ($t_b^2 : t_a^2 : t_c^2 \sim 4000 : 2 : 1$), the non-superconducting analogue of the high-T_c cuprate $YBa_2Cu_4O_8$, as a function of disorder content, introduced either through atomic-site substitution or electron irradiation [1, 2]. A common single disorder threshold is found to drive interchain and inchain resistivities into a low temperature regime where they display $d\rho/dT < 0$. The survival of a large magnetoresistance of orbital origin reveals the itinerancy of the electronic system not to be suppressed by the presence of disorder [3]. We propose an interpretative scenario based on a microscopic electronic fragmentation of the metallic chains, though in contrast to many previous theoretical proposals, coherent hopping between chains appears to remain a relevant perturbation within the disordered system.

[1] New J. Phys. 8 (2006) 172-183; [2] Phys. Rev. Lett. vol. 99, 136402 (2007); [3] Phys. Rev. Lett. vol. 98, 146601 (2007).

TT 34.18 Thu 18:45 H 2053

Dynamics of correlated charge carriers in the close proximity to the Mott-Hubbard transition — •Michael Dumm[1], D. Faltermeier[1], S. Yasin[1], N. Drichko[1], M. Dressel[1], and J. Merino[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid 28049, Spain

We explored the dynamics of correlated charge carriers in close proximity to the Mott-Hubbard transition experimentally and theoretically in the quasi two-dimensional organic conductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_x$Cl$_{1-x}$ ($x = 0.73$ and 0.85). In the dc and optical conductivity data, we observe typical signatures of Fermi liquid behavior below the characteristic temperature $T^* \approx 30$ K and frequency $\nu^* \approx 400$ cm^{-1}: a T^2 and ν^2 dependence in resistivity and scattering rate, respectively and a substantial enhancement of the effective mass of the correlated carriers once we approach the metal-to-insulator transition by increasing U/t, i. e. by decreasing the Br content. The experimental results obtained by infrared spectroscopy agree well with DMFT calculations of a Hubbard model on a frustrated square lattice. Both, temperature and frequency dependence of optical conductivity and effective charge carrier number are successfully described by the theoretical model. If the temperature is increased above T^*, the Drude peak observed in the optical data at $T < T^*$ and $\nu < \nu^*$ vanishes and the optical spectral weight of the correlated carriers decreases indicating a gradual destruction of the quasiparticles.

TT 35: Transport: Nanoelectronics I - Quantum Dots, Wires, Point Contacts 3

Time: Thursday 14:00–18:30 Location: H 3010

TT 35.1 Thu 14:00 H 3010

Conductance of gold nanojunctions thinned by electromigration — •Regina Hoffmann[1,2], Daniel Weissenberger[2,3], Jacques Hawecker[2,3], Dominik Stöffler[1,2], and Hilbert v. Löhneysen[1,2,4] — [1]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe — [2]DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe — [3]Laboratorium für Elektronenmikroskopie, Universität Karlsruhe, 76128 Karlsruhe — [4]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe

Electromigration can in principle be used to fabricate arrays of nanocontacts for single-molecule junctions on the same chip, in contrast to the mechanically controllable break-junction technique. With this method, a Au nanowire prepared by electron beam lithography is heated resistively until thermally activated atoms diffuse under the influence of electromigration forces. Eventually, a nanogap is formed that can host a molecule. We report conductance histograms before a nanogap is formed that show oscillations as a function of the conductance for contacts in the ballistic regime. Obviously, heating enhances the probability of the atoms to reach equilibrium positions. The oscillations of the histogram as a function of the conductance have a period of slightly less than 1 G_0. This is typical for atomic shell structures. Similar oscillations have been observed for work-hardened Au wires while annealed Au shows oscillations typical for electronic shell structures [1].

[1] I.K. Yanson et al., Phys. Rev. Lett. 95, 256806 (2005).

TT 35.2 Thu 14:15 H 3010

Fabrication of nano-electrodes by means of controlled electrochemical deposition of gold — •Conrad R. Wolf, Daniel Gerster, Klaus Thonke, and Rolf Sauer — Institut für Halbleiterphysik, Universität Ulm, 89069 Ulm

In the emerging fields of nano- and molecular electronics a strong need for nano-electrodes arises from the wish to contact objects such as quantum dots or single molecules. In this contribution we show the use of a controlled electrochemical deposition scheme to fabricate stable electrodes with spacings below 10 nm. In our experiments we start with a pair of gold electrodes separated by a 200 nm gap prepared by electron beam lithography. These electrodes are immersed into a solution of KI and I_2 in ethanol which has been saturated by dissolving gold in it [1]. Both nano-electrodes are connected to the same DC potential, while an AC voltage between them is used to in-situ monitor the conductance with a lock-in amplifier. For the deposition a DC voltage is applied to the counter electrode until the recorded conductance reaches the desired value. It is also possible to reversibly close and open the electrode gap by applying positive and negative

voltages, respectively, to the counter electrode. With this technique gaps of around 1 nm can be realized, as conductance measurements after rinsing and drying as well as SEM micrographs show. When the electrodes are grown together slowly, we observe a step-wise increase in the conductance which corresponds to integer multiples of the conductance quantum $2e^2/h$.

[1] A. Umeno and K. Hirakawa, Appl. Phys. Lett. 86, 143103 (2005).

TT 35.3 Thu 14:30 H 3010

Electrical conductance through nanocontacts between fcc(100) electrodes of gold — •Daniela Koudela[1], Olga Lopez-Acevedo[1], Michael Walter[1], and Hannu Häkkinen[1,2] — [1]Department of Physics, Nanoscience Center, P.O. Box 35, FIN-40014 University of Jyväskylä — [2]Department of Chemistry, P.O. Box 35, FIN-40014 University of Jyväskylä

Both experimental and theoretical work has been done to explain conductance curves for metal nanowires, giving presently a good model that allows to explain experimental results microscopically. For one atom contacts it has moreover been shown, theoretically and experimentally, a strong relation between the number of valence orbitals of the single atom and the maximum value of the conductance that can be obtained [1].

We have studied Au nanowires of different lengths connected to fcc(100) tips corresponding to possible configurations in the elongation process. For those systems we have calculated the self-consistent potential obtained with Density Functional Theory and used it to calculate the conductance using the recursion-transfer-matrix method [2]. Our results show that though gold has formally only one valence electron (6s), for wires shorter than 3 atoms there are 3 (partially) open eigenmodes. [3]

[1] E. Scheer et al., Nature 394, 154 (1998)

[2] M. Brandbyge, K. W. Jacobsen, J. K. Norskov, Phys. Rev. B 55, 2637 (1997)

[3] O. Lopez-Acevedo et al., in preparation.

TT 35.4 Thu 14:45 H 3010

Ohmic current trough 1D quantum constrictions in the non-linear regime — •Afif Siddiki, Sefa Arslan, and Andreas Weichselbaum — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilans-Universität, München

The electron and current density distributions in the close proximity of quantum point contacts (QPCs) are investigated. A three dimensional Poisson equation is solved self-consistently to obtain the electron density and potential profile in the absence of an external magnetic field for gate and etching defined devices. We observed the surface charges and their apparent effect on the confinement potential, when considering the (deeply) etched QPCs. In the presence of an external magnetic field, we investigated the formation of the incompressible strips and their influence on the current distribution both in the linear response and out of linear response regime. A spatial asymmetry of the current carrying incompressible strips, induced by the large source drain voltages, is reported for such devices in the non-linear regime.

