TT 44: Poster Session Correlated Electrons

Time: Thursday 10:00–13:00 Location: P1

TT 44.1 Thu 10:00 P1

NRG calculations of the magnetization of Kondo impurities in an external field — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, D-33615 Bielefeld, Germany

The deposition of magnetic molecules on suitable substrates represents one possibility to solve the problem of addressing individual molecules so that they might be used for information storage or quantum computing purposes. However, the magnetic properties of the molecules, which for example determine the dependence of magnetization on temperature and applied field and which are crucial for such applications, will in general be influenced by the interaction with the substrate. The goal of our ongoing investigations is to better understand the form and extent of this effect.

In an attempt to theoretically approach the problem, we study single-impurity Kondo models in an external magnetic field whose impurity consists of several exchange-coupled spins and is supposed to represent a magnetic molecule. We then focus on the impurity magnetization and compare the behavior of the free and deposited molecule (the impurity) for each model.

In order to obtain reliable approximations for the thermodynamic limit of interest, i.e. the infinitely extended substrate, we carry out the calculations using Wilson's Numerical Renormalization Group (NRG). NRG is by now a well established method and has been significantly improved in the last five years. As an additional benefit, it allows us to study the impurity magnetization both as function of temperature and magnetic field.

TT 44.2 Thu 10:00 P1

Real-space Kondo correlations — •Michael Becker, Andrew Mitchell, and Ralf Bulla — Universität zu Köln

We investigate real-space Kondo correlations in various impurity models. Any physical quantity in real space can be calculated from purely local impurity correlators. In the simplest (but most revealing) example of the Anderson model, the density variation around the impurity is related to the impurity Green function, which we calculate accurately via the numerical renormalization group technique. Signatures of the 'free orbital', 'local moment' and 'strong coupling' fixed points are evident in real space, with characteristic length scales R_{FO} and R_{LM} being associated with each at $T = 0$. The 'local moment cloud' is an exponentially extended object with $R_{LM} \sim 1/T_K$; Kondo screening itself occurring for $r \gg R_{LM}$. As the temperature is increased, the Kondo effect is destroyed, as manifest in real space by the divergence of R_{LM}, implying that the uncompensated moment due to the impurity becomes infinitely extended. The familiar RG picture known for other classic models is similarly apparent in real space. In particular, the phase transition in the pseudogap Anderson model (realised here for an impurity in graphene) is associated with a diverging length scale; and the existence of both 'local moment' and 'overscreening' clouds are demonstrated in the two-channel Kondo model.

TT 44.3 Thu 10:00 P1

Coupled Spins in a Dissipative Environment — •Etienne Gärtner, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zülpicherstr. 77 50937 Cologne, Germany

One of the fascinating consequences of quantum mechanics is that different coupled subsystems can become entangled. A classic example is a quantum impurity coupled to a dissipative environment (the standard spin-boson model). Here we consider the natural extension of this scenario, studying the entanglement generated between two impurities which are coupled to a common bosonic bath. This two-spin-boson model is analysed in detail using the bosonic numerical renormalization group (NRG) technique, with the Von Neumann entropies and phase diagram extracted directly. Recently the question has been posed as to whether a common bath could also generate entanglement between spatially separated spins. To address the question of the lenghtscale for such entanglement, we couple the spins to 1 or 2 dimensional bosonic host lattices, and calculate the dependence of physical properties on impurity separation. To this end, we extend the bosonic NRG to deal with the two-bath effective model that results.

TT 44.4 Thu 10:00 P1

Kondo physics with variational matrix-product states — •Andrej Schwabe and Michael Potthoff — I. Institut Theoretische Physik, Universität Hamburg, Hamburg, Deutschland

The screening of an impurity spin by conduction band electrons, known as the Kondo effect, is a typical many-particle phenomenon which still raises basic questions. We apply our variational matrix-product states code (VMPS [1,2]) which is based on the implementation of the corrected one-site algorithm [3] and exploits $U(1)$ symmetries. We present calculations for an impurity coupled locally to a finite, but long uncorrelated nano chain as well as calculations for an inhomogeneous two-leg Hubbard-type model with site and leg dependent Hubbard-U.
Our study focuses on the spin correlation functions, which show the emergence of the Kondo screening cloud, and comprises the investigation of its dependence on the position of the impurity, the Kondo coupling, and the length of the chain. The results are compared to previous studies [4,5]. We discuss the interference of the Kondo clouds of several impurities coupled to the chain, and the competition with the magnetic exchange coupling between the impurities (RKKY).
[1] U. Schollwoeck, arXiv:1008.3477v1 (2010)
[2] F. Verstraete et al., Advances in Phys. **57**, 143 (2008)
[3] S. R. White, Phys. Rev. B **72**, 180403 (2005)
[4] T. Hand et al., Phys. Rev. Lett. **97**, 136604 (2006)
[5] A. Holzner et al., Phys. Rev. B **80**, 205114 (2009)

TT 44.5 Thu 10:00 P1

Kondo effect in single wall carbon nanotubes with ferromagnetic contacts — Markus Gaass[1], •Daniel Steininger[1], Andreas K. Hüttel[1], Kicheon Kang[1,3], Ireneusz Weymann[2,4], Jan von Delft[2], and Christoph Strunk[1] — [1]Universität Regensburg, Germany — [2]Ludwig-Maximilians-Universität München, Germany — [3]Chonnam National University, Gwangju 500-757, Korea — [4]Adam Mickiewicz University, 61-614 Poznań, Poland

We investigate the influence of ferromagnetic contacts on the Kondo effect in quantum dots formed in SWCNTs. For this purpose we use $Pd_{0.3}Ni_{0.7}$, a ferromagnetic alloy known for providing sufficiently transparent interfaces to CNTs [1,2]. Transport spectroscopy shows a conductance anomaly around zero bias in every second Coulomb diamond. The ferromagnetic contacts cause two peaks at finite bias which can be rejoined by a finite magnetic field. The size and sign of the splitting as well as its dependence on gate voltage can be explained by spin-dependent renormalization processes of the quantum dot level that include two contributions. One, independent of gate voltage, arises from the macroscopic magnetization of the leads. The other contribution, showing a gate dependence, stems from the polarization of the spins at the Fermi energy. The data are compared to numerical renormalization group calculations. In addition, we observe a fine structure in the spectra indicating a complex level structure which may result from curvature-induced spin-orbit interaction.
[1] J.R. Hauptmann, et al., Nature Phys. **4**, 373 (2008)
[2] L. Hofstetter, et al., Phys. Rev. Lett. **104**, 246804 (2010)

TT 44.6 Thu 10:00 P1

Superconductivity in the Kondo lattice model — •Oliver Bodensiek[1], Rok Žitko[1,2], and Thomas Pruschke[1] — [1]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

We study the Kondo lattice model with an additional attractive interaction among the conduction-band electrons by means of dynamical mean-field theory in combination with the numerical renormalization group method. In the normal phase we observe a strong dependency of the low-energy scale on the attractive interaction. Thus, there exists a delicate interplay between the attractive interaction and the antiferromagnetic Kondo exchange, which results in a critical interaction, above of which the Fermi surface collapses because the spins become effectively decoupled from the conduction electrons. Additionally, we allow for a s-wave superconducting phase, which appears to be split at the point of the underlying Fermi surface collapse. We discuss the interplay between attractive interaction an Kondo exchange and its pertinence to phonons in heavy fermion physics.

TT 44.7 Thu 10:00 P1

Magnetic phase transitions in CePdAl — •S. Woitschach[1], O. Stockert[1], V. Fritsch[2], N. Bagrets[2], H. v. Löhneysen[2], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

The heavy fermion system CePdAl in its hexagonal modification shows antiferromagnetic order below $T_N = 2.7$ K and is located close to quantum criticality. By applying hydrostatic pressure or by concentration tuning via alloying Ni on the Pd site, T_N decreases continuously and finally a quantum critical point is approached. In this system geometrical frustration is present, as inferred from neutron scattering, and might play a role in tuning the groundstate. Several magnetically ordered phases have been observed in CePdAl, but so far no detailed measurements of the B-T phase diagram and the magnetic anisotropy have been performed. Here, we report on measurements of the heat capacity of a Czochralski-grown CePdAl single crystal to determine the B-T phase diagram. Especially we focus on the anisotropy for magnetic fields applied along the c-axis or in the basal plane.

TT 44.8 Thu 10:00 P1

Investigating the large degeneracy Kondo lattice metamagnet CeTiGe: Crystal growth and doping studies — •T. Gruner[1], N. Caroca-Canales[1], J. Sereni[2], M. Deppe[1], and C. Geibel[1] — [1]MPI für Chemische Physik fester Stoffe, 01187, Dresden, Germany — [2]Centro Atomico Bariloche, 8400, S. C. de Bariloche, Argentina

CeTiGe is a paramagnetic Kondo lattice system with a large orbital degeneracy involved in the formation of the heavy Fermion ground state. Recently we discovered that this compound presents a huge metamagnetic transition at $B_{\mathrm{MMT}} \approx 13\,\mathrm{T}$, with much larger anomalies in magnetization, magnetoresistance and magnetostriction than in the archetypical Kondo lattice metamagnet $CeRu_2Si_2$. Since CeTiGe forms in a pronounced peritectic reaction the growth of single crystals is difficult. We therefore studied the Ce-Ti-Ge ternary metallographic phase diagram to get a sound basis for future crystal growth attempts. Preliminary results of growth experiments based on these studies are promising and shall be discussed. Furthermore, Ti-rich CeTiGe was recently reported to present a high temperature phase crystallizing in the closely related CeScSi structure type. In order to study this structural instability and the effect on the physical properties, we studied the effect of substituting Sc for Ti, since pure CeScGe crystallizes in the CeScSi structure type. In well annealed samples we observed a two phase region in the range 10 % - 25 %-Sc-substitution. Preliminary investigations of the $CeSc_xTi_{1-x}Ge$ alloy suggest it is a promising candidate for the observation of a ferromagnetic quantum critical point in a large degeneracy Kondo lattice system.

TT 44.9 Thu 10:00 P1

CeCo(As/P)O pnictides: complex interplay of 4f and 3d magnetism as seen from NMR (^{31}P, ^{59}Co and ^{75}As). — •Michael Baenitz[1], Rajib Sarkar[1], Eva Brüning[1], Asok Poddar[2], Chandan Majumdar[2], Anton Jesche[1], Cornelius Krellner[1], Cristoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]ECMP Division, Saha Institute of Nuclear Physics, Kolkata, India

The coupling of the magnetic sub-systems of Co-3d and Ce-4f ions in the compounds CeCoAsO and CeCoPO is studied by using the local NMR probe. The magnetic order in such 3d-4f systems is rather complex depending on the inter-3d, inter-4f ion exchange coupling and the intra 3d-4f - ion coupling (polarization). Sometimes two separated transitions could be found (for example CeFeAsO). For CeCo(P/As)O only a single ferromagnetic transition is found at about 75 K [1, 2]. Here CeCoPO is of special interest because strong correlations (Kondo interaction) became evident at low temperatures [2]. Furthermore, recent low field magnetization results indicate a more complex type of magnetic order. One scenario is a crossover from a canted or antiferromagnetic type at low fields to a field polarized ferromagnetic type of order at higher fields.

[1] Phys. Rev. B 82, 054423 (2010)
[2] Physica B, 404 (2009) 3206.

TT 44.10 Thu 10:00 P1

Magnetic properties of CeTPO (T = Co,Ru,Os) phosphides studied by muon spin relaxation — •Johannes Spehling[1], Cornelius Krellner[2], Hubertus Luetkens[3], Til Dellmann[1], Anton Jesche[2], Christoph Geibel[2], and Hans-Henning Klauss[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232, Villingen, Switzerland — [3]Max-Planck-Institut für Chemische Physik fester Stoffe Dresden

We have investigated the magnetic ground state properties in the pnictide systems CeTPO with T = Co,Ru,Os by means of zero field (ZF) and weak transverse field muon spin relaxation (muSR). For CeCoPO, magnetic order of the Co-3d moments below 75 K is found as evidenced by the observation of a spontaneous muon spin precession frequency. A second muon frequency below 45 K suggests a spin reorientation transition. No clear indication for Ce-4f magnetic ordering is found. In contrast, for CeRuPO and CeOsPO ZF-muSR shows Ce-4f magnetic order below 15 K and 4.5 K, respectively. Here, no magnetic order of the d electronic moments is observed. This is consistent with macroscopic results [1-3]. For all systems, the temperature dependence of the magnetic order parameter (muon precession frequency) suggests a peculiar interplay between the transition metal d and rare earth Ce-4f electronic subsystems.

