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 **q** which agrees well with the experimental values of **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 **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 $Sr_{14}Cu_{24-x}Zn_xO_{41}$ ($0 \leq x \leq 0.75$) 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.