TT 35.5 Thu 15:00 H 3010

Maximally-localized Wannier functions within the FLAPW method applied to ballistic transport in thin metallic wires — •Y. Mokrousov[1], N.-P. Wang[1], F. Freimuth[2], B. Hardrat[1], S. Blügel[2], and S. Heinze[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

We report on the development of a ballistic transport code for one-dimensional systems based on maximally-localized Wannier functions (MLWFs) [1] constructed within the full-potential linearized augmented plane-wave (FLAPW) method [2,3]. We describe the details of the MLWFs construction from the FLAPW wavefunctions choosing a monoatomic Pt chain as a model system. For the calculation of ballistic transport, we apply the Landauer formalism using Green's functions. The Hamiltonian of the system including a scattering region attached to semi-infinite leads is constructed from the MLWFs which serve as a localized basis set. The open boundary conditions are treated by replacing the leads by their self-energies obtained via the decimation technique. From the Green function we can immediately calculate the conductance of the system. As a first application of the approach, we study the transition from the contact to the tunneling regime in thin Pt wires by a stretched bond.

[1] N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)

[2] Y. Mokrousov *et. al.*, Phys. Rev. B 72, 045402 (2005)

[3] www.flapw.de

15 min. break

TT 35.6 Thu 15:30 H 3010

A nonequilibrium functional renormalization group study of the single impurity Anderson model — •Severin G. Jakobs, Mikhail Pletyukhov, Herbert Schoeller, and Volker Meden — Institut für Theortische Physik A, RWTH Aachen, Germany

We apply a nonequilibrium version of the functional renormalization group [1] to the problem of transport through the single impurity Anderson model at finite bias voltage, temperature and magnetic field. Apart from the flow of the self energy we investigate the flow of the frequency dependent two-particle vertex.

[1] S. G. Jakobs, V. Meden, H. Schoeller, Phys. Rev. Lett. **99**, 150603 (2007)

TT 35.7 Thu 15:45 H 3010

Novel iterative path-integral scheme for interacting quantum dots out of equilibrium — •Stephan Weiss, Jens Eckel, Michael Thorwart, and Reinhold Egger — Inst. f. Theoret. Physik IV, Heinrich-Heine Universität Düsseldorf

We have developed a novel numerically exact method to evaluate fermionic many-body path-integrals. This method (IPI), see also [1] allows to give benchmark results for the observables of interest, e.g. the current. We perform simulations for real-time path-integrals on the Keldysh contour in a non-equilibrium situation. As application, we focus on the single site Anderson impurity model, subject to an applied bias voltage. We calculate the steady state current as a function of various system parameters, such as gate voltage ϵ_0, temperature T, on-dot Coulomb interaction U and external magnetic field B. Furthermore we obtain the nonlinear differential conductance in the coherent tunneling regime as a function of these parameters.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, submitted.

TT 35.8 Thu 16:00 H 3010

Competition between superconductivity and Kondo effect in a carbon nanotube quantum dot — Alexander Eichler[1], •Markus Weiss[1], Stefan Oberholzer[1], Christian Schönenberger[1], Alfredo Levy-Yeyati[2], Juan Carlos Cuevas[2], and Alvaro Martin-Rodero[2] — [1]Departement Physik, Universität Basel, Klingelbergstr. 82, CH-4056 Basel, Switzerland — [2]Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, E-28049 Madrid, Spain

We present nonlinear transport measurements on a carbon nanotube contacted to superconducting electrodes. At low temperatures, the nanotube acts as a quantum dot with intermediate contact transparencies. While level spacing and the charging energy dominate, the contact transparencies are large enough for higher order processes like the Kondo effect to occur. With superconducting electrodes, signs of the superconducting gap become visible in nonlinear transport, and additional subgap features due to multiple Andreev refections appear. In addition, we see a striking difference between even and odd charge states, with the first Andreev process at $V=\Delta/e$ being strongly enhanced in states with odd electron number. Although direct signs of the Kondo effect, as the Kondo ridge around zero bias, are suppressed, we argue that this even-odd asymmetry is due to a hidden Kondo resonance that, due to contact asymmetries, survives only on one contact, and leads to strongly enhanced transport at $V=\Delta/e$.

We find good agreement of our data with a single impurity Anderson model solved in a Slave Boson mean field approach.

TT 35.9 Thu 16:15 H 3010

Interaction Effects on Transport through an Electronic Mach-Zehnder Interferometer — •Vitaly Golovach and Florian Marquardt — Department of Physics, Arnold-Sommerfeld-Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstrasse 37, 80333 Munich, Germany

We study theoretically transport through an electronic Mach-Zehnder interferometer in the presence of Coulomb interaction inside the interferometer, using a discrete wave-packet model. We find that the mutual capacitance between the arms of the interferometer leads to

a suppression of the visibility of the Aharonov-Bohm oscillations at a large source-drain bias $\Delta\mu \gg \hbar v_F/L$, where L is the length of the arms and v_F is the electron drift speed. Our numerical simulations indicate that the visibility of the Aharonov-Bohm oscillations is a non-analytic function of the mutual capacitance strength, in the limit $\Delta\mu \to \infty$.

TT 35.10 Thu 16:30 H 3010

Effect of Magnetic field on edge channel interference in an electronic Mach-Zehnder interferometer — •Leonid Litvin, Andreas Helzel, Peter Tranitz, Werner Wegscheider, and Christoph Strunk — Institute of experimental and applied physics, University of Regensburg, D-93040 Regensburg, Germany

We study an electronic Mach-Zehnder Interferometer (MZI) employing the edge channels of a two-dimensional electron gas in the quantum Hall regime and quantum point contacts as tuneable beam splitters. In this system interference contrast up to 80% can be achieved at low temperatures. Two interferometers with the arm length of 14 and 9 μm were investigated. We found that the interference contrast depends strongly on interferometer size and filling factor. High visibility is restricted to a rather small interval of magnetic field, which approximately ranges from filling factor 2 to 1, with maximum near 1.5. The temperature dependences of visibility taken at fixed magnetic field show exponential damping above ≈45 mK. Below this value the visibility has much weaker T-dependence. This implies that two energy scales are responsible for the decay of visibility.

TT 35.11 Thu 16:45 H 3010

Bulk-edge coupling in the non-abelian $\nu = 5/2$ quantum Hall interferometer — •Bernd Rosenow[1], Bertrand I. Halperin[1], Steven H. Simon[2], and Ady Stern[3] — [1]Physics Department, Harvard University, Cambridge, MA 02138 — [2]Lucent-Alcatel Bell Laboratories, Murray Hill NJ, 07974 — [3]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

Recent schemes for probing non-abelian statistics in the $\nu = 5/2$ quantum Hall effect are based on geometries where current-carrying quasiparticles flow along edges that encircle N_{qp} bulk quasiparticles, which are localized. Here we consider one such scheme, the Fabry-Perot interferometer. In the limit of weak back-scattering, when N_{qp} is even the two back-scattering amplitudes interfere coherently, while when N_{qp} is odd they are incoherent, and thus do not interfere. In the former case, the back-scattered current oscillates with the area of the cell, while in the latter case it does not. This difference reflects the non-abelian nature of the quasiparticles.

In a real system, some degree of coupling between the edge and quasiparticles localized in the bulk is unavoidable. One may suspect that such a coupling would blur the distinction between bulk and edge quasiparticles and endanger the possibility of observing the even-odd effect. We find that at weak coupling the interference signal is indeed degraded, while for strong enough coupling the bulk quasiparticle becomes essentially absorbed by the edge and the even-odd effect survives. Furthermore, we find that the strength of the coupling can be tuned by the source-drain voltage.

15 min. break

TT 35.12 Thu 17:15 H 3010

Critical conductance of a one-dimensional doped Mott insulator — •Markus Garst[1], Dmitry Novikov[2], Ady Stern[3], and Leonid Glazman[2] — [1]Institut für Theoretische Physik, Universität zu Köln, 50938 Köln — [2]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [3]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We consider the two-terminal conductance of a one-dimensional Mott insulator close to the commensurate-incommensurate quantum phase transition to a conducting state (arXiv:0708.0545). We treat the leads as Luttinger liquids. At a specific value of compressibility in the leads, corresponding to the Luther-Emery point, the conductance can be computed in terms of a scattering problem of non-interacting fermions with charge $e/\sqrt{2}$. The Mott insulator can be approximated as an effective point scatterer with a strongly energy dependent scattering matrix. At the Luther-Emery point, the temperature dependence of the conductance across the quantum phase transition is then described by a Fermi function. The deviation from the Luther-Emery point in the leads results in an interaction among the fermionic scattering states and changes the temperature dependence qualitatively. In the metallic state, the low-temperature conductance is determined by the properties of the leads, and is described by the conventional Luttinger liquid theory. In the insulating state, conductance still occurs via activation of $e/\sqrt{2}$ charges, and is independent of the Luttinger liquid compressibility.