[1] Phys. Rev. B 76, 104418 (2007)
[2] Phys. Rev. Lett. 100, 066401 (2008)
[3] Physica B 404, 3206 (2009).

TT 44.11 Thu 10:00 P1

^{27}Al NMR/NQR study on $R\mathrm{Ru_2Al_{10}}$ (R: La, Ce) and $R\mathrm{Fe_2Al_{10}}$ (R: Y, Yb). — •Panchanana Khuntia[1], Michael Baenitz[1], Rajib Sarkar[1], André Strydom[2], and Frank Steglich[1] — [1]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Physics Department APK, University of Johannesburg, P.O. Box 524, Auckland Park 2006, South Africa

Ternary orthorhombic aluminides of $R\mathrm{T_2Al_{10}}$ type (R:Ce, Yb, T: Fe, Ru, Os) are currently attracting much interest because of a number of exotic properties such as anomalously high magnetic ordering temperatures in $CeRu_2Al_{10}$ [1] and $CeOs_2Al_{10}$, and strongly hybridized Kondo insulating state in $CeFe_2Al_{10}$. The Fe-Al systems are of special interest because YFe_2Al_{10} is claimed being located close to a Fe-based ferromagnetic instability at very low temperature [2]. Here pronounced non Fermi liquid (NFL) phenomena are observed. For $YbRh_2Si_2$ this NFL behaviour is associated to strong ferromagnetic fluctuations (see ^{29}Si NMR in [3]). Our spin relaxation study on YFe_2Al_{10} gives strong evidence for Fe based ferromagnetic fluctuations evolving towards low temperature in small fields. $YbFe_2Al_{10}$ is a weak Kondo coupled heavy fermion system where no traces of Fe-magnetism could be found [2].

[1] Physica B, 404(2009)2981
[2] Phys. Stat. Solidi 4, No. 12, 356-358(2010)
[3] PRL 89, 107202(2010)

TT 44.12 Thu 10:00 P1

Exotic Heavy-Fermion Behaviour of the Filled Skutterudite $SmPt_4Ge_{12}$ — •Roman Gumeniuk[1], Walter Schnelle[1], Michael Nicklas[1], Helge Rosner[1], Michael Schöneich[2], and Andreas Leithe-Jasper[1] — [1]MPI Chemische Physik fester Stoffe, Dresden — [2]Anorganische Chemie, TU Dresden

Samarium-filled platinum-germanium skutterudite $SmPt_4Ge_{12}$ was prepared at high pressure and temperature (5.0 GPa, 1070 K). The compound is isotypic with $LaFe_4P_{12}$ (cubic, space group $Im\bar{3}$, a = 8.6069(4) Å). X-ray absorption spectroscopy measurements show that samarium in $SmPt_4Ge_{12}$ has a temperature-independent intermediate valence ($\nu = 2.90 \pm 0.03$). Van-Vleck paramagnetism is observed above ∼50 K. The low-temperature specific heat displays a broad anomaly around at 2.9 K and a large linear coefficient $\gamma' = 450\ \mathrm{mJ\,mol^{-1}K^{-2}}$ suggesting heavy-fermion behaviour. Electrical resistivity shows a temperature dependence reminiscent of the Kondo effect. Density functional calculations result in an electronic structure that is, apart from the Sm $4f$ contributions, very similar to $LaPt_4Ge_{12}$.

TT 44.13 Thu 10:00 P1

Tuning the magnetism in $YbRh_2Si_2$ via isoelectronic transition metal (Co, Ir) substitutions: a ^{59}Co- and ^{29}Si-NMR study — •Michael Baenitz, Cornelius Krellner, Panchanana Khuntia, Christoph Geibel, and Frank Steglich — Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

$YbRh_2Si_2$ is unique among heavy fermion systems because of its proximity to a quantum critical point (QCP) in the Doniach-type phase diagram. Pronounced non-Fermi-liquid (NFL) behavior was observed. ESR as well as the ^{29}Si-NMR spin-lattice relaxation (SLR) gave strong evidence that the NFL behavior is closely related to the presence of strong ferromagnetic fluctuations competing with antiferromagnetic ones [1,2]. Here we present a ^{59}Co- and ^{29}Si-NMR study on the

$x = 0, 0.07, 0.12$ and 1 samples of the $Yb(Rh_{1-x}Co_x)_2Si_2$ alloy together with ^{29}Si-NMR results on the pure $YbIr_2Si_2$.The isoelectronic substitution of the smaller Co ion on the Rh site promotes the AF order whereas the substitution of the larger Ir ion strengthen the Kondo interaction. As a consequence the SLRs $^{29}(1/T_1)$ as well as the spin-spin relaxation rates $^{29}(1/T_2)$ are damped for the $YbIr_2Si_2$ system, which allows to study the ^{29}Si-NMR in great detail up to room temperature.

[1] Phys. Rev. Lett. 91, 156401 (2003)
[2] Phys. Rev. Lett. 89, 1072021 (2002)

TT 44.14 Thu 10:00 P1

Magnetism and valence fluctuations in $Eu(Rh_{1-x}Ir_x)_2Si_2$ single crystals — •Silvia Seiro and Christoph Geibel — MPI-CPfS, Nöthnitzer Strasse 40, 01187 Dresden, Germany

Valence instabilities and intermediate valence in rare earth intermetallics RT_2Si_2, R being a rare earth element with instable 4f-shell like Ce, Eu and Yb, and T a transition metal, have been focus of research for the last three decades. In particular, much attention has been drawn by the suppression of the magnetic order of the localized f moments and the associated transition from a small to a large Fermi surface, which can be induced in Ce and Yb compounds by varying some external parameter such as pressure, composition or magnetic field. Due to the unavailability of high quality single crystals, however, the properties of homologue Eu compounds remain comparatively unexplored. We report the synthesis of $Eu(Rh_{1-x}Ir_x)_2Si_2$ single crystals and their physical properties as they evolve from divalent Eu antiferromagnetism for $x = 0$ to intermediate valence behavior for $x = 1$.

TT 44.15 Thu 10:00 P1

Magnetic excitations in $YbCo_2Si_2$ — •O. Stockert[1], A. Haase[1], K. Schmalzl[2], C. Krellner[1], N. Mufti[1], and C. Geibel[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France

Quantum phase transitions and their origin are still open issues of current research in condensed matter physics. Although $YbRh_2Si_2$ is a model system to study quantum criticality, microscopic studies by neutron scattering are prevented because of the large absorption of Rh for neutrons, the small ordered moment and the small available samples. Instead, we investigated $YbCo_2Si_2$ being isoelectronic and isostructural to $YbRh_2Si_2$. $YbCo_2Si_2$ orders antiferromagnetically below $T_N \approx 1.7$ K in an incommensurate structure and changes to a commensurate structure below $T_L \approx 0.9$ K. Using inelastic neutron scattering we studied in detail the spin excitations in the low temperature commensurate phase. Well-defined spin excitations exhibiting distinct dispersion have been detected. The results contribute to the general understanding of the magnetic interactions in $YbCo_2Si_2$.

TT 44.16 Thu 10:00 P1

Phase diagram of $CePt_3B_{1-x}Si_x$ — •Daniela Rauch[1], Matthias Bleckmann[1], Stefan Süllow[1], Moo Sung Kim[2], Meigan Aronson[2,3], and Ernst Bauer[4] — [1]TU Braunschweig, Institute for Physics of Condensed Matter, Braunschweig, Germany — [2]Brookhaven National Laboratory, Condensed Matter Physics and Materials Science Department, New York, USA — [3]Stony Brook University, Department of Physics and Astronomy, New York, USA — [4]TU Vienna, Institute of Solid State Physics, Vienna, Austria

The non-centro symmetric system $CePt_3Si$ shows an unconventional heavy-fermion superconducting ground state ($T_c = 0.75$ K), in coexistence with an antiferromagnetic phase below $T_N = 2.2$ K. In contrast, $CePt_3B$ exhibits a complex magnetically ordered state at low temperatures, with an antiferromagnetic phase below $T_N = 8$ K and a second weakly ferromagnetic transition below $T_C \approx 5$ K.

Here we report a study of the magnetic phase diagram of the alloying series $CePt_3B_{1-x}Si_x$. From our investigation we find the antiferromagnetism of $CePt_3B$ to transform into the analagous phase of $CePt_3Si$. In contrast, we observe a supression of the ferromagnetically ordered phase above a critical Si concentration $x_c \approx 0.5$. We discuss the relationship of superconductivity and magnetism of the alloying series.

TT 44.17 Thu 10:00 P1

Exotic field induced phases in UPt_2Si_2 — •D. Schulze Grachtrup[1], M. Bleckmann[1], B. Willenberg[1], H. Rakoto[2], I. Sheikin[3], Y. Skourski[4], M. Bartkowiak[4], J.A. Mydosh[5], and S. Süllow[1] — [1]IPKM, TU Braunschweig, Germany — [2]LNCMI, Toulouse, France — [3]LNCMI, Grenoble, France — [4]HLD, Dresden, Germany — [5]LION, Leiden University, Netherlands

Tetragonal UPt_2Si_2 has been characterized as a moderately mass enhanced antiferromagnetic compound ($T_N = 32$ K), which in low magnetic fields resembles other materials such as URu_2Si_2 [1-3]. Here,we present an extensive study of resistivity and magnetization of single crystalline UPt_2Si_2 in high magnetic fields up to 50 T. Initially we find the phase transition at $T_N = 32$ K in zero field to shift down to lower temperatures with increasing field for both crystallographic axes. Below $\sim$ 15 K and for $B//a$ we see this transition to split up and become hysteretic, forming a new and distinct high field phase between $\sim$38T and $\sim$45T. Similarly, with $B//c$ we also find a splitting resulting in a new high field phase between $\sim$24 T and $\sim$31 T. Moreover, below 5K our measurements along the c axis show even more structure, indicating at least one more high field phase between $\sim$29 T and $\sim$33 T. Altogether, our data reveal a rich magnetic high field phase diagram, which resembles some observations made for URu_2Si_2 [4].

[1] S. Süllow *et al.*, J. Phys. Soc. Jpn. **77** (2008) 024708
[2] N. Johannsen *et al.*, Phys. Rev. B **78** (2008) 121103(R)
[3] R. A. Steeman *et al.*, J. Phys.: Condens. Matter **2** (1990) 4059
[4] K. H. Kim *et al.*, Phys. Rev. Lett. **91** (2003) 256401

TT 44.18 Thu 10:00 P1

Dynamics of the Periodic Anderson Model: exhaustion effects and the interplay of scales — •Lucas Hollender, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zülpicherstr. 77 50937 Cologne, Germany

We are investigating the paramagnetic periodic Anderson model within the framework of dynamical mean field theory, using Wilson's numerical renormalization group approach to obtain the self energy of the effective impurity model. We examine the exhaustion scenario where the conduction band is progressively emptied. Here our main interest lies in the existence of the Kondo scale and its connection to the coherence scale. We also consider a bipartite system (with two sublattices comprising inequivalent impurity sites), and study the interplay of Kondo and lattice coherence scales. Furthermore we increase the distance of the impurities to simulate dilute impurity systems, trying to find the crossover from the lattice system to the dilute impurity system.

TT 44.19 Thu 10:00 P1

Quantum Phase Transition between Semimetal and Superfluid in a Dirac Cone Model — •Benjamin Obert[1], Philipp Strack[1], So Takei[2] und Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart Germany — [2]University of Maryland, USA

We analyse a two-dimensional Dirac cone model which undergoes a quantum phase transition between a semimetal and a superfluid. We compute fluctuation effects by using flow equations derived within the functional renormalization group (fRG) framework [1]. Near the quantum critical point (QCP) fluctuations lead to non Fermi liquid behaviour. The superfluid correlation length is infinite not only at the quantum critical point, but everywhere in the semimetallic phase.

[1] P. Strack, S. Takei, W. Metzner, Phys. Rev. B **81**, 125103 (2010)

TT 44.20 Thu 10:00 P1

Quantum critical dynamics in the one-dimensional spin chain systems CuPzN and $(phzH)_2CuCl_4$ — •H. Kühne[1,3], M. Günther[1], H.-H. Klauss[1], A.A. Zvyagin[2], J. Litterst[3], S. Grossjohann[4], W. Brenig[4], A.P. Reyes[5], P.L. Kuhns[5], C.P. Landee[6], and M.M. Turnbull[6] — [1]IFP,TU Dresden — [2]ILTPE,Kharkov,Ukraine — [3]IPKM,TU Braunschweig — [4]IThP,TU Braunschweig — [5]NHMFL,Tallahassee,USA — [6]DoP,Worcester,USA

We present a comprehensive NMR study of the field-driven quantum phase transitions in the spin=1/2 chain systems CuPzN and $(phzH)_2CuCl_4$. The static and dynamic experimental NMR properties are compared with both quantum Monte Carlo calculations and Luttinger liquid theory. CuPzN is known to be one of the best realizations of the antiferromagnetic S=1/2 Heisenberg chain (AFHC) model with a low coupling constant J. The zero temperature saturation field B_c = 14.6 T corresponds to a quantum critical point, where the system is driven from a Luttinger liquid state to ferromagnetic polarization. In the vicinity of this point in the corresponding B- and T- parameter space, a divergent behavior of the nuclear ^{1}3C-spin-lattice relaxation rate is observed and in good agreement with theory. $(phzH)_2CuCl_4$

is a recently synthesized spin chain system. ^{1}H- and ^{3}5Cl-NMR experiments yield a field- and temperature dependent behavior of $1/T_1$ similar to that of CuPzN. But, in contrast, a pronounced second maximum is observed at about 3/4 of the saturation field $B_c = 12.2$ T. This effect is not found in the local or macroscopic magnetization, suggesting a more complicated magnetic interaction scheme.

TT 44.21 Thu 10:00 P1

Accurate Determination of the Gauss-Transition in the Anisotropic Spin-One Chain — •Shijie Hu[1,2], Bruce Normand[2], and Xiaoqun Wang[2] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Department of Physics, Renmin University of China

We have investigated ground-state properties and thermodynamic properties of the uniaxial anisotropic spin-one Heisenberg chain using the density matrix renormalization group method and the transfer matrix renormalization group method. We found that the gap depending on D around the Ising critical point $D_{c1} = -0.3145(1)$ is well described by a linear function. By contrast, the critical point $D_{c2} = 0.9684(2)$ cannot easily be obtained by any physical quantities except for the entanglement entropy. Simultaneously x-axis string order parameter which is used to define the Haldane phase with an incomplete $Z_2 \times Z_2$ symmetry and the scaling behavior of the spin susceptibility at low temperature are also exhibited.

TT 44.22 Thu 10:00 P1

Relation between crystal structure, magnetism and electronic properties in layered ruthenates — •Johanna Brand[1], Anna Silex[1], Karsten Binder[1], Yvan Sidis[2], Arsen Gukasov[2], Beatrice Gillon[2], Satoru Nakatsuji[3], Naoki Kikugawa[4], Andrew Mackenzie[4], Fumihiko Nakamura[5], and Markus Braden[1] — [1]II. Physik, Uni Köln — [2]LLB, Saclay — [3]ISSP, Tokio — [4]Univ. of St. Andrews — [5]ADSM, Hiroshima

Layered ruthenates exhibit a close coupling between crystal structure and magnetic and electronic properties, which strengthens the interest in these materials arising from the superconductivity in Sr_2RuO_4 and Ca_2RuO_4. By substituting Sr through isovalent Ca in Ca_2RuO_4 one tunes the system from the superconductor into a highly anomalous metal with heavy-fermion like properties and finally into an antiferromagnetic Mott insulator. The MIT in Ca_2RuO_4 can not only be induced by Sr-doping, heating and pressure but also by the application of an electric field. A part of the sample transforms into the metallic phase under the application of moderate electric fields, this phase is characterized by a longer c-lattice parameter and it can be cooled far below room temperature when a finite current density is maintained. At low temperature there is coexistence of the metallic phase and the insulating phase. Doping $Ca_3Ru_2O_7$ with Ti significantly stabilizes a weakly non-metallic phase as seen both in the transition temperature and in the resistivity jump. This effect is especially prominent at a substitution of 10

TT 44.23 Thu 10:00 P1

Low-frequency optics on $Sr_{1-x}Ca_xRuO_3$ — •Diana Geiger[1], Marc Scheffler[1], Martin Dressel[1], Melanie Schneider[2], and Philipp Gegenwart[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

The pseudo-cubic perovskite ruthenates $SrRuO_3$ and $CaRuO_3$ have attracted interest due to their unconventional electronic properties. For both materials, non-Fermi liquid behavior has been reported in previous optical studies. In addition to these compounds, the doping series $Sr_{1-x}Ca_xRuO_3$ offers a rich phase diagram: going from the itinerant ferromagnet $SrRuO_3$ to the paramagnet $CaRuO_3$, a quantum phase transition is expected at $x \approx 0.8$.

Using different approaches of optical spectroscopy, we studied thin-film samples of the $Sr_{1-x}Ca_xRuO_3$ system, which were prepared by metalorganic aerosol deposition. In order to be sensitive to the low energy scales expected close to the quantum phase transition, we address the THz and GHz frequency ranges at temperatures down to 2K. We present optical data, in particular the frequency-dependent conductivity, and discuss it in the framework of the extended Drude model and possible non-Fermi liquid behavior.

TT 44.24 Thu 10:00 P1

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

The series $Sr_{1-x}Ca_xRuO_3$ shows a continuous evolution from itinerant electron ferromagnetism with $T_C \approx 160$ K (x = 0) towards a paramagnetic metallic state at x = 1. For thin films, which have been grown epitaxially on $SrTiO_3$ and $NdGaO_3$ substrates by metalorganic aerosol deposition technique, we present electrical transport measurements extended to mK temperatures and in applied magnetic fields. We also investigated nonlinear transport at high current densities in the non-Fermi liquid regime for microstructured thin films. Work supported by DFG through SFB 602, TP A19."

TT 44.25 Thu 10:00 P1

Quantum criticality in $Sr_3Ru_2O_7$ studied by measurements of the magnetocaloric effect — •Manuel Mchalwat[1], Yoshi Tokiwa[1], R.S. Perry[2,3], Y. Maeno[3], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Scottish Universities Physics Alliance, School of Physics, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, Scotland — [3]International Innovation Center and Department of Physics, Kyoto University, Kyoto 606-8501, Japan

The tetragonal ruthenate $Sr_3Ru_2O_7$ displays itinerant electron metamagnetism and the formation of a novel phase close to a presumed quantum critical point (QCP). Here, we address quantum criticality by measurements of the adiabatic magnetocaloric effect, determined using an alternating field method. Our results indicate universal scaling behavior over several decades in temperature over magnetic field in agreement with the predictions of the Hertz-Millis scenario for an itinerant two-dimensional metamagnetic ($z = 3$) QCP.

Work supported by the DFG through SFB 602 and research unit 960 (Quantum phase transitions).

TT 44.26 Thu 10:00 P1

Low-temperature electrical resistivity of $Yb(Rh_{0.95}Fe_{0.05})_2Si_2$ — •Maik Schubert, H.S. Jeevan, Yoshi Tokiwa, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

We report measurements of the electrical resistivity $\rho(T, B)$ on a single crystal of $Yb(Rh_{0.95}Fe_{0.05})_2Si_2$ at temperatures down to 15 mK and in magnetic fields up to 2 T. The Fe-doping has a threefold effect: (i) an increase of the residual resistivity similar as found for respective Co or Ir doping, (ii) a decrease of the Kondo temperature due to the chemical pressure effect, like it has been found for the respective Co doping, and (iii) a slight shift of the Fermi energy corresponding to the doping of 0.1 holes per unit cell. This latter effect suppresses the antiferromagnetic ordering despite the expected increase of T_N due to chemical pressure. Furthermore, we observe a moderate shift of the energy scale $T^*(B)$ with $B^*(T \to 0) = 0.03$ T. At lowest temperatures, the electrical resistivity follows Fermi liquid behavior $\Delta\rho = A(B)T^2$ both above and below 0.03 T with a divergence of the coefficient A upon approaching the critical field from both sides.

Work supported by the DFG through SFB 602 and research unit 960 (Quantum phase transitions).

TT 44.27 Thu 10:00 P1

Structural and magnetic transitions in YbPd — •Stefanie Grünheit[1], Hirale S. Jeevan[1], Devashibhai T. Adroja[2], Yoshifumi Tokiwa[1], Christian Stingl[1], Aziz Daoud-Aladine[2], and Philipp Gegenwart[1] — [1]1. Physikalisches Institut, Georg-August-Universität Göttingen — [2]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OXII, 0QX, United Kingdom

The cubic YbPd is a unique strongly-correlated electron system which shows structural and magnetic transitions upon cooling to low temperatures [1]. However, the nature of the magnetic and the atomic structure at low T has not been solved yet. We synthesized YbPd polycrystals and investigated their physical properties by electrical resistivity, magnetic susceptibility, specific heat and thermal expansion measurements. Furthermore, neutron scattering experiments were performed down to 20 mK in order to obtain microscopic information on the different phase transitions. At low temperatures, the Sommerfeld coefficient of YbPd is of the order of 200 mJ/(mol K^2) suggesting that YbPd is a moderately heavy fermion system. A reduced entropy of about one quarter of $R \log 2$ at 1.9 K is found. Remarkably this value is consistent with a structure with only half of the Yb-Ions contributing to the magnetic entropy.

Work supported by DFG through research unit 960 (Quantum phase

transitions).
[1] P. Bonville et al., Phys. Rev. Lett. 57 (1986) 2733.

TT 44.28 Thu 10:00 P1

^{31} P NMR study on $Eu(Ni_{1-x}Fe_x)_2P_2$: from valence fluctuations to ferromagnetic order — •Michael Baenitz[1], Ramesh Nath[2], Rajib Sarkar[1], Hirale Jeevan[3], Philipp Gegenwart[3], Zarkir Hossain[4], Nubia Caroca-Canales[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI-CPfS , 01187 Dresden, Germany. — [2]IISER-TVM, Trivandrum-695016, India. — [3]1. Phys. Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany. — [4]Dept. of Physics, Indian Institute of Technology, Kanpur 208016 India.

Among unstable f shell sytems the magnetic phase diagram of Eu systems differs from that of Ce, Yb or U systems. In contrast to these systems the Eu valence mostly could not be tuned (by substitutions or external pressure) continuously between the magnetic ($Eu^{+2}, J = 7/2$) and the non magnetic ($Eu^{+3}, J = 0$) state. Instead of that, first order valence transitions (like in $EuNi_2(Si/Ge)_2$) or an unstable, fluctuating valence (VF) at high temperatures (like in $EuCu_2Si_2$) are rather common. For $EuCu_2Si_2$ we have shown that upon Ge substitution the VF are suppressed and a small Kondo regime exist in the phase diagram before entering the antiferromagnetic ordered state on the Ge rich side. For the valence fluctuator $EuNi_2P_2$ the question arises whether a Kondo regime exists upon Fe substitution. In contrast to the $EuCu_2(Si/Ge)_2$ series the end point of the study here, $EuFe_2P_2$, is ferromagnetically ordered. This brings up the question of competition and/or coexistence of ferromagnetic and Kondo type of interactions in this new series. ^{31} P NMR measurements are carried out on $Eu(Ni_{1-x}Fe_x)_2P_2$ samples with $x = 0, 0.15, 0.5$ and 1.

TT 44.29 Thu 10:00 P1

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

The tetragonal organic system $NiCl_2$-4SC$(NH_2)_2$ (known as DTN) is a quantum paramagnet where the Ni atoms form $S = 1$ dimers which are weakly coupled along the crystallographic c axis. The Ni^{2+} single ion anisotropy $D = 8.9$ K opens an energy gap between the $S_z = 0$ ground state and the $S_z = \pm 1$ first excited state. When a magnetic field H is applied along c, it closes the gap and induces a transition into an XY-antiferromagnetic ordered state at low temperatures. For $T = 0$ the critical field $Hc_1 \approx 2$ T. Such a quantum critical point belongs to the $d = 3$ and $z = 2$ universality class and the following theoretical laws are predicted: The magnetization $M \propto T^{d/z}$, the phase boundary line $(H - Hc_1) \propto T_c^{d/z}$, the thermal and magnetic Grüneisen ratios, Γ and Γ_H, are expected to follow T^{-1}. We present measurements of the magnetization, specific heat and thermal expansion in the temperature range $0.05 \leq T \leq 5$ K across Hc_1 and analyse the critical behavior of Γ and Γ_H at Hc_1.