TT 35.13 Thu 17:30 H 3010

Conductivity of a disordered fermion-gaugefield system — •Thomas Ludwig[1], Igor V. Gornyi[2], Alexander D. Mirlin[2,3], and Peter Woelfle[3] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Institut fuer Nanotechnologie, Forschungszentrum Karlsruhe, Germany — [3]Institut fuer Theorie der kondensierten Materie, Universitaet Karlsruhe, Germany

We present a discussion of the interaction correction to conductivity in a disordered system of fermions interacting via a Chern-Simons gauge field. To first order in the interaction, we find a large positive Hartree correction to the conductivity. To account for higher orders in the interaction, we discuss effects of dephasing (at high temperatures) and screening (at low temperatures) on the Hartree correction. At sufficiently high temperatures, the Hartree correction is strongly suppressed by dephasing. At very low temperatures, the correction changes its sign to negative due to screening.

TT 35.14 Thu 17:45 H 3010

Quantum Transport in a Multi Particle Triple Quantum Dot — •Pöltl Christina, Emary Clive, and Brandes Tobias — Institut für Theoretische Physik, Hardenbergstr. 36, D-10623 TU Berlin, Germany

It is known that in the transport through triple quantum dot systems so-called dark states can occur [1, 2]. An electron entering such a state is trapped in the quantum dot system due to destructive interference and this leads to a blockade in current. Such states have previously been discussed only in the strong Coulomb blockade regime, where at most one excess electron is present in the system at any one time.

In this contribution, we discuss the effects of relaxing this condition, and permit multiple dot-occupancies. We use an number-resolved master equation approach to calculate the current, noise and counting statistics of the system, and show how the experimentally relevant quantities show a combination of dark-state and multiple-occupancy effects. We also consider signatures of electronic entanglement in the system.

[1] B. Michaelis, C. Emary and C. W. J. Beenakker, Europhys. Lett., 73 (5), pp. 677-683 (2006)

[2] C. W. Groth, B. Michaelis, and C. W. J. Beenakker, Phys. Rev B 74, 125315 (2006)

TT 35.15 Thu 18:00 H 3010

Electron Bunching in Stacks of Coupled Quantum Dots — •Sigmund Kohler[1], Rafael Sánchez[2], Peter Hänggi[1], and Gloria Platero[2] — [1]Institut für Physik, Universität Augsburg — [2]Instituto de Ciencia de Materiales, CSIC, Madrid, Spain

In recent measurements of the electrical current through transport channels that are formed by self-assembled double quantum dots, super-Poissonian noise has been observed [1]. In this system, two physical ingredients seems to play a crucial role, namely Coulomb interaction between electrons in neighbouring transport channels and, as well, the coupling of the electrons to substrate phonons. In a corresponding theoretical analysis [2], we study the transport properties of two double quantum dots in a parallel arrangement, in which the transport channels can block each other. Our results show that phonon emission and absorption, however, can suspend this blocking, which leads to "phonon-induced channel opening". This also affects the shot noise: For asymmetric coupling between the dots and the respective lead, the current noise is sub-Poissonian for resonant tunnelling, but super-Poissonian in the vicinity of the resonances. The both experimentally and theoretically observed asymmetry of the peaks at low temperatures stems from spontaneous emission.

[1] P. Barthold, F. Hols, N. Maire, K. Pierz, and R. J. Haug, Phys. Rev. Lett. **96**, 246804 (2006).

[2] R. Sánchez, S. Kohler, P. Hänggi, and G. Platero, arXiv:0706.2950 [cond-mat].

TT 35.16 Thu 18:15 H 3010

Violation of Wiedemann-Franz Law in a Single-Electron Transistor — •Björn Kubala[1,2], Jürgen König[1], and Jukka Pekola[3] — [1]TP III, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, 80333 Munich, Germany — [3]Low Temperature Labora-

tory, Helsinki University of Technology, PO BOX 3500, 02015 TKK, Finland

We study the influence of Coulomb interaction on the thermoelectric transport coefficients for a metallic single-electron transistor [1]. By performing a perturbation expansion up to second order in the tunnel-barrier conductance, we include sequential and cotunneling processes as well as quantum fluctuations that renormalize the charging energy and the tunnel conductance. We find that Coulomb interaction leads to a strong violation of the Wiedemann-Franz law: the Lorenz ratio becomes gate-voltage dependent for sequential tunneling, and is increased by a factor 9/5 in the cotunneling regime. Finally, we suggest a measurement scheme for an experimental realization.

[1] B. Kubala, J. König, and J. Pekola, arXiv:0709.4181 (unpublished).

TT 36: Superconductivity: Properties, Electronic Structure, Order Parameter

Time: Friday 10:15–13:00 Location: H 0104

TT 36.1 Fri 10:15 H 0104

Electron-Phonon interaction in electron-doped graphites — •Lilia Boeri[1], Ole Krogh Andersen[1], Jun Sung Kim[1], Reinhard Kremer[1], Giovanni B. Bachelet[2], and Matteo Giantomassi[3] — [1]Max-Planck-Institut für FestkörperForschung, Stuttgart, Germany — [2]INFM SMC and Dipartimento di Fisica, Università "la Sapienza", Roma, Italy — [3]UPCM, Université Catholique de Louvain, Louvain-la-Neuve,Belgium

The discovery of superconductivity in MgB_2 has initiated a thorough search for new electron-phonon ($e-ph$) superconductors, particulary among hexagonal layered compounds.

In this talk I will describe, using *ab-initio* methods, the electron-phonon properties of two classes of recently discovered superconductors, namely alkali-earth intercalated graphites (highest T_c 15.1 K for CaC_6)and metal-intercalated ternary compounds of the form: MaAlSi (highest T_c=7.8 K for CaAlSi).

TT 36.2 Fri 10:30 H 0104

Anisotropic s-wave superconductivity in graphite intercalation compounds: CaC_6 and SrC_6 — •Jun Sung Kim[1], Lilia Boeri[1], Feridoon Razavi[2], and Reinhard Kremer[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraβe 1, D-70569 Stuttgart, Germany — [2]Department of Physics, Brock University, St. Catharines, Ontario, L2S 3A1, Canada

We have investigated the anisotropy of the superconducting properties for newly-discovered superconducting graphite intercalation compounds, CaC_6 and SrC_6 using specific heat (C_p). The electronic C_p for CaC_6 shows an exponential temperature dependence at low temperatures, consistent with a fully gapped s-wave superconducting order parameter. However, the detailed comparison with an isotropic superconducting gap model shows significant deviation between experiment and theory. From the magnetic field dependence of C_p, the anisotropy of upper critical fields (H_{c2}) for CaC_6 is ~ 5, consistent with that obtained from the magnetic field dependence of Sommerfeld coefficient, but much larger than that of SrC_6. In comparison with electronic structure calculations, we found that the isotropic gap model cannot explain observed superconducting properties, suggesting significant anisotropy in the superconducting gap for both CaC_6 and SrC_6. Recent investigations on a directional point-contact spectroscopy on CaC_6 along the c-axis and ab-plane will also be discussed.