TT 44.30 Thu 10:00 P1

Field and concentration dependent scaling behavior of the thermal expansion near the quantum critical point of $CeCu_{6-x}Au_x$ — •Sebastian Zaum[1,2], Kai Grube[1], Roland Schäfer[1], Veronika Fritsch[2], Thomas Wolf[1], Peter Schweiss[1], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe, Germany

The heavy-fermion system $CeCu_{6-x}Au_x$ exhibits long-range antiferromagnetic order at $x > 0.1$. The order can be suppressed by hydrostatic or chemical pressure, through the variation of the Au content, as well as by the application of a magnetic field. The quantum critical point at the onset of antiferromagnetism leads to non-Fermi liquid behavior visible in thermodynamic and transport properties. Among these, the thermal expansion offers a particularly sensitive probe to study the quantum critical scaling behavior due to the strong pressure dependence of the Kondo effect in heavy-fermion materials. To shed light on the difference between the two control parameters, pressure and magnetic field, we studied the scaling behavior of the thermal expansion on $CeCu_{6-x}Au_x$ single crystals with varying Au content as a function of the magnetic field in the temperature range between 40 mK and 10 K.

TT 44.31 Thu 10:00 P1

Thermal expansion and magnetostriction of $Yb_2Fe_{12}P_7$ single crystals — •Kai Grube[1], Sebastian Zaum[1,2], Roland Schäfer[1], Peter Schweiss[1], R. E. Baumbach[3], M. B. Maple[3], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76128 Karlsruhe, Germany — [3]Department of Physics, University of California, San Diego, La Jolla, California 92093, USA

The noncentrosymmetric heavy-fermion compound $Yb_2Fe_{12}P_7$ exhibits a magnetic transition at ≈ 1 K. Recent resistivity measurements [1] reveal non-Fermi-liquid behavior in an extended temperature and field range. From the unusual low-temperature behavior it was concluded that $Yb_2Fe_{12}P_7$ belongs to the growing class of compounds in which the non-Fermi-liquid behavior does not conform to the standard QCP scenario which can be described by the Hertz-Millis-Moriya theory. We report on thermal expansion and magnetostriction measurements in a temperature range of $40\,\text{mK} < T < 10$ K and magnetic fields of up to 14 T parallel and perpendicular to the hexagonal c axis. From the data we construct (T, B) phase diagrams for both field directions. The Grüneisen ratio calculated from our measurements is comparatively small and does not diverge for $T \to 0$. It gives, therefore, no evidence for a nearby pressure-induced quantum critical point.
[1] R. E. Baumbach et al., Phys. Rev. Lett. 105, 106403 (2010).

TT 44.32 Thu 10:00 P1

flow equations approach to one dimensional quantum Ising model — •Amin Kiani[1], Farhad Shahbazi[2], and Seyed Akbar Jafari[3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of physics, Isfahan University of Technology, Isfahan, Iran — [3]Department of physics, Sharif University of Technology, Tehran, Iran

One dimensional quantum Ising model with nearest neighbor interaction in transverse magnetic field is one of the simplest spin models which undergoes quantum phase transition. This model has been solved with different methods exactly. In this paper, we solve this model in uniform magnetic field $-Jg\sigma_n^x$ exactly with new method called Continuous Unitary Transformations (CUT) or Flow equations and obtain the expectation values of $\langle\sigma_n^x\rangle$, $\langle\sigma_n^z\rangle$ and $\langle\sigma_n^x\sigma_{n+j}^x\rangle$. Then we apply this method on one dimensional Quantum Ising model in staggered magnetic field $(-1)^n Jg\sigma_n^x$. We observed that both models have the same critical properties as we expected. Moreover we observe that the spontaneous symmetry breaking cannot be derived from CUT.

TT 44.33 Thu 10:00 P1

Broadband dielectric spectroscopy on multiferroic compounds — •Daniel Niermann, Max Schalenbach, Christoph Grams, Florian Waschkowski, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Deutschland

Studying the dynamic dielectric response of given materials provides extensive insight in charge-carrier properties and involved relaxation processes. It was recently shown on the example of the perovskite rare-earth manganites that the occurrence of the multiferroic phase transition is often coupled to characteristic changes of relaxation dynamics [1]. We studied the frequency dependent dielectric properties of the multiferroic compounds $LuFe_2O_4$ and $MnWO_4$. To cover a wide frequency range from mHz to several GHz different setups for low-frequency impedance analysis and microwave spectroscopy were used. For the microwave regime we show transmission-measurements using a new microstrip-sampleholder, which allows a high measuring sensitivity for high-impedance samples. The measurements are performed at cryogenic temperatures down to 1.8K and high magnetic fields up to 14T. This work was supported by the DFG through SFB 608.
[1] F. Schrettle et al., *Phys. Rev. Lett.*, **102** (2009) 207208

TT 44.34 Thu 10:00 P1

Phase diagram of $NaFe(WO_4)_2$ — •Yvonne Sanders[1], Stephanie Orbe[1], Oliver Heyer[1], Sven Jodlauk[2], Sebastian Albiez[2], Petra Becker[2], Ladislav Bohatý[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Institut für Kristallographie, University of Cologne, Germany

Multiferroic materials show simultaneous ferroelectric and magnetic order, which are strongly coupled to each other. A well-known model system is $MnWO_4$ with only one kind of magnetic ions and three magnetically ordered phases below ∼13 K. Here, the multiferroic behavior of one of these phases arises from an incommensurate spin spiral structure. Much less is known about the double tungstate $NaFe(WO_4)_2$, which has a structure closely related to $MnWO_4$. While in $MnWO_4$ sheets || (100) of MnO_6 zig-zag chains alternate with similar sheets of WO_6, in $NaFe(WO_4)_2$ an alternating sheet sequence FeO_6-WO_6-NaO_6-WO_6 - is found. Consequently, the a lattice parameter is doubled and the magnetic subsystem is diluted. The ordering temperature in $NaFe(WO_4)_2$ is reduced to $T_N \approx 4$K. The magnetic structure in zero magnetic field is reported to be collinear antiferromagnetic, but the H-T phase diagram has not been published so far. Here, we present a detailed study of this phase diagram obtained by high-resolution thermal expansion and magnetostriction measurements. We find pronounced hysteresis effects, which resemble those observed in other multiferroic materials.

Supported by the DFG through SFB 608.

TT 44.35 Thu 10:00 P1

Evidence for local lattice distortions in giant magnetocapacitive $CdCr_2S_4$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[2], Yurii Pashkevich[3], Alois Loidl[4], and Vladimir Tsurkan[4,5] — [1]ILTPE NAS, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]DonFTI NAS, Ukraine — [4]EP V, Univ. Augsburg, Germany — [5]IAP AS, Moldova

Pronounced anomalies in intensity, frequency, and width of optical phonon modes were observed in the $CdCr_2S_4$ spinel. To explain the colossal magnetocapacitive effects in $CdCr_2S_4$ we developed a scenario based on hybridization effects to be in accordance with the observed enhanced polarizabilities of certain Cr-S displacements and evidence for symmetry reduction.

Work supported by DFG.

TT 44.36 Thu 10:00 P1

Tunnel-spectroscopy of tunable granular metals prepared by focused electron beam induced deposition — •Dirk Klingenberger, Fabrizio Porrati, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, D-60438 Frankfurt am Main

For the fabrication of platinum containing granular metals we used a focused electron beam and the precursor trimethyl-methylcyclopentadienyl-platinum injected into a vacuum chamber nearby the focal area of the beam. The granular metals are composed of platinum nanocrystallites, embedded in a carbonaceous matrix. Post-growth electron irradiation manipulates the surrounding matrix and allows us - via the radiation dose - to fine tune the sample's conductivity from the insulating to the metallic regime. The deposits were written onto oxidized aluminum contacts to create planar tunnel junctions. Differential conductance measurements have been performed at different temperatures utilizing a He4 cryostat to investigate the sample's density of states. So the current theory of granular metals can be tested. Especially, the behavior of the Coulomb blockade was analyzed for the different conductivity regimes.

TT 44.37 Thu 10:00 P1

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

The quasi two-dimensional organic charge-transfer salt κ-$(ET)_2Cu[N(CN)_2]Cl$ exhibits a rich pressure vs. temperature phase diagram, including Mott-insulating and metallic phases separated by a first order transition line. By applying moderate pressures of ∼ 30 MPa (300 bar), the ratio of the kinetic energy to the onsite Coulomb repulsion t/U can be changed sufficiently to cross this phase transition line. Our objective is to study the effect of carrier doping and the accompanying changes of the first-order transition line and its second-order critical endpoint. We used X-ray irradiation [1] to introduce charge carriers into the material, doping it away from half filling. We will present resistivity data for the temperature range $5\text{K} < T < 60\text{K}$ and for pressures up to 50 MPa for κ-$(ET)_2Cu[N(CN)_2]Cl$ crystals at various doping levels and discuss the accompanied changes in the p-T-phase diagram.

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

TT 44.38 Thu 10:00 P1

Correlated heterostructures with dynamical mean field theory — •Christoph Schütte and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The interfaces between different materials in a three-dimensional nanostructures give rise to interesting electronic phenomena such as metallic or even superconducting layers between insulators. We calculate the electrical resistivity and the Hall coefficient for different heterostructures as a function of temperature. The interactions in the structure may be described by the Hubbard model with an additional self-consistent treatment of long-range Coulomb interactions in a Hartree approximation. Inhomogeneous Dynamical Mean Field Theory (DMFT) is employed to calculate the electronic structure of such a multilayered device in 3 spatial dimensions. The subsequent single impurity Anderson model (SIAM) is solved with the numerical renormalisation group (NRG), a non-perturbative method which yields the accurate low-temperature properties.

TT 44.39 Thu 10:00 P1

Stripline-based resonant microwave spectroscopy to study interacting electron systems — •Christian Fella, Marc Scheffler, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

While conventional optical spectroscopy is well suited to study solids on energy scales dominated by band structure, it cannot access many correlated electron states. For such compounds relevant energies are often of the order of 0.1 meV or below, corresponding to frequencies of 30 GHz and below. To study the frequency-dependent conductivity of such materials, microwave experiments have to be carried out at several frequencies and at low temperatures. Here we present an experimental approach for cryogenic microwave spectroscopy on metals which is based on a 1D stripline resonator. Since the sample under study acts as ground plane, the only requirement for the geometry of the sample is a flat surface of sufficient size. To address both the frequency and temperature dependence of the sample, we measure several modes of the resonator at frequencies from 2 to 20 GHz and between room temperature and ^{4}He temperatures. We present different resonator designs (based on commercial high-frequency laminates as well as on vapor-deposition of metals onto sapphire substrates), discuss their sensitivity and range of applicability for different samples, and compare them to other experimental techniques for microwave studies on metals at low temperatures.

TT 44.40 Thu 10:00 P1

Infrared properties of magnetite under pressure — •Jihaan Ebad-Allah[1], Leonetta Baldassarre[1], Michael Sing[2], Ralph Claessen[2], Vic Brabers[3], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [3]Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, the Netherlands

Magnetite (Fe_3O_4) crystallizes in the inverse cubic spinel structure and undergoes a Verwey transition at $T_v \approx 120$ K at ambient pressure. By applying pressure, T_v decreases with increasing pressure according to the phase diagram proposed in [1]. In addition, it was recently suggested that at room temperature (RT) magnetite undergoes a pressure-induced phase transition from the inverse spinel to the normal spinel structure above 6 GPa, without a change in the lattice symmetry. This proposal is, however, controversially discussed [2].

We studied the electronic and vibrational properties of magnetite by infrared reflectance measurements. First, in order to verify the conduction mechanism via polaron hopping and to search for possible signatures of the phase transition at around 6 GPa, we measured the RT reflectance as a function of pressure. Secondly, we carried out the low-temperature reflectance measurements under pressure in the far-infrared range to check the effect of high pressure on T_v and the splitting of the phonon modes.