TT 36.3 Fri 10:45 H 0104

Superconducting properties of CaC_6 — •Antonio Sanna[1,2], Gianni Profeta[3], Andrea Floris[2], Andrea Marini[4], Eberhard K.U. Gross[2], and Sandro Massidda[1] — [1]Università degli studi di Cagliari, Italy. — [2]Freie Universität Berlin, Germany. — [3]Università degli studi dell'Aquila, Italy. — [4]University of Rome Tor Vergata, Italy.

We present first-principles calculations of the superconducting properties of CaC_6[1], obtained within the density functional theory of superconductivity (SCDFT). We find an anisotropic gap which is larger on the Fermi surface sheet with interlayer character. In contrast to MgB_2 the intraband anisotropy is large and the gaps on the three Fermi surface sheets overlap. The resulting critical temperature of 9.5 K is in good agreement with the experimental value of 11.5 K.

We show that anisotropy improves the agreement between calculated and experimental specific heat and is consistent with tunnelling experiments. A direct evidence of the gap anisotropy in CaC_6 has been recently observed in directional point contact measurements[2].

We also investigate the system under pressure in order to analyse the increase of the superconducting critical temperature reported experimentally[3] but not reproduced in the McMillan approach. Within our SCDFT implementation we intend to improve the theoretical description with respect to previous studies introducing an ab-initio and pressure-dependent Coulomb interaction.

[1] A. Sanna *et al.*, Phys. Rev. B **75**, 020511 (2007).
[2] R. Gonnelli *et al.*, arXiv 0708.0921.
[3] A. Gauzzi *et al.*, Phys. Rev. Lett. **98**, 067002 (2007).

TT 36.4 Fri 11:00 H 0104

High-pressure study of layered bulk phases of elemental boron — •Jens Kunstmann[1], Lilia Boeri[1], and Jens Kortus[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Inst. für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany

The valence shell of boron contains less electrons than available orbitals, which results in very complex bulk structures, primarily consisting of B_{12} icosahedra. But boron is relatively little studied and many properties such as the phase diagram, the ground state structure, and its high-pressure behavior are unknown. Recently two discoveries put elemental boron into the scientific focus. One is that it becomes superconducting under high pressure. The other one is that small clusters form two-dimensional sheet-like structures, as suggested by theoretical studies of Boustani and Quandt in the mid-1990s. The high-pressure superconductivity is not fully understood so far, because the corresponding crystal structures are still under debate. Hence before solving the problem of understanding the coupling mechanism for superconductivity one has to solve first the problem of determining the crystal structure. The existence of sheet-like clusters poses the question if boron sheets, similar to graphene, or layered bulk phases, similar to graphite, may also exist for boron. Therefore our study tries to approach the following questions: What do such layered bulk structures look like? What are their stabilities in comparison with other bulk phases? Are they dynamically stable and if yes, are they responsible for the high-pressure superconductivity of elemental boron?

TT 36.5 Fri 11:15 H 0104

Electrons, phonons and superconducting properties of CaBeSi — •A. Floris[1], C. Bersier[1], A. Sanna[1,2], G. Profeta[3], A. Continenza[3], E.K.U. Gross[1], and S. Massidda[2] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Germany — [2]INFM SLACS and Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari, Italy — [3]C.A.S.T.I. - INFM and Dipartimento di Fisica, Università degli studi dell'Aquila, Italy

We present first-principles calculations on the normal and superconducting state of $CaBe_xSi_{2-x}$ $(x = 1)$[1,2], in the framework of the density functional theory for superconductors (SCDFT)[3,4] . CaBeSi is isostructural and isoelectronic to MgB_2 and this makes possible a direct comparison of the electronic and vibrational properties and the electron-phonon interaction of the two materials. Although our calculations show that CaBeSi has a low critical temperature ($T_c \approx 0.6$ K), it exhibits a complex gap structure, with *three* gaps at the Fermi level. Besides the two σ and π gaps, present also in MgB_2, the appearance of a third gap is related to the anisotropy of the Coulomb repulsion, acting in different way on the bonding and antibonding electronic π states.

[1] N. May *et al.*, Z. Naturforsh. B **2**, 1947 (1977).
[2] F. Sano *et al.*, CP850 Low Temperature Physics: 24^{th} International Conference on Low Temperature Physics, 2006.
[3] M. Lüders *et al.*, Phys. Rev. B, **72**, 024545 (2005).
[4] M. A. L. Marques *et al.*, Phys. Rev. B, **72**, 024546 (2005).

15 min. break

TT 36.6 Fri 11:45 H 0104

Superconductivity in the new filled skutterudites $M\mathbf{Pt_4Ge_{12}}$ (M = La, Pr, Sr, Ba) — •Walter Schnelle, Roman Gumeniuk, Helge Rosner, Michael Nicklas, Andreas Leithe-Jasper, and Yuri Grin — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

New germanium-platinum compounds with the filled-skutterudite crystal structure were synthesized [1]. The crystal structure and composition were investigated by X-ray diffraction and microprobe analysis. Magnetic susceptibility, specific heat, and electrical resistivity measurements evidence superconductivity in $LaPt_4Ge_{12}$ and $PrPt_4Ge_{12}$ below 8.3 K. The parameters of the normal and superconducting states were established. Strong coupling and a crystal electric field singlet groundstate is found for the Pr compound. Electronic structure calculations show a large density of states at the Fermi level [1]. Similar behavior albeit with lower T_c was observed for $SrPt_4Ge_{12}$ and $BaPt_4Ge_{12}$ [1,2].

[1] R. Gumeniuk *et al.* Phys. Rev. Lett. submitted. ArXiV 0710.1413v1.

[2] R. Gumeniuk *et al.* Poster, this conference.

TT 36.7 Fri 12:00 H 0104

Eliashberg Theory of Superconductivity and Inelastic Scattering by Rare-Earth Impurities in the Filled Skutterudite $\mathbf{La_{1-x}Pr_xOs_4Sb_{12}}$ — •Jun Chang[1], Ilya Eremin[1,2], Peter Thalmeier[3], and Peter Fulde[1] — [1]Max-Planck Institut fur Physik komplexer Systeme, D-01187 Dresden, Germany — [2]Institute fur Mathematische und Theoretische Physik, TU-Braunschweig, D-38106 Braunschweig, Germany — [3]Max-Planck Institut fur Chemische Physik fester Stoffe, D-01187 Dresden, Germany

We study the influence of inelastic rare-earth impurity scattering on electron-phonon mediated superconductivity and mass renormalization in $(La_{1-x}Pr_x)Os_4Sb_{12}$ compounds. Solving the strong coupling Eliashberg equations we find that the dominant quadrupolar component of the inelastic scattering on Pr impurities yields an enhancement of the superconducting transition temperature T_c in $LaOs_4Sb_{12}$ and increases monotonically as a function of Pr concentration. The calculated results are in good agreement with the experimentally observed $T_c(x)$ dependence. Our analysis suggests that phonons and quadrupolar excitations cause the attractive electron interaction which results in the formation of Cooper pairs and singlet superconductivity in $PrOs_4Sb_{12}$.

TT 36.8 Fri 12:15 H 0104

Evidence for an Fulde-Ferrell-Larkin-Ovchinnikov state in a layered organic superconductor — •B. Bergk[1], P. H. M. Böttger[1], R. Lortz[2], Y. Wang[2], A. Demuer[3], I. Sheikin[3], G. Zwicknagl[4], Y. Nakazawa[5], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, FZ Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Condensed Matter Physics, University of Geneva, CH-1211 Geneva, Switzerland — [3]Grenoble High Magnetic Field Laboratory, CNRS, 38042 Grenoble, France — [4]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [5]Department of Chemistry, Osaka University, 1-1, Machikaneyama, Toyonaka, Osaka, Japan

We present specific heat and torque-magnetization data of the layered organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ in high magnetic fields up to 28 T and at low temperatures down to 1.5 K. The magnetic field was aligned perfectly parallel to the superconducting planes of the sample. In that orientation and at low temperatures the upper critical field, B_{c2}, gets close to the Pauli limit which is about 21 T. But instead of the expected saturation at this field value we observe an upturn of B_{c2} towards low temperatures. This comes along with a change of the order of the phase transition from second order to first order. In addition, another first-order phase transition appears below B_{c2} in the superconducting state. These features strongly point to the formation of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase in the state above the Pauli limit. Our results are in line with the behaviour predicted for FFLO states in two-dimensional systems.

TT 36.9 Fri 12:30 H 0104

Electron Phonon Interaction and Superconductivity in Nb and Pb investigated with Neutron Resonance Spin Echo Spectroscopy — •Pegor Aynajian[1], Thomas Keller[1,2], Lilia Boeri[1], Klaus Habicht[3], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkrperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]ZWE FRMII, TUM, Lichtenbergstrasse 1, D-85748 Garching, Germany — [3]3Hahn-Meitner-Institut, Glienicker Strasse 100, D-14109 Berlin, Germany

The momentum and temperature dependency of the phonon lifetime of the transverse acoustic branches along the [110] and [100] directions in Pb and Nb were studied using the high resolution neutron resonance spin-echo, triple-axis technique. Several anomalies were observed, which can in part be assigned to Kohn anomalies. The most striking feature both in Nb and Pb is a Kohn anomaly sitting at a phonon energy corresponding to the superconducting energy gap 2D(T = 0). This arises the question if 2D is limited by a Kohn anomaly.

TT 36.10 Fri 12:45 H 0104

Localized superconductivity in TiN thin films — •Ante Bilušić[1], Tatyana Baturina[2], Tatyana Mironov[2], Florian Otto[1], Mikhaïl Baklanov[3], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]IMEC, Leuven, Belgium

We present a low-temperature investigation of transport and magnetic properties of TiN thin films in the critical region of the disorder driven superconductor-insulator transition (SIT). At zero magnetic field, the superconducting and insulating phases are sharply separated, indicating the absence of the intermediate metallic state in the SIT. Electrical conductivity of the insulating films is thermally activated. Films closer to the critical level of disorder show a huge positive magnetoresistance (MR) at low, and a negative MR for high fields. Films being deeper on the insulating side of the SIT critical region exhibit negative MR only. At low temperatures, differential conductance curves of insulating samples show a depinning threshold V_T, below which the conductance is immeasurably small. Threshold V_T depends in a nonmonotonic way on magnetic field. This can be explained in terms of recent theory [1], which relies on the competition of Coulomb charging and Josephson coupling in arrays of Josephson junctions.

[1] M. V. Fistul, V. M. Vinokur, and T. I. Baturina, arXiv:0708.2334v2 (unpublished)

TT 37: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Friday 10:15–13:00 Location: H 2053

TT 37.1 Fri 10:15 H 2053

Quantum Transport through Nanodevice — •Frithjof Anders — Institut für Theoretische Physik, Universität Bremen, P.O. Box 330 440, D-28334 Bremen

The electronic transport though nanodevices such as quantum dots and carbon nanotubes are dominated by their small capacitance at low temperatures. The Kondo effect is now a classical hallmark of many-body physics in nanoscale devices governing the crossover between the Coulomb blockade regime and perfect transmission. We present numerical renormalization group (NRG) calculation for the temperature evolution zero-bias conductance which agrees beautifully with recently published experiments on semiconducting carbon nanotube quantum dots.

Furthermore, we discuss a novel approach to steady-state non-equilibrium dynamics at finite bias, based on a combination of an NRG approach to open quantum system and the recently developed time-dependent NRG. The current-voltage characteristics can be obtained for a tunneling junctions as well as symmetric single-electron transistors at arbitrarily low temperatures.

TT 37.2 Fri 10:30 H 2053

Transport through Semiconductor Nanowire Quantum Dots in the Kondo Regime — •Stefan Schmaus, Verena Koerting, and Peter Wölfle — Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany

Recent experiments on quantum dots made of semiconductor nanowires in the Coulomb blockade regime have shown the influence of several approximately equidistant levels on the conductance. We study a model with three levels occupied by three electrons. At finite bias voltage charge energy conserving excitations into several higher lying states occur leading to features in the differential conductance. We restrict our study to the six lowest lying states by performing a Schrieffer-Wolff type projection onto this subspace. The emerging effective Kondo Hamiltonian is treated in non-equilibrium perturbation theory in the coupling to the leads. For convenience we use a pseudoparticle representation and an exact projection method. The voltage-dependence of the occupation numbers is discussed. The density matrix on the dot turns out to be off-diagonal in the dot eigenstate Hilbert space in certain parameter regimes. The dependence of the differential conductance on magnetic field and temperature is calculated in lowest order in the dot-lead coupling and the results are compared with experiment.

TT 37.3 Fri 10:45 H 2053

Stable Two-Channel Kondo Fixed Point of an SU(3) Quantum Defect in a Metal: Renormalization-Group Analysis and Conductance Spikes — •Katinka Ballmann, Tobias Langenbruch, Michael Arnold, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

We propose a physical realization of the two-channel Kondo (2CK) effect, where a rotational defect in a metal has a unique ground state and twofold degenerate excited states [1]. In a wide range of parameters the interactions with the electrons renormalize the excited doublet downward below the bare defect ground state, thus stabilizing the 2CK fixed point. In addition to the Kondo temperature T_K the three-state defect exhibits another low-energy scale, associated with ground-to-excited-state transitions, which can be exponentially smaller than T_K. Using the perturbative nonequilibrium renormalization group we demonstrate that this can provide the long-sought explanation of the sharp conductance spikes observed by Ralph and Buhrman in ultrasmall metallic point contacts. In addition, we investigate the effect of an applied magnetic field coupling to the angular magnetic moment of the defect, lifting the degeneracy of the excited states, which can lead to a splitting of the sharp conductance spikes even when the Zeeman energy is less than T_K.

[1] M. Arnold, T. Langenbruch, and J. Kroha, PRL **99**, 18660 (2007).

TT 37.4 Fri 11:00 H 2053

Non-Equilibrium Scaling 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

By using infinitesimal unitary transformations (flow equations) [1] we derive a perturbative scaling picture of a Kondo dot in a magnetic field. Within this single scaling picture we are able to study both equilibrium and non-equlibrium (dc voltage bias) situations. As main result, we work out the spin-spin correlation function and the T-Matrix as functions of magnetic field, voltage bias and temperature.

This work is a generalization of the previous flow equation analysis of the non-equilibrium Kondo Model [2].

[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)

TT 37.5 Fri 11:15 H 2053

Coupled-Cluster Method for the Anderson Impurity Model — •Jin-Jun Liang, Clive Emary, and Tobias Brandes — Sekr. PN 7-1, Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 BERLIN

The coupled-cluster method (CCM) is one of the most powerful and numerically accurate approximation methods for describing many-body quantum systems. It is popular in nuclear physics, quantum chemistry and quantum magnetism. However, the method has been rarely applied to models with continua, like the Anderson impurity model. In this talk, we will present our work on applying the CCM to the Fano-Anderson model and the Anderson model with Coulomb interaction. Results are mainly for ground state properties, including ground state energies and impurity occupation numbers. The method will also be compared with some other more traditional methods in quantum impurities, such as Green's function and self-consistent perturbation theory.

15 min. break

TT 37.6 Fri 11:45 H 2053

Quantum systems coupled to baths: A novel Chebyshev space description — •Andreas Alvermann and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany

We propose a new concept for the dynamics of a quantum bath, the Chebyshev space method. Relying on Chebyshev expansions the Chebyshev space representation of the bath degrees of freedom has very favorable properties with respect to extremely precise and efficient numerical calculations of groundstate properties, static and dynamical correlations, and time-evolution for a great variety of quantum systems. In particular we can address important topics like transport through quantum systems coupled to fermionic baths, the solution of quantum impurity models, or the non-equilibrium dynamics of mesoscopic devices coupled to leads.