[1] G. Kh. Rozenberg et al., Phys. Rev. Lett. **96**, 045705 (2006).
[2] S. V Ovsyannikov et al., J. Phys.: Condens. Matter **20**, 172201 (2008).

TT 44.41 Thu 10:00 P1

On the development of orbital order domains across the Verwey transition in magnetite — •M. Döhler[1], C. F. Chang[1],

M. Buchholz[1], C. Trabant[1,2], T. Kachel[2], N. Pontius[2], M. Beye[2,3], F. Sorgenfrei[4], W. Schlotter[3], S. de Jong[3], R. Kukreja[3], B. Bräuer[3], S. Hossain[3], C. Back[3], A. Scherz[3], D. Zhu[3], J. Turner[3], W.-S. Lee[3], Y.-D. Chuang[3], O. Krupin[3], P. Vogt[1], W. Wurth[4], A. Föhlisch[2], J. B. Goedkoop[5], H. A. Dürr[3], and C. Schüssler-Langeheine[2,1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Helmholtz-Zentrum Berlin — [3]SLAC RSXS collaboration, USA — [4]Universität Hamburg and CFEL — [5]Van der Waals-Zeeman Institute, Universiteit van Amsterdam

The Verwey transition in magnetite (Fe_3O_4) involves a symmetry reduction from cubic to monoclinic and the formation of orbital order at low temperatures. In the low-temperature phase orbital-order domains form. We used resonant soft x-ray diffraction to study how this orbital-order domain pattern changes in the vicinity of the Verwey transition. We found that very close to the transition the domains become mobile, which we assign to fluctuations between the high- and the low-temperature phase. In order to understand how the domain pattern changes when the transition is driven by a fs-infrared-laser pulse, we carried out a time-resolved resonant soft x-ray diffraction experiment at the LCLS. We find that the IR-pulse affects mainly the peak intensity and much less the correlation length of orbital order. Supported by the DFG through SFB 608 and by the BMBF project 05K10PK2.

TT 44.42 Thu 10:00 P1

Orbital occupation and magnetic moments of tetrahedrally coordinated iron in $CaBaFe_4O_7$ — •Nils Hollmann[1], Zhiwei Hu[1,2], Hua Wu[1], Martin Valldor[1], Navid Qureshi[1], Thomas Willers[1], Yi-Ying Chin[1], Julio Criginski Cezar[3], Arata Tanaka[4], Nicholas Brookes[3], and Liu Hao Tjeng[1,2] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany — [3]European Synchrotron Radiation Facility, Boîte Postale 220, 38043 Grenoble Cédex, France — [4]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

$CaBaFe_4O_7$ is a mixed-valent transition metal oxide having both Fe^{2+} and Fe^{3+} ions in tetrahedral coordination. Here we characterize its magnetic properties by magnetization measurements and investigate its local electronic structure using soft x-ray absorption spectroscopy at the Fe $L_{2,3}$ edges, in combination with multiplet cluster calculations. We discuss the x-ray linear dichroism, finding that the Fe^{2+} ion in the unusual tetrahedral coordination is Jahn-Teller active with the high-spin $e^2_\uparrow t^3_{2\uparrow} e^1_\downarrow$ configuration having a x^2-y^2-like electron for the minority spin. With x-ray magnetic circular dichroism it is deduced that there is an appreciable orbital moment of about $L_z = 0.36$ caused by multiplet interactions, thereby explaining the observed magnetic anisotropy. $CaBaFe_4O_7$ might offer new opportunities to explore charge, orbital and spin physics in tetrahedrally coordinated transition metal ions. *This work is supported by the SFB through SFB 608.*

TT 44.43 Thu 10:00 P1

Charge, orbital and spin ordering in 214- manganites, nickelates and cuprates investigated by neutron and x-ray scattering — •A. Bielefeld[1], H. Ulbrich[1], D. Senff[1], A. C. Komarek[1], P. Steffens[2], Y. Sidis[3], and M. Braden[1] — [1]II. Phys. Institut, Universität zu Köln — [2]ILL, Grenoble (France) — [3]LLB, Saclay (France)

The coupling of charges and magnetic moments in numerous transition-metal compounds leads to a complex ordering with checkerboard or stripe like patterns. For nickelates and cuprates stripe states has been intensively studied particularly due to the possible implications for high T_c superconductivity. We have studied the mixed order of electronic, orbital and magnetic degrees of freedom in the planar compounds $La_{2-x}Sr_xReO_4$ (Re = Mn, Ni, Cu). For the manganites we have examined half (x=0.5), electron-doped (x<0.5) and overdoped (x>0.5) systems. For x=0.5, the equal amount of Mn^{3+} and Mn^{4+} ions leads to a checkerboard ordering of charges. The spins of the Mn^{3+} and Mn^{4+} order in an antiferromagnetic CE-type structure following the orbital order [1-3]. For the overdoped-system we find an incommensurate stripe-like coupling of four order parameters: charges, orbitals and magnetic ordering of Mn^{3+} and Mn^{4+} [4]. The formation of stripes in overdoped manganites is similar to stripe phases in nickelates. In 214-cuprates, incommensurate magnetic ordering leads to the forming of diagonal stripes.

[1] J.B. Goodenough, Phys. Rev. 100, 564 (1955).
[2] D. Senff et al., Phys. Rev. Lett. 96, 257201 (2006).
[3] D. Senff et al., Phys. Rev. B 77, 184413 (2008).
[4] H. Ulbrich et al., arXiv: 1008.4496

TT 44.44 Thu 10:00 P1

Temperature-dependent near-edge x-ray absorption fine structure of $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ — •Stephan Uebe[1,2], Andrea Assmann[1,2], Michael Merz[1], Markus Wissinger[1,2], Hilbert von Löhneysen[1,3], Sebastian Hühn[4], Vasily Moshnyaga[4], Peter Nagel[1], and Stefan Schuppler[1] — [1]KIT, Institut für Festkörperphysik, Karlsruhe — [2]KIT, Fakultät für Physik, Karlsruhe — [3]KIT, Physikalisches Institut, Karlsruhe — [4]Universität Göttingen, Physikalisches Institut, Göttingen

All members of the $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ (LPCMO) doping series are strongly correlated electron systems where the electron-electron interaction gives rise to the macroscopic feature of colossal magnetoresistance (CMR). Changing the La/Pr ratio allows for tuning the electron-phonon coupling and thereby T_C.

Thin films of LPCMO were grown on MgO by the Metalorganic Aerosol Deposition technique. The temperature-dependent near-edge x-ray absorption fine structure of the samples was recorded with special emphasis on a double-peak structure that emerges when cooling below T_C.

This feature is known to be specific for CMR manganites and different scenarios have been suggested in literature to explain this change in the electronic structure, being obviously concomitant with the MI phase transition.

Based upon our experimental findings, we will discuss the various scenarios and their respective implications.

TT 44.45 Thu 10:00 P1

On the coupling of spin and charge order in the stripe phase of layered nickelates — •Pascal Vogt[1], Christoph Trabant[1,2], Marcel Buchholz[1], Chun-Fu Chang[1], Niko Pontius[2], Marita Döhler[1], Enrico Schierle[2], Justina Schlappa[1,2], Agung Nugroho[3], Mohamed Benomar[1], Alexander Komarek[1], Ralf Feyerherm[2], Liu Hao Tjeng[1,4], Markus Braden[1], and Christian Schüssler-Langeheine[1,2] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Instiut Teknologi Bandung, Indonesia — [4]MPI for Chemical Physics of Solids, Dresden, Germany

Stripe order is a complex pattern of spins and charge in the CuO_2-planes of doped layered cuprates and NiO_2 planes of the isostructural nickelates. Neutron diffraction finds that spin order decays at about 40 K lower temperatures than charge order, while stripe-like magnetic correlations can be found up to higher temperatures. In resonant soft x-ray diffraction this difference between the two orders is less pronounced, but an intriguing loss of spatial coherence at low temperatures is found for both orders, which is not seen by neutron diffraction. In order to understand the interplay between spin and charge order better, we carried out a comparative study of the temperature dependence of both signals as well of their non-equilibrium behaviour upon pumping with a ps-IR-laser pulse. Preliminary results show that both degrees of freedom behave in a similar way. Supported by the DFG through SFB 608, by the BMBF through projects 05 S3XBA/5 and 05 KS7PK1, and by the HZB.

TT 44.46 Thu 10:00 P1

Investigation of the Electronic Structure and the Role of Cationic Disorder in $LaAlO_3$ - $SrTiO_3$ Heterointerfaces by Soft X-ray Spectroscopy — •Andreas Koitzsch[1], Johannes Ocker[1], Martin Knupfer[1], Martina Dekker[1], Kathrin Dörr[1], Bernd Büchner[1], and Patrick Hoffmann[2] — [1]IFW Dresden, P. O. Box 270116, 01171 Dresden, Germany — [2]Hemlholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The structure of $LaAlO_3$ / $SrTiO_3$ interfaces is under intense discussion due to the appearance of metallic conductivity, magnetism and superconductivity. The most important phenomena supposed to be crucial for the observed effects are the polar catastrophe, the formation of oxygen vacancies and the intermixing of La and Sr at the interface. However, at present there is no consensus about the driving force of the unusual properties. Here we apply on and off resonant photoemission to differently prepared $LaAlO_3$ / $SrTiO_3$ interfaces. In particular we study the behavior of the valence band, the Ti 2p, Sr 3d and La 4d lines. Significant differences are found as a function of sample treatment and photon energy. A model of the interface structure is developed.

TT 44.47 Thu 10:00 P1

Design and realization of a torque magnetometer for magnetization studies on $LaAlO_3$-$SrTiO_3$ interfaces — •Matthias Brasse, Marc A. Wilde, and Dirk Grundler — Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str.1, D-85747 Garching b. München, Germany

Two-dimensional electron systems (2-DESs) have been found to form at the interface between the otherwise insulating oxides $LaAlO_3$ and $SrTiO_3$. The strongly correlated electron system show metallic and superconducting phases. The magnetic properties of the 2-DESs interface are under debate. We intend to use highly sensitive micromechanical torque magnetometry to measure the magnetization of correlated electron states in the 2-DESs formed at the interface between $SrTiO_3$ and $LaAlO_3$. This will allow us to address different phenomena such as the de Haas-van Alphen effect, dia- and paramagnetism in superconducting states, spontaneous magnetization in case of correlated magnetism as well as magnetic hysteresis and anisotropy. Methods and results of ongoing measurements will be presented. We thank S. Thiel and the group of J. Mannhart from the University of Augsburg for sample preparation. This work is supported by the DFG via TRR 80.

TT 44.48 Thu 10:00 P1

Thermal conductivity of $BaCo_2V_2O_8$ — •Gerhard Kolland, Sandra Niesen, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

$BaCo_2V_2O_8$ is a quasi one-dimensional antiferromagnetic Ising-like spin-chain. The chain can be described by an effective S=1/2 1D XXZ model with coupling constant $J \simeq 65\,\mathrm{K}$ and anisotropy parameter $\epsilon = 0.46$. Parallel to the c axis the magnetization saturates at $H_{s||} \simeq 23\,\mathrm{T}$ and perpendicular to the c axis at $H_{s\perp} \simeq 41\,\mathrm{T}$. At zero field, the system orders at $T_N = 5.4\,\mathrm{K}$. The Néel order is suppressed by a magnet field with very different rates depending on the direction of the applied field. We measured the thermal conductivity parallel ($\kappa_{||}$) and perpendicular ($\kappa_\perp$) to the chains in the temperature range from room temperature down to 250 mK. For both directions, we observe a sharp anomaly at T_N and two maxima, one in the ordered phase and one above. In the ordered phase, the thermal conductivity is isotropic ($\kappa_{||} = \kappa_\perp$), while above T_N, $\kappa_{||}$ is significantly higher than $\kappa_\perp$. As this may suggest an additional magnetic contribution to $\kappa_{||}$ in the disordered phase, we compare our data to numerical calculations of the anisotropic κ using the 1D XXZ model Hamiltonian. Moreover, we analyze the field dependence of κ for different directions of the applied magnetic field. *Supported by the DFG through SFB 608.*

TT 44.49 Thu 10:00 P1

Synthesis and characterization of low dimensional magnetic spin systems — •Johanna Frielingsdorf, Ralf Müller, Simon Scharffe, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

The physics of low-dimensinal spin systems is fundamentally controlled by quantum fluctuations and therefore a hot topic. Thus, the preparation of materials with suitable magnetic subsystems, that experimentally realize various theoretical model hamiltonians, is highly desireable. The synthesis and characterization of spin-chain systems such as $BaCo_2V_2O_8$, $BaMn_2V_2O_8$, $SrMn_2V_2O_8$, $CoNb_2O_6$, and Cs_2CoCl_4 is subject of this poster. These compounds provide transition-metal oxides with partly filled 3d shells and hence are suitable to study spin systems from S=1/2 to 5/2. $BaCo_2V_2O_8$, as a quasi one-dimensional S=1/2 Ising system, belongs to the alkaline earth (A)- transition metal(M)- vanadates $AM_2V_2O_8$. $BaMn_2V_2O_8$ on the other hand is an S=5/2 nearly isotropic Heisenberg system. $CoNb_2O_6$, known as columbite, is a quasi one-dimensional Ising ferromagnet and shows a complex interplay of quantum criticality and geometrical frustration. A quasi one-dimensional frustrated XY antiferromagnet is represented by Cs_2CoCl_4, where a spin-liquid ground state can be reached by applying magnetic fields.
This work is supported by the DFG through SFB 608.