TT 37.7 Fri 12:00 H 2053

Matrix product state comparison of the numerical renormalization group and the density matrix renormalization group — •Hamed Saberi, Andreas Weichselbaum, and Jan von Delft — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Wilson's numerical renormalization group (NRG) method for solving quantum impurity models can be turned into a variational method within the set of so-called matrix product states (MPS) with significantly more flexibility and efficient use of numerical resources. White's density matrix renormalization group (DMRG) for treating quantum lattice problems can likewise be reformulated in terms of MPSs. Thus, the latter constitute a common algebraic structure for both approaches. We exploit this fact to compare the NRG approach for the single-impurity Anderson model to the DMRG approach. We explore to what extent NRG results can be improved upon systematically by performing a variational optimization in a space of variational matrix product states of the same structure as those used by NRG. We also compare the truncation schemes of NRG and DMRG, which are formulated in terms of energy eigenvalues or density matrix eigenvalues, respectively, and establish how many of the latter need to be kept to reproduce NRG eigenspectra using DMRG.

TT 37.8 Fri 12:15 H 2053

Dephasing rates within nonequilibrium RG: A generic approach — •Frank Reininghaus, Herbert Schoeller, and Thomas Korb — Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany

We consider a generic model for a local quantum system coupled to reservoirs and present a general solution to the problem how relaxation and dephasing rates can be implemented within nonequilibrium renormalization group. Generalizing previous RG-methods [1,2] to a specific frequency representation and using a cutoff on the imaginary frequency axis [3], we show that decay rates always cut off the RG flow and find the physical meaning of these rates. We illustrate the method for the nonequilibrium Kondo model.

[1] Herbert Schoeller and Jürgen König, Phys. Rev. Lett. **84**, 3686 (2000)

[2] Thomas Korb, Frank Reininghaus, Herbert Schoeller, and Jürgen König, Phys. Rev. B **76**, 165316 (2007)

[3] Severin G. Jakobs, Volker Meden, and Herbert Schoeller, Phys. Rev. Lett. **99**, 150603 (2007)

TT 37.9 Fri 12:30 H 2053

Kondo screening cloud in a one-dimensional wire: Numerical renormalization group study — •László Borda — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany — Department of Theoretical Physics, TU Budapest, H1111 Budapest, Budafoki út 8. Hungary

We study the Kondo model -a magnetic impurity coupled to a one-dimensional wire via exchange coupling- by using Wilson's numerical renormalization group technique. By applying an approach similar to which was used to compute the two-impurity problem we managed to improve the poor spatial resolution of the numerical renormalization group method. In this way we have calculated the impurity-spin-conduction-electron-spin correlation function which is a measure of the Kondo compensation cloud whose existence has been a long-standing

problem in solid-state physics. We also present results on the temperature dependence of the Kondo correlations.

TT 37.10 Fri 12:45 H 2053

Low temperature Kondo phyiscs in mesoscopic systems — •Rainer Bedrich, Sebastien Burdin, and Martina Hentschel — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

We study the Kondo effect in a quantum dot with discrete energy levels coupled to a single magnetic impurity. The electronic occupation can be changed by tuning the gate voltage that is applied to the dot. Solving the Hamiltonian within a mean-field approximation, we compute various physical quantities, e.g. the magnetic susceptibility, the conductance and the local density of states in the Kondo regime. Finite size effects lead to deviations from the universal behavior which would be expected for a bulk system. They are investigated by varying the number of energy levels and the mean level spacing.

TT 38: Matter At Low Temperature: Quantum Liquids, Bose-Einstein Condensates, Ultra-cold Atoms, ...

Time: Friday 10:15–13:00 Location: H 3010

TT 38.1 Fri 10:15 H 3010

Supersolid Bose-Fermi Mixtures in Optical lattices — •Irakli Titvinidze, Michiel Snoek, and Walter Hofstetter — Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany

We study a mixture of strongly interacting bosons and fermions with on-site repulsion in a three-dimensional optical lattice. We apply a generalized DMFT (gDMFT) scheme, which is exact in infinite dimensions and reliably describes the full range from weak to strong coupling. In first instance we restrict ourselves to the case of a mixture of bosons and spinless fermions at half filling. In this case a supersolid forms for weak Bose-Fermi repulsion, in which bosonic superfluidity coexists with charge-density wave order. For stronger interspecies repulsion the bosons become localized while the charge density wave order persists. The system is unstable against phase separation for weak repulsion among the bosons. Extending this to the case of spinfull fermions, we also find an antiferromagnetic phase.

[1] I. Titvinidze, M. Snoek, and W. Hofstetter; preprint: arXiv:0708.3241

TT 38.2 Fri 10:30 H 3010

Noise correlation for fermions with attractive interactions confined in one-dimensional optical lattices — •Farshid Karim Pour[1], Stefan Wessel[1], Marcos Rigol[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany. — [2]Department of Physics, University of California, Santa Cruz, 1156 High Street Santa Cruz, CA 95064, USA

Using quantum Monte Carlo simulations, we study the behavior of the one-dimensional attractive fermionic Hubbard model in different confinement potentials. Studying the noise correlation function we show that the signals for charge-density wave and superconductivity can clearly be seen in the noise correlation function for such fermionic systems. We show that density-density and pairing correlation functions are characterized by the anomalous dimension K_ρ of a corresponding periodic system. This allows us to determine conditions for a supersolid state inside a trap. We find that, eventhough the SU(2) symmetry is broken by the confining potential, density-desity and pairing correlations can decay with exactly the same exponent, hence giving rise to a (quasi-)supersolid in 1D[1].

[1] F. Karim Pour, M. Rigol, S. Wessel, A. Muramatsu, PRB **75**, 161104(R) (2007)

TT 38.3 Fri 10:45 H 3010

FFLO states in a one-dimensional lattice with polarized, trapped fermions and attractive interactions — •Fabian Heidrich-Meisner[1] and Adrian Feiguin[2] — [1]Institut für Theoretische Physik C, RWTH Aachen, 52064 Aachen, Germany — [2]Microsoft Station Q, University of California, Santa Barbara, CA 93106, USA

We study the properties of a one-dimensional (1D) gas of fermions focusing on the case of unequal spin populations and strong attractive interaction. While the emergence of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states has previously been predicted from mean-field and local density approximation studies, here [1], we address this problem by means of a quasi-exact numerical method, the density matrix renormalization group technique. In the low density regime, the system phase-separates into a well defined superconducting core and a fully polarized metallic cloud surrounding it. We argue that the superconducting phase corresponds to a 1D analogue of the FFLO state, with a finite center-of-mass momentum that scales linearly with the magnetization. Moreover, we find that the spatial decay of pair correlations follows a power law. In the large density limit, the system allows for four phases: in the core, we either find a Fock state of localized pairs or a metallic shell with spin-down fermions moving in a fully filled background of spin-up fermions. As the magnetization increases, the Fock state disappears to give room for a metallic phase, with a partially polarized superconducting FFLO shell and a fully polarized metallic cloud surrounding the core.

[1] A.E. Feiguin, F. Heidrich-Meisner, arXiv:0707.4172.

TT 38.4 Fri 11:00 H 3010

Spin - charge separation in ultracold two-component Bose-gases — •Adrian Kleine[1], Corinna Kollath[2], Ian P. McCulloch[3], Thierry Giamarchi[2], and Ulrich Schollwöck[1] — [1]Institut für Theoretische Physik C, RWTH Aachen, D-52056 Aachen, Germany — [2]DPMC-MaNEP, University of Geneva, CH-1211 Geneva, Switzerland — [3]School of Physical Sciences, University of Queensland, Brisbane, Qld 4072, Australia

The experimental search for signatures of spin-charge separation, a hallmark feature of one-dimensional interacting electron systems, is a key topic in strongly correlated electron physics. The recent progress in ultracold atom realizations allows for both interaction parameters to be fine-tuned and to trap atoms in quasi one dimensional set-ups, hence opening a novel path towards the observation of spin charge separation. Here we theoretically study a two-component system of bosonic ultracold atoms in the framework of the Bose-Hubbard model. We show that even close to a competing phase separation regime, such a model features spin charge separation [1]. To this end, we determine the real-time evolution of a single particle excitation and the single-particle spectral function using density-matrix renormalization group techniques. In anticipation of experimental realizations we calculate the velocities for spin and charge perturbations for a wide range of parameters.