TT 44.50 Thu 10:00 P1

Thermodynamic properties of the XY-spin-$\frac{1}{2}$ chain system Cs_2CoCl_4 — •Oliver Breunig, Daniel Löwen, Ralf Müller, Oliver Heyer, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany

Cs_2CoCl_4 contains $CoCl_4$ tetrahedrons, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split up by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The lowest doublet is separated from the second by approximately 14 K, such that at low enough temperatures the system can be described by the one-dimensional spin-$\frac{1}{2}$ XY model. The intra-chain exchange constant being much stronger than the coupling between the chains suppresses the antiferromagnetic order to $T_N \simeq 220$ mK. Here, we present measurements of specific heat and magnetization in a temperature range from about 0.3 to 20 K. The one-dimensional magnetism is reflected by a pronounced maximum in c_p around 1 K. The zero-field data are well described by numerical calculations yielding an intra-chain exchange constant $J/k_B \simeq 2.5$ K. In magnetic fields the specific heat changes drastically, as the system undergoes a quantum phase transition to a fully polarized state at fields of about 2 T. We compare our experimental data for different field directions to numerical calculations.
This work was supported by the DFG through SFB 608.

TT 44.51 Thu 10:00 P1

Strong Electron Correlations in a Two-Dimensional Electron System on a Surface — •Philipp Höpfner[1], Jörg Schäfer[1], Thomas Schramm[1], Max Herpich[1], Gang Li[2], Werner Hanke[2], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Institut für Theoretische Physik und Astronomie, Universität Würzburg

A truly two-dimensional system with strong electron-electron correlation effects can be generated in dilute atomic adlayers on surfaces. An intriguing experimental realization is the Sn/Si(111)-($\sqrt{3} \times \sqrt{3}$) system. Interestingly, this triangular lattice naturally implies spin frustration. Contrary to the naive expectation of a metallic system, there have been recent indications that it is a Mott insulator at low temperature, based on scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) [1]. However, spectral weight and temperature-dependent changes are largely not understood yet.

Here, we present new data on this system from both STS and ARPES. We find that Sn/Si(111) shows an apparent low-temperature band gap of order 1 eV. It is retained even at room temperature, yet accompanied by changes in the spectral weight. ARPES reveals a surface state of rather narrow band width, which may be attributed to the lower Hubbard band. In comparison to recent advances in theoretical treatments of the triangular lattice, e.g., by dynamical mean field theory, the general trend of the findings can be reproduced, and implications for potential antiferromagnetic order at the surface are discussed.
[1] S. Modesti *et al.*, Phys. Rev. Lett. **98**, 126401 (2007).

TT 44.52 Thu 10:00 P1

Thermal expansion under pressure - test measurements on Azurite $[Cu_3(CO_3)_2(OH)_2]$ — •Rudra Sekhar Manna and Michael Lang — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany

Thermal expansion measurements provide a sensitive tool for exploring a material's thermodynamic properties. Particularly strong effects in the expansivity are expected in cases where the Grüneisen parameter is large or even diverges. The latter situation is encountered upon approaching a quantum phase transition [1] or a finite-temperature critical end point [2], by, *e.g.*, the application of hydrostatic pressure. Here we report on the realization of a dilatometer designed for measurements under Helium-gas pressure p $\leq$ 2.5 kbar. For test measurements, a single crystal of Azurite $[Cu_3(CO_3)_2(OH)_2]$ - a realization of a one-dimensional distorted Heisenberg chain - has been used, where significant pressure effects are expected.
[1] L. Zhu *et al.*, Phys. Rev. Lett. **91**, 066404 (2003).
[2] L. Bartosch *et al.*, Phys. Rev. Lett. **104**, 245701 (2010).

TT 44.53 Thu 10:00 P1

Investigatons of modified interlayer coupling in the anisotropic antiferromangnet $[Cu(pyz)_2(HF_2)]SbF_6$ — •R. Beyer[1], J.L. Manson[2], J.A. Schlueter[3], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor (HLD), Forschungszentrum Dresden-Rossendorf (FZD), Dresden, Germany — [2]Department of Chemistry and Biochemistry, EasternWashington Univ., Cheney, USA — [3]Materials Science Division, Argonne National Laboratory, Argonne, USA

In recent years, many synthetic strategies have emerged with regard to the crystal engineering of functional magnetic materials. The group of J.L. Manson *et al.* were able to grow single crystals of a quasi-2D antiferromagnet $[Cu(pyz)_2(HF_2)]SbF_6$ and a defective polymorphic pen-

dant $[Cu_2(pyz)_4F(HF)(HF_2)](SbF_6)_2$ where 50% of the HF_2^- links are broken, leading to two crystallographically unique Cu^{2+} sites. The chemical composition remains unchanged, the structural configuration indicates a minor Jahn-Teller distortion. We studied the two branches of this compound by means of magnetization and specific heat measurements, in order to get a better understanding of the importance of H-F hydrogen bonds for establishing long-range magnetic ordering in polymeric quantum magnets. Part of this work has been supported by EuroMagNET II.

TT 44.54 Thu 10:00 P1

Doping dependence of collective spin states in $LaCoO_3$ — •A. Alfonsov[1], E. Vavilova[1,2], V. Kataev[1], A. Podlesnyak[3], E. Pomjakushina[4], and B. Büchner[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, RAS, 420029 Kazan, Russia — [3]Oak Ridge National Laboratory, P.O. BOX 2008 MS6494 Oak Ridge TN 37831-6494, USA — [4]ETH Zurich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

We have shown recently that a small Sr doping of $LaCoO_3$ yields the spin-state polaron with a big spin value and substantial spin orbital coupling [1]. The Sr for La substitution provides the hole doping due to different valency of Sr and La. In addition, it gives rise to a distortion of the crystal field around the doped ion due to the mismatch of ionic radii. The present work is aimed to discriminate between the effect of the charge (hole- or electron) doping and the effect of structural distortion. For that we have carried out a comparative high field electron spin- (ESR), nuclear magnetic resonance (NMR) and static magnetization study of lightly doped samples of $La_{0.998}A_{0.002}CoO_3$ (A = Sr, Ca, Y, Sn, Ce). We will discuss the role of the heterovalent hole- (Sr^{2+}, Ca^{2+}) and electron doping (Sn^{4+}, Ce^{4+}) as well as the homovalent doping with Y^{3+} ($r^{\rm ion}_{\rm Y^{3+}} \ll r^{\rm ion}_{\rm La^{3+}}$) for the formation of the spin-state polaron in $LaCoO_3$.

[1] A. Podlesnyak et al., Phys. Rev. Lett. **101**, 247603 (2008)

TT 44.55 Thu 10:00 P1

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

We report on detailed experimental and theoretical studies on the magnetic properties of Li_2CuO_2. This compound serves as a simple, but representative model system for an interesting class of spin-chain materials. Their magnetic properties are determined by strong nearest-neighbor ferromagnetic interactions in the chain which are frustrated by an antiferromagnetic (afm) coupling to next-nearest-neighbors. The competition of interactions can induce incommensurate correlations in the chain. On the example of Li_2CuO_2 we illustrate on the basis of our thermodynamical and inelastic neutron scattering data, how relatively weak inter-chain couplings can prevent incommensurate long-range order and determine solely the saturation field [1,2]. In particular, we discuss the influence of the inter-chain couplings onto the magnetic phase transitions.

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

TT 44.56 Thu 10:00 P1

Magnetic and Thermal properties of a Honeycomb lattice system Li_2IrO_3 — •Soham Manni, Yogesh Singh, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Recently Ir based oxides have come into prominence because the interplay between spin-orbit and electronic correlations can lead to a novel Mott insulating state. Sr_2IrO_4 and Na_2IrO_3 are two such examples.

Na_2IrO_3 is an insulator which shows frustrated magnetic interactions which lead to an antiferromagnetic ordering below T_N = 15K even though the magnetic interactions are relatively strong as seen by the Weiss temperature of θ = - 120 K.

Applying pressure is one way to tune an insulator to a metallic state. We have synthesized Li_2IrO_3 in an attempt to apply chemical pressure to Na_2IrO_3. We present results of our transport, magnetic, and thermal property measurement with emphasis on how the magnetic and transport properties change when compared to Na_2IrO_3.

TT 44.57 Thu 10:00 P1

Quasi-1D Transport Measurements on $(TMTTF)_2X$ under Hydrostatic Pressure — •Karl Schrem, Eva Rose, Gabi Untereiner, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

The charge transfer salts $(TMTTF)_2X$ and $(TMTSF)_2X$ are model compounds for low-dimensional strongly correlated electron systems where the interplay of electronic, spin and lattice degrees of freedom together with changes of dimensionality result in a rich temperature-pressure phase diagram. All $(TMTTF)_2X$ compounds are located on the quasi-one dimensional part of the phase diagram and develop a charge-ordered phase at different temperatures $T_{\rm CO}$, except $(TMTTF)_2ClO_4$ and $(TMTTF)_2Br$. In the group with non-centrosymmetric anions (X=ClO_4, BF_4, ReO_4) one can observe anion ordering for $T < T_{\rm AO}$, resulting in a doubling of the unit cell. The different phases can easily be tuned both by chemical and hydrostatic pressure. We investigated several non-centrosymmetic compounds by carrying out electrical transport measurements under hydrostatic pressure up to 12 kbar and down to 4.2 K along different crystal axis. Our measurements show the changes in band width and dimensionality by pressure and its consequences on correlation effects, such as charge order. The shift of $T_{\rm AO}$ and the modification of the related transport characteristics stress the importance of the coupling between electronic system and the lattice.

TT 44.58 Thu 10:00 P1

Doping effects on the non-linear transport in blue bronze — •Ali Al-Hadeethi[1], Duminik Grund[1], Song Yue[2], Martin Dressel[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

When low-dimensional metals are cooled, they often undergo a phase transition to an insulating state exhibiting a new type of order. A famous example is the blue bronze $K_{0.3}MoO_3$, which undergoes a Peierls transition at $T_P \approx 180$ K to a charge-density-wave (CDW) state. In this work, the temperature dependence of the dc resistivity and the non-linear transport properties in pure, Rb-doped, and W-doped blue bronze single crystals is presented. Our measurements show that substituting K by Rb and Mo by W shifts T_P to lower values and smears out the metal-insulator transition. At temperatures below T_P nonlinear conductivity due to charge transport by the CDW is observed, when the applied electric field exceeds the so-called first threshold field. The temperature dependence of the first threshold field is presented for all studied samples. Furthermore, the temperature dependence of the second threshold field, which is usually attributed to the onset of coherent CDW sliding, is discussed.

TT 44.59 Thu 10:00 P1

Quantitative measurement of low temperature magnetisation by a caloric technique — •Hanjo Ryll[1,2], Klaus Kiefer[1], Christian Rüegg[3], Simon Ward[3], Karl Krämer[4], and Tobias Müller[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Technische Universität Berlin, Germany — [3]London Centre for Nanotechnology and Department of Physics and Astronomy, Great Britain — [4]Universität Bern, Switzerland — [5]Universität Kassel, Germany

Measurements of absolute magnetisation at very low temperatures and in high magnetic fields are notoriously difficult. The magnetocaloric effect (MCE) offers an alternative approach, which is applicable down to the mK temperature range. A quantitative MCE measurement is performed by precisely determining the temperature difference between sample and thermal bath with a well known thermal resistivity between bath and calorimeter. This allows for the measurement of the heat (δQ) generated or absorbed by the sample for a changing field (δB). Using Maxwell's relations, the MCE yields the derivative of magnetisation with respect to temperature: $(\delta Q/\delta B)/T = -(\partial M/\partial T)|_B$. Integration directly provides the uniform magnetisation $M(B,T)$. The necessary integration constant is obtained by a magnetisation measurement at higher temperatures, for example by a vibrating sample magnetometer (VSM). The method was applied to the metal-organic spin ladder material $(C_5H_{12}N)_2CuCl_4$. Magnetisation and MCE data between 0.3 K and 3 K are shown as an example, together with quantitative modeling of these quantities for a perfect spin ladder.

TT 44.60 Thu 10:00 P1

Tensor network states for lattice systems — •Stefan Depenbrock and Ulrich Schollwöck — Physics Department, Arnold Sommerfeld Center for Theoretical Physics, LMU München

Tensor network decompositions offer an efficient description of many-body states on a lattice that can capture the essential physics of these systems. Here, we apply the projected entangled pair state (PEPS) algorithm to finite spin and fermion systems on a square lattice.

TT 44.61 Thu 10:00 P1

Strong correlations in spinful quantum wires with multiple dynamics — •Tobias Meng[1], Mehul Dixit[2], Julia Meyer[3], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [2]Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA — [3]SPSMS, CEA-INAC/UJF-Grenoble 1, 38054 Grenoble, France

We consider a quantum wire of electrons and focus on the quantum phase transition from a strictly one-dimensional to a quasi one-dimensional electron liquid. In the low-density limit, this transition corresponds to the deformation of the 1D Wigner crystal to a zig-zag arrangement of the electrons described by an Ising order parameter. The critical properties are governed by the charge degrees of freedom, of which the spin sector remains essentially decoupled. The interaction between critical fluctuations and the gapless plasmon mode leads to an enhanced SU(2) symmetry and a suppression of the characteristic velocity. At higher densities, the electrons form one-dimensional subbands. At the transition, the second band gets filled as a function of the external gate voltage. Electrons at the bottom of the second band interact strongly due to the diverging density of states and become impenetrable. This stabilizes the electron liquid as it hinders pair-tunneling processes between the bands which generate an attractive interaction. The impenetrable electrons in the second band are further screened by plasmon excitations and the resulting polarons finally undergo a Lifshitz transition. We discuss the resulting phase diagram as a function of transverse confinement and density of the electrons.

TT 44.62 Thu 10:00 P1

Properties of dimerized n-leg spin 1/2 ladders — •Kris Cöster and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The Heisenberg model on quasi one-dimensional ladder structures is expected to be interesting since it interpolates between the purely one-dimensional case having fractional excitations and the two-dimensional system displaying long-range order. In recent years there has been a big process in the theoretical and experimental understanding of the two-leg ladder. But the microscopic determination of the excitation spectrum and the spectral properties of n-leg ladders is very challenging.

Here we approach the general case by studying dimerized n-leg ladders with n=3,4,5,6. To this end we use perturbative continuous unitary transformations (pCUTs) with advanced graph techniques to obtain an effective quasi-particle description. We calculate the one- and two-triplon properties. Special regard is paid to binding effects between two triplons with total spin zero which is of direct relevance for optical spectroscopy on such systems.

TT 44.63 Thu 10:00 P1

Finite-size scaling analysis of the frustrated square-lattice Heisenberg model — •Burkhard Schmidt, Mohammad Siahatgar, and Peter Thalmeier — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The two-dimensional frustrated next nearest neighbor Heisenberg model on the square lattice is a prime example for a spin system where quantum fluctuations can either destroy or stabilize magnetic order. The phase boundaries and staggered moment dependence on the frustration ratio J_2/J_1 of the exchange constants are fairly well understood both from approximate analytical and numerical methods. We use exact diagonalization for finite clusters for an extensive investigation of the more general $J_{1a,b}$-J_2 model to clarify the dependence of ground-state energy and ordered moment on exchange frustration and anisotropy. Exact diagonalization is an unbiased approach, however it is restricted to small tiles, and we have to account for finite-size effects. We therefore introduce a systematic way of uniquely generating all possible tilings of the square lattice, define a *compactness* parameter for selecting the tiles to be included into the scaling procedure and, for this low symmetry model, define a controlled procedure for the finite size scaling that is compatible with the possible magnetic phases. We apply the scaling procedure to the ground-state energy, the static structure factor, and the static long-distance correlation function of the $J_{1a,b}$-J_2 model at different characteristic points in the parameter space of the Hamiltonian. The tile size dependence of the ordered moment is derived from the latter two quantities.

TT 44.64 Thu 10:00 P1

Time-dependent exact diagonalization for the simulation of RIXS in 1-D systems — •Stefanos Kourtis, Maria Daghofer, and Jeroen van den Brink — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

We present a method for numerical simulation of resonant inelastic X-ray scattering (RIXS). Using time-dependent exact diagonalization, we take explicitly into account the finite lifetime of the core-hole present in the intermediate state of the process and study its effect on observables. We report preliminary results for the spin and charge excitations of a one-dimensional chain at quarter filling and compare them to various approximations used. In particular, we study to what extent the finite lifetime affects direct RIXS and possibly leads to differences between the expected outcome and the charge response function.

TT 44.65 Thu 10:00 P1

Transport simulations in quasi-one-dimensional correlated quantum systems — •Alex Cojuhovschi[1], Malcolm Einhellinger[1], Eric Jeckelmann[1], Sabine Tornow[2], and Gertrud Zwicknagl[2] — [1]Leibniz Universitaet Hannover — [2]TU Braunschweig

We present a powerful numerical approach for studying spin and charge transport in quasi-one-dimensional correlated quantum many-body systems. The time-evolving block decimation (TEBD) method [1] is used to simulate the quantum dynamics of finite-size systems which are driven out of equilibrium by a sudden change in applied voltage potentials. Thanks to the natural parallelizability of the TEBD algorithm large systems can be simulated efficiently on modern high-performance parallel computers. Using a finite-size analysis based on an analogous classical model, steady-state transport properties are obtained from the quasi-stationary properties calculated with TEBD for finite systems.

To assess the capability and limitation of our approach we investigate the transient and steady-state transport properties of various correlated quantum systems such as Luttinger liquids and dot-lead systems and compare our results with exact results for non-interacting systems as well as field-theoretical predictions and time-dependent numerical renormalization group simulations for interacting systems. \newline [1] G. Vidal, PRL 91, 147902 (2002); 93, 040502 (2004)

TT 44.66 Thu 10:00 P1

Quantum relaxation in the XY chain with free boundaries — •Benjamin Blass and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

We study the quantum relaxation in the spin-1/2 XY chain with free boundaries in a longitudinal field. The system is described by $\hat{H} = -\frac{J}{2}\sum_{i=1}^{L-1}\left[\frac{1+\gamma}{2}\hat{\sigma}_i^x\hat{\sigma}_{i+1}^x + \frac{1-\gamma}{2}\hat{\sigma}_i^y\hat{\sigma}_{i+1}^y\right] - \frac{h}{2}\sum_{i=1}^{L}\hat{\sigma}_i^z$. By preparing the system in an eigenstate (e.g., the ground state) of the Hamiltonian for given parameters γ_0, J_0 and h_0 and then suddenly changing (i.e., quenching) the parameters to γ, J and h, the system evolves dynamically according to the Schrödinger equation into a stationary (i.e., time translational invariant) state, which is characterized by a length and time scale depending on the quench parameters. Due to the free boundaries, the local order parameter has a time and space dependent profile, which is computed. The issues of thermalization (or the lack thereof) as well as recurrence within a finite system are discussed.

TT 44.67 Thu 10:00 P1

Band renormalization for systems on anisotropic triangular lattices — •Andrea Di Ciolo, Luca F. Tocchio, and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt Am Main, Germany.

We consider electronic systems on anisotropic triangular lattices, i.e. with hopping t on two bonds of the unit cell and t' on the last bond.

We apply the renormalized mean-field theory to the Hubbard model [see F. C. Zhang, et al., Supercond. Sci. Tech. 1, 36 (1988)] and our analytical results are to be compared with Variational Monte Carlo findings.

The renormalization of the band structure and the evolution of the

Fermi surface are investigated as due to electronic correlations.

In particular, motivated by former studies for 2D-systems on square lattices [C. Gros et al., Proc. Natl. Acad. Sci. U.S.A. 103, 14928 (2006)] and 1D-systems [L. F. Tocchio et al., Phys. Rev. B 81, 205109 (2010)], we explore the issue of the underlying Fermi surface (Luttinger surface) for insulating states on triangular lattices.

TT 44.68 Thu 10:00 P1

Response of Jahn-Teller inhomogeneities to uniaxial strain. — •Joaquin Miranda Mena — German Research School for Simulation Sciences and RWTH Aachen University, 52425 Jülich

Using Monte Carlo simulations we study the effect of uni-axial strain in a two-dimension electron-phonon Hamiltonian with long-range Coulomb interaction. Lattice effects are introduced in form of Jahn-Teller (JT) polarons. In the absence of strain we observe that charge clustering is accompanied with a strong suppression of single particle density of states (DOS) for high doping and low temperatures. Remarkably, these clusters take stripe forms when the JT attraction and the Coulomb repulsion are similar in magnitude. In this work we report how the map of lattice distortions and DOS are modified in the presence of the uniaxial strain. In the case of ferro-distortive JT attraction we observe orbital ordering and no changes of cluster shapes. The presence of the strain is mainly reflected in DOS of unoccupied states. In the case of antiferro-distortive JT attraction, clusters start to melt with increasing strain.

TT 44.69 Thu 10:00 P1

Functional RG for spin chains — Kimmo Sääskilahti[1], •Stefan Göttel[2], Dirk Schuricht[2], Sabine Andergassen[2], and Carsten Honerkamp[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen, Germany — [2]Institut für Theorie der statistischen Physik, RWTH Aachen, Germany

We apply a recently developed functional RG (fRG) scheme [1] for quantum spin systems to one-dimensional spin chains. Based on an auxiliary fermion representation, the derived flow equations allow for a systematic resummation of perturbation series in the spin-spin interactions. The computed observables include the ground-state energy and the spin-spin correlation function as a function of the spin anisotropy. Comparing to exact results from Bethe Ansatz and DMRG calculations, we assess the accuracy of the obtained results. The importance of the Katanin modification in the truncated fRG scheme is addressed.
[1] J. Reuther und P. Woelfe, Phys. Rev. B 81, 144410 (2010)

TT 44.70 Thu 10:00 P1

Quantum phase transitions in anisotropic Heisenberg antiferromagnetic chains — •David Peters — Institut für Theoretische Physik der Phasenübergänge, RWTH Aachen

Using (infinite) density matrix renormalization group calculations, ground state properties of the spin–1 Heisenberg chain with exchange and quadratic single-ion anisotropies in an external field are studied, for special choices of the two kinds of anisotropies[1]. In particular, the ground state phase diagrams comprise antiferromagnetic, spin-liquid (or spin-flop), half-magnetization-plateau, and supersolid (or biconical) phases. Especially, studying various quantities, including spin-spin correlations, interesting features of the spin-liquid and supersolid phases are identified. Properties of the quantum chains are compared to those of corresponding classical spin chains.
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TT 44.71 Thu 10:00 P1

Magnetic susceptibility and spin-wave properties of two-band Hubbard models — •Ernst von Oelsen, Jörg Bünemann, and Götz Seibold — Institut für Physik, BTU Cottbus, Postfach 101334, 03013 Cottbus

We present result on the magnetic susceptibility and the spin-wave properties of two-band Hubbard models in two, three, and infinite dimensions. As a method we use the recently developed generalisation of the time-dependent Gutzwiller theory for multi-band models. Our findings are compared with those of a Hartree-Fock based random phase approximation, which is the standard textbook method for the calculation of two-particle response functions. Like in the corresponding ground-state theories we find significant differences between both methods quantitatively as well as qualitatively.