[1] A. Kleine et al. to appear in Phys. Rev. A, preprint arXiv:0706.0709

TT 38.5 Fri 11:15 H 3010

Trionic phase of the attractive SU(3)-Hubbard model — •Guido Klingschat and Carsten Honerkamp — Theoretische Physik, Universität Würzburg

Recently, a quantum phase transition from a color superfluid to a colorless phase with conglomerates of 3 fermions on a single site ('trions') has been proposed to occur in the attractive SU(3)-Hubbard model [Rapp et al., Phys. Rev. Lett. 98, 160405 (2007)]. Here we analyze the properties of the trionic phase using exact diagonalization. We determine the spectral function of single particle and trionic excitations, and compute spatial correlations. This way we can characterize the effective quasiparticles of the strong coupling phase.

15 min. break

TT 38.6 Fri 11:45 H 3010

Circulating currents in fermionic bilayers — •Alexei Kolezhuk — Institut für Theoretische Physik C, RWTH Aachen, Germany

It is shown that fermionic polar molecules or atoms in a bilayer optical lattice can undergo the transition to a state with circulating currents, which spontaneously breaks the time reversal symmetry. The bilayer

lattice design is proposed, estimates of relevant temperature scales are given and experimental signatures of the circulating current phase are identified. Related phenomena in bosonic and spin systems with ring exchange are discussed.

TT 38.7 Fri 12:00 H 3010

Vorticity in rotating 2D Bose-Einstein condensates in the regime of strong coupling — •Tanja Rindler-Daller — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany

When Bose-Einstein condensates are subjected to an external rotation different vortex structures appear depending on the applied angular velocity Ω. We study the ground state within the Gross-Pitaevskii theory in the limit of large coupling constant for condensates which are confined in (asymptotically) homogeneous trap potentials [1,2]. We identify three regimes in Ω, which are characterized by a distinctive behaviour in the density profile and vortex structures, by rigorous estimates.

[1] M.Correggi, T.Rindler-Daller, J.Yngvason, J.Math.Phys. 48, 042104 & 102103 (2007)

[2] T.Rindler-Daller, accepted by Physica A

TT 38.8 Fri 12:15 H 3010

Shuttle for cold atoms: atomic quantum dot inside Bose Josephson junction. — •Anna Posazhennikova[1], Uwe R. Fischer[2], and Christian Iniotakis[3] — [1]Physikalisches Institut, Universitaet Bonn, Germany — [2]Institut fuer Theoretische Physik, Eberhard-Karls-Universitate Tuebingen, Germany — [3]ETH Zuerich, Institut fuer Theoretische Physik, Zuerich, Switzerland

We study an atomic quantum dot representing a single hyperfine "impurity" atom which is coherently coupled to two well-separated Bose-Einstein condensates. It is demonstrated that the quantum dot by itself can induce coherent oscillations of the particle imbalance between the condensates even when the conventional tunneling between the two condensates is exponentially small and can be completely neglected. In the limit of noninteracting condensates, we provide an analytical solution to the coupled nonlinear equations of motion which is in agreement with the full numerical treatment.

TT 38.9 Fri 12:30 H 3010

Condensate formation in Bose-gas upon cooling — •Roman Saptsov[1], Efim Brener[1], and Sergey Iordanskiy[2] — [1]IFF, FZ-Jülich, Jülich, Germany — [2]Landau Istitute for Theoretical Physics, Moscow, Russia

The mechanism for the transition of a Bose gas to the superfluid state via thermal fluctuations is considered. It is shown that in the process of external cooling some critical fluctuations (instantons) are formed above the critical temperature. The probability of the instanton formation is calculated. It is found that this probability increases as the system approaches the transition temperature.

TT 38.10 Fri 12:45 H 3010

Construction of an optical dipole trap for studying bosonic mixtures — •Lars Steffens[1,2], Shincy John[1], Claudia Weber[1], Artur Widera[1], Manfred Fiebig[2], and Dieter Meschede[1] — [1]IAP, Universität Bonn, Wegelerstr. 8, 53115 Bonn, Germany — [2]HISKP, Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany

Because of their well controlable behaviour, ultracold atomic gases are a useful tool for studying quantum mechanical many body systems. A variety of problems of solid state physics could be modelled by using systems of ultracold gases. In addition, studying *mixtures* of ultracold gases lead to an improved understanding of quantum mechanical multi component systems. Up to now, mostly boson-fermion mixtures were considered while only little research has been done on boson-boson mixtures of different atomic species. Here the construction of an simple optical dipole trap designed for Feshbach spectroscopy of Rb-Cs mixtures is presented. The response of the atomic species to the light field is discussed. A precise simulation of the optical potential by a 3D-simulation of the light field including aberration and diffraction effects is given. These results can be used as a basis for the construction of other dipole potential setups that can be used to describe a broad variety of external parameters.

TT 39: Transport: Nanoelectronics II - Spintronics and Magnetotransport

Time: Friday 10:15–13:00 Location: EB 202

Invited Talk TT 39.1 Fri 10:15 EB 202

EuO_{1-x} Epitaxially Integrated with Silicon — •Andreas Schmehl[1,2], Stefan Thiel[2], Christoph Richter[2], Ross Ulbricht[1], Tassilo Heeg[1], Marco Liberati[3], Martin Röckerath[4], Sebastian Mühlbauer[6], Peter Böni[6], Yuri Barash[5], Jürgen Schubert[4], Yves Idzerda[3], Jochen Mannhart[2], and Darrell G. Schlom[1] — [1]Pennsylvania State University, University Park, PA, USA — [2]Universität Augsburg, Augsburg — [3]Montana State University, Bozeman, MT, USA — [4]Forschungszentrum Jülich, Jülich — [5]Russian Academy of Sciences, Chernogolovka, Russia — [6]Technische Universität München, Garching

The ferromagnetic semiconductor EuO is well known for its outstanding magneto-transport and magneto-optical properties, but for decades its instability in air has prevented the thorough exploration of this exciting material. Exploiting oxide MBE and advanced capping techniques, we are now able to epitaxially integrate EuO with a multitude of substrates including silicon and GaN and pattern it using photolithography. Using Andreev reflection spectroscopy, we demonstrate that these films have spin-polarizations exceeding 90%, rendering EuO a very promising candidate to establish spin-selective ohmic contacts to silicon. A novel patterning process, combining *insitu* ion etching and sputtering, allows for the patterning of the films, paving the way to exploit EuO in semiconductor-based spintronic devices as well as in devices making use of its exceptional magneto-transport and magneto-optical properties.

TT 39.2 Fri 10:45 EB 202

Simultaneous ferromagnetic semiconductor-metal transition in Gd-doped EuO — •Michael Arnold and Johann Kroha — Physikalisches Institut, Universität Bonn

At room temperature, europium oxide, EuO, is a paramagnetic semiconductor with a large band gap of 1.2 eV which undergoes a ferromagnetic ordering transition at a Curie temperature of $T_C = 69$ K. Upon minute electron doping, this transition turns into a simultaneous ferromagnetic semiconductor-metal transition, with nearly 100 % of the conduction electrons polarized and a huge magnetoresistance effect. This has made EuO a prototypical material for possible spintronics applications.

Here we present a general framework for describing this phase transition in Gd-doped EuO. This system is described by a Heisenberg lattice of the Eu 4f moments S=7/2, a conduction band (which in the high-temperature phase is empty), and singly occupied impurity levels in the gap, provided by the Gd 5d orbitals. The theory correctly describes detailed experimental features of the conductivity and of the magnetization, in particular the enhancement of T_C by a minute Gd doping concentration. The existence of correlation-induced local moments on the impurity sites is essential for this description. We also predict that the ferromagnetic semiconductor-metal transition can be switched by applying a gate voltage to EuO films.

TT 39.3 Fri 11:00 EB 202

Effect of spin-orbit coupling on transport through ferromagnetic atomic-sized contacts — •Michael Häfner[1,2,3], Janne Viljas[1,2], and Juan Carlos Cuevas[3,1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Institut für Nanotechnologie, FZ Karlsruhe, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid

Based on a tight-binding model we analyze the effect of spin-orbit coupling on the transport through ferromagnetic atomic-sized contacts. Our calculation shows a strong dependence of the conductance on the direction of magnetization. The results suggest that the anisotropic magnetoresistance found in recent experiments on transport through ferromagnetic atomic-sized contacts [1] stems from the spin-orbit coupling.

[1] K. Bolotin et al., Phys. Rev. Lett. **97**, 127202 (2006)

TT 39.4 Fri 11:15 EB 202

Spin transport across double quantum dots and carbon nanotubes — •S. Koller, R. P. Hornberger, G. Begemann, A. Donarini, and M. Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

Spin polarized transport through nanostructures is a topic attracting increasing interest. Utilizing not only the charge, but also the electron's spin degree of freedom opens various potential applications in spintronics as well as in quantum computing. Among the promising candidates for future electronic devices are e.g. carbon nanotubes as well as semiconducting quantum dots. By employing the reduced density matrix technique, we have developed a quite general model for spin dependent transport across nanostructures weakly coupled to ferromagnetic electrodes with both collinear or non-collinear magnetization directions. The model can be applied e.g. to single or double quantum dots [1] as well as to carbon nanotubes. For the two latter systems, the low bias conductance as a function of gate voltage exhibits a characteristic repeating pattern of four peaks distinct in height, possessing certain mirror symmetries representing electron-hole-symmetries. For devices like spin valve transistors, the tunnelling magnetoresistance (TMR) is a decisive parameter. It is found that the TMR is heavily influenced by a Zeeman splitting of energy levels, which in fact is not only crucial for the occurence of negative TMR, but also found to break the electron hole-symmetries. Overmore, in the nonlinear bias regime, negative differential conductance arises for non-collinear polarizations.

[1] R. P. Hornberger et al., in preparation.

15 min. break

TT 39.5 Fri 11:45 EB 202

Adiabatic pumping through a quantum-dot spin valve — •Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[2] — [1]Département de Physique Théorique, Université de Genève, Switzerland — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Germany

We investigate the adiabatically pumped current through a quantum-dot spin-valve setup, consisting of a quantum dot coupled to two differently polarized ferromagnetic leads (F-dot-F). We therefore resort to a real-time diagrammatic technique in the adiabatic limit, taking into account the Coulomb interaction on the dot exactly. On one hand we investigate the influence of the lead polarizations and of the on-site Coulomb interaction on the pumped charge. On the other hand we are interested in the influence of the pump mechanism on the average dot polarization during a pumping cycle. In the case where only one lead is ferromagnetic and the other one is a normal metal (F-dot-N), we extend our analysis to spin pumping, where we are in particular interested in the ratio between pumped spin and pumped charge.

TT 39.6 Fri 12:00 EB 202

Electrically driven spin dynamics in disordered electron systems — •Mathias Duckheim and Daniel Loss — Department of physics, University of Basel, CH-4056 Basel, Switzerland

A key principle of many spintronics applications is the coherent control of spins at the nanometer scale using electric fields. However, with no direct electrical coupling to the spin available, indirect mechanisms are necessary to achieve this task.

In this talk we discuss the possibility of coherent spin control using electric-dipole-induced spin resonance[1-4](EDSR) and the magneto-electrocal effect[5]. We investigate the spin polarization and the associated spin-Hall current due to EDSR and study the disorder-induced broadening of the resonance due to the D'yakonov-Perel mechanism, which limits the efficiency of EDSR[3] drastically. We show[4] that these limitations can be partially circumvented by exploiting the interference of different spin-orbit interaction mechanisms and give a phenomenological description of the spin dynamics that recovers the diagrammatic linear response calculation for a weak electric field but extends to the non-equilibrium situation of strong driving.

[1] R. L. Bell, Phys. Rev. Lett. **9**, 52 (1962).
[2]Y. K. Kato and R. C. Myers and A. C. Gossard and D. D. Awschalom, Nature **427**, 50 (2004).
[3] M. Duckheim and D. Loss, Nature Phys. **2**, 195 (2006).
[4] M. Duckheim and D. Loss, Phys. Rev. B **75**, 201305(R) (2007).
[5] V. M. Edelstein, Solid State Comm. **73**, 233 (1990).

TT 39.7 Fri 12:15 EB 202

Photon-assisted spin transport in a two-dimensional electron gas: spin-polarized current and spin valve effect — •Mikhail Fistul[1] and Konstantin Efetov[1,2] — [1]Theoretische Physik III, Ruhr-Universität Bochum, Germany — [2]L. D. Landau Institute for Theoretical Physics, Moscow, Russia

We study spin-dependent transport in a two-dimensional electron gas subject to an external step-like potential $V(x)$ and irradiated by an electromagnetic field (EF). In the absence of EF the electronic spectrum splits into spin sub-bands originating from the "Rashba"spin-orbit coupling. We show that the resonant interaction of propagating electrons with the component EF parallel to the barrier induces a *non-equilibrium dynamic gap* ($2\Delta_R$) between the spin sub-bands. Existence of this gap results in coherent spin-flip processes that lead to a spin-polarized current and a large magnetoresistance, i.e the spin valve effect. These effects may be used for controlling spin transport in semiconducting nanostructures, e.g. spin transistors, spin-blockade devices etc. , by variation of the intensity S and frequency ω of the external radiation.

TT 39.8 Fri 12:30 EB 202

Transport through Inhomogeneous Magnetization Textures - Domain-Wall Resistance — •Christian Wickles and Wolfgang Belzig — Universität Konstanz, Fachbereich Physik, 78457 Konstanz, Germany

We microscopically derive a transport equation for the conduction electrons in ferromagnetic materials with inhomogeneous magnetisation profiles featuring spin-flip scattering at magnetic impurities. In the diffusive limit, we calculate the conductance through a domain-wall and find that the domain-wall resistance can be positive or negative. In the limit of long walls we find analytical expressions which differ from previous works, which used less general models or different theoretical frameworks.

TT 39.9 Fri 12:45 EB 202

Extracting current-induced spins: spin boundary conditions at narrow Hall contacts — •Matthias Scheid[1], Inanc Adagideli[1], Michael Wimmer[1], Gerrit E. W. Bauer[2], and Klaus Richter[1] — [1]Universität Regensburg, Institut für theoretische Physik, 93040 Regensburg, Germany — [2]Kavli Institute of Nanoscience, TU Delft, Lorentzweg 1, 2628 Delft, The Netherlands

We consider the possibility to extract spins that are generated by an electric current in a disordered two-dimensional electron gas with Rashba/Dresselhaus spin orbit interaction (R2DEG) in the Hall geometry. In that respect we discuss boundary conditions for the spin accumulations between a spin orbit (SO) coupled region and a contact without SO coupling, i.e. a normal two-dimensional electron gas (2DEG). We demonstrate that in contrast to contacts that extend along the whole sample, a spin accumulation can diffuse into the normal region through finite contacts and be detected by e.g. ferromagnets. For an impedance-matched narrow contact the spin accumulation in the 2DEG is equal to the current induced spin accumulation in the bulk of R2DEG up to a geometry-dependent numerical factor.

[1] I. Adagideli, M. Scheid, M. Wimmer, G.E.W. Bauer, and K. Richter, New J. Phys. **9**, 382