TT 44.72 Thu 10:00 P1

Investigation of giant spin rings with DMRG — •Jörg Ummethum and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld

Giant antiferromagnetic molecules like Fe_{18} [1], which consists of 18 $s = 5/2$ spins on a ring, are much too large for exact diagonalization so that simplifying models or approximate numerical methods like Quantum Monte Carlo or DMRG have to be used. For one-dimensional systems DMRG is known to yield very accurate results.

We use static and dynamical DMRG methods to investigate the low-lying spectrum of a Heisenberg spin ring consisting of 18 spins (neglecting the small single-ion anisotropy which is present in Fe_{18}) with spin quantum numbers $s = 1/2$ and $s = 5/2$. We calculate the lowest energies in subspaces of total magnetic quantum number, the $T = 0$ magnetization curve, and the spectral function $S^{zz}(q, \omega)$ for different values of q. Since the momentum of the ground state is known, the momenta of low-lying excited states in the $S = 1$ subspace can be calculated by looking for peaks in $S^{zz}(q, \omega)$.

We find that the lowest energies in subspaces of total magnetic quantum number form a rotational band and that transitions from the $S = 0$ ground state to the $S = 1$ ground state within the first rotational band are dominant. This agrees with the results of [2] where much smaller spin rings have been investigated using exact diagonalization.
[1] O. Waldmann, T. C. Stamatatos, G. Christou, H. U. Güdel, I. Sheikin, and H. Mutka, Phys. Rev. Lett. 102, 157202 (2009)
[2] O. Waldmann, Phys. Rev. B 65, 024424 (2001).

TT 44.73 Thu 10:00 P1

Factorization of time-dependent correlation functions for the central spin model — •Fabian Güttge, Jasmin V. Jäger, and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The spin of an electron trapped in a semiconductor quantum dot has been suggested as a possible realisation of a solid-state qubit. The major source of decoherence in such devices is the hyperfine coupling to the nuclear spins. We model this system by a central spin coupled to a finite number of independent nuclear bath spins. The time-dependent two-, three and four-particle correlation functions are calculated using exact diagonalization. We investigate under which conditions the correlation functions can be factorized by neglecting higher order cummulant corrections. This provides information about the applicability of equation of motion decoupling schemes which scale linear with the number of bath spins.

TT 44.74 Thu 10:00 P1

Thermal relaxation and heat transport in spin ice $Dy_2Ti_2O_7$ — •Bastian Klemke[1,2], M. Meissner[1,2], P. Strehlow[2,3], K. Kiefer[1], S. A. Grigera[4,5], and D. A. Tennant[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Technische Universität Berlin — [3]Physikalisch Technische Bundesanstalt, Institut Berlin — [4]School of Physics and Astronomy, St. Andrews, UK — [5]Instituto de Física de Líquidos y Sistemas Biológicos, CONICET, UNLP, La Plata, Argentina

The thermal properties of single crystalline $Dy_2Ti_2O_7$ have been studied at temperature below 30 K and magnetic fields applied along [110] direction up to 1.5 T. Based on a thermodynamic field theory (TFT) various heat relaxation and thermal transport measurements were analysed. So we were able to present not only the heat capacity of $Dy_2Ti_2O_7$, but also for the first time the different contributions of the magnetic excitations and their corresponding relaxation times in the spin ice phase. In addition, the thermal conductivity and the shortest relaxation time were determined by thermodynamic analysis of steady state heat transport measurements. Finally, we were able to reproduce the temperature profiles recorded in heat pulse experiments on the basis of TFT using the previously determined heat capacity and thermal conductivity data without additional parameters. Thus, TFT has been proved to be thermodynamically consistent in describing three thermal transport experiments on different time scales. The observed temperature and field dependencies of heat capacity contributions and relaxation times indicate the magnetic excitations in the spin ice $Dy_2Ti_2O_7$ as thermally activated monopole-antimonopole defects.

TT 44.75 Thu 10:00 P1

Collective orbital excitations in $GdVO_3$ — •Michael Voigt[1], Luis Mäder[1], Konstantin Shportko[1], Graeme R. Blake[2], Nandang Mufti[2], Agustinus A. Nugroho[2,3], Thomas T. M. Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]University of Groningen — [3]Institut Teknologi Bandung

In the vanadates (RVO$_3$) orbital interactions are expected to be especially strong. In the compounds YVO$_3$ and HoVO$_3$ these interactions lead to two different phases of orbital ordering (OO), one in an intermediate temperature range with G-type OO and one low-temperature phase with C-type OO. [1] In these orbitally ordered states, one expects novel collective excitations, so called orbitons, which are analogous to spin waves in a magnetically ordered state.

Previous optical measurements of YVO$_3$ and HoVO$_3$ have shown a striking feature at 0.4 eV with polarization $E \parallel c$ in the intermediate phase which is interpreted as bi-orbiton excitation. [2] Furthermore a second interesting feature at 0.55 eV with polarization $E \parallel a$ is observed. The interpretation of this feature is still a puzzle.

We show the optical conductivity $\sigma(\omega)$ of GdVO$_3$ single crystals for the mid-infrared range and temperatures from 10 K to 300 K. In GdVO$_3$, G-type OO (the intermediate phase of YVO$_3$) extends down to the lowest temperatures, offering additional information on the excitations discussed above.

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[2] Benckiser *et al.*, NJP **10**, 053027 (2008)

TT 44.76 Thu 10:00 P1

Looking for orbiton dispersion features in GdVO$_3$ with the aim of RIXS — •Pasquale Marra[1], Krzysztof Wohlfeld[1], Jeroen van den Brink[1], Luis Maeder[2], Komalavalli Thirunavukkuarasu[2], Marco Moretti Sala[3], Giacomo Ghiringhelli[3], Thorsten Schmitt[4], and Marcus Grueninger[2] — [1]IFW Dresden — [2]Universität zu Köln — [3]Politecnico di Milano — [4]PSI Villigen

We compute the theoretical RIXS spectra for the *dd* excitations at the vanadium L_3 edge in GdVO$_3$, as a function of energy and momentum transfer, by factorizing the RIXS spectral function into two parts: (i) a single-site part with a core hole present and (ii) a lattice part without the core hole. The obtained results are compared with the direct measurements on the compound for four different angles, carried out with SAXES at the ADDRESS beamline (PSI Villigen, Switzerland). The experimental spectra show a shoulder at low energy with a clearly visible shift corresponding to different momentum transfers. We investigate the possible origin of this shift, in order to distinguish between a crystal field effect (weight transfer between two or more different peaks) and an orbiton dispersion feature predicted by the superexchange mechanism for $3d^2$ degenerate electrons in V^{3+} ions.

TT 44.77 Thu 10:00 P1

Spin excitations in the antiferromagnetic and antiferroquadrupolar phase of CeB$_6$ — •G. Friemel[1], Y. Li[1], A. Invanov[2], V. B. Filipov[3], N. Yu. Shitsevalova[3], N. E. Sluchanko[4], and D. S. Inosov[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Institut Laue-Langevin, 6 rue Jules Horowitz, F-38042 Grenoble Cedex 9, France — [3]I. N. Frantsevich Institute for Problems of Material Science, National Academy of Sciences of Ukraine, ul. Krzhizhanovskogo 3, Kiev, 03680, Ukraine — [4]A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, ul. Vavilova 38, Moscow, 119991 Russia

We present inelastic neutron scattering studies on CeB$_6$, a rare earth hexaboride. In zero field CeB$_6$ exhibits a paramagnetic phase at high temperatures and orders antiferromagnetically below $T_N = 2.3$K. However, below $T_Q = 3.2$K a peculiar "antiferroquadrupolar" (AFQ)-phase of the cerium ions appears, whose nature is so far controversial. Multipolar excitations in zero field have been theoretically predicted and partially studied. The mechanism behind this type of ordering is still in question since spin excitation data is sparsely available. Therefore, we present a first comprehensive temperature and energy dependent mapping of the spin excitations in the AFM and AFQ phases, which are dominated by a pronounced inelastic intensity in the vicinity of the AFQ wavevector (1/2 1/2 1/2) and which quickly disappear in the paramagnetic phase upon warming above T_Q.

TT 44.78 Thu 10:00 P1

Low temperature thermal and electrical transport properties of ZrZn$_2$ in high magnetic field — •Yang Zou[1,3], Mike Sutherland[1], Stephen Hayden[2], Daniel Rothfuss[3], Andreas Fleischmann[3], F. Malte Grosche[1], and Christian Enss[3] — [1]Cavendish Laboratory, University of Cambridge, United Kingdom — [2]Department of Physics, University of Bristol, United Kingdom — [3]Kirchhoff-Institut, Universität Heidelberg, Germany

Laudau's Fermi-liquid theory has been proven remarkably successful in describing the properties of metals at low temperatures. Unlike most metals, the low temperature band ferromagnet ZrZn$_2$ appears to violate Fermi-liquid behaviour over a wider temperature range at low temperature. In order to investigate the nature of the Fermi-liquid breakdown in this material, the electrical and thermal transport properties of ZrZn$_2$ were investigated over a wide range of magnetic field. An experimental technique to measure the thermal conductivity down to 100 mK has been set up and tested. In zero field our measurements confirm the finding reported in [1] that, to leading order in temperature T, the electrical and effective thermal resistivities at low temperature take a $T^{5/3}$ and T form, respectively. These are the signatures of a marginal Fermi-liquid, predicted to occur close to a ferromagnetic quantum critical point by spin fluctuation theory. In contrast, we find that at finite magnetic field the electrical and effective thermal resistivities assume quadratic temperature dependencies, consistent with a return to conventional Fermi-liquid behaviour.

[1] Smith et al. Nature 455, 7217 (2008)

TT 44.79 Thu 10:00 P1

Low temperature spin excitation spectrum of FeSi by polarized neutron spectroscopy — •Sven Krannich[1], Yvan Sidis[2], Jean-Michel Mignot[2], Daniel Lamago[1,2], Frank Weber[1], Alexander Ivanov[3], and Paul Steffens[3] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, 76021 Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA-Saclay, F-91191 Gif sur Yvette Cedex, France — [3]Institute Laue Langevin, 156X, 38042 Grenoble Cedex 9, France

We investigated the spin excitation spectrum of FeSi using the thermal triple axis neutron spectrometer IN20 at the Institute Laue Langevin, Grenoble, with polarization analysis. FeSi displays a behavior which has, so far, only been observed in f-electron containing Kondo insulators. Therefore, it has often been claimed to be the first 3d system belonging to this class of materials [1]. A temperature dependent energy gap was observed in optical spectroscopy [2], but measurements of inelastic magnetic scattering via neutrons have been restricted to T $\geq$ 150 K so far [3] and did not report gap signatures. We measured magnetic scattering between room temperature and T = 15 K over a large energy range up to energies of 80 meV. Particular attention was devoted to possible spin-exciton formation at energy transfers below the gap value at low temperatures as observed in the Kondo-insulator YbB$_{12}$ [4].

[1] D. Mandrus et al., Phys. Rev. B 51, 4763 (1995)
[2] D. Menzel et al., Phys. Rev. B 79, 165111 (2009)
[3] K. Tajima et al.,Phys. Rev. B 38, 6954 (1988)
[4] K. S. Nemkovski et al., Phys. Rev. Lett. 99, 137204 (2007)

TT 44.80 Thu 10:00 P1

Dynamic triple-helix spin clusters in the paramagnetic phase of MnSi — •A. Hamann[1], D. Lamago[2], Th. Wolf[1], H. v. Löhneysen[1], and D. Reznik[3] — [1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Laboratoire Léon Brillouin, CEA Saclay, France — [3]Department of Physics, University of Colorado, Boulder, USA

MnSi exhibits helical magnetic order at low temperatures and ambient pressure with underlying Fermi-liquid (FL) properties. At high pressures an exotic magnetic state forms referred to as partial order [1], where the helical propagation vector becomes disordered. Non-FL temperature dependence of the electrical resistivity appears nearby in the phase diagram. Our numerical calculations show that isotropic nearest-neighbor spin interactions in MnSi favor a glassy aggregation of topological magnetic clusters that we call triple-helices. They are similar to double helices well known from blue phases of liquid crystals [2] and have the spectral signature of partial order. Their stability increases as their size decreases. This model may explain most of the puzzling properties of MnSi including the non-FL behavior and the two-component phase transition that was revealed by specific heat [3]. Our detailed neutron scattering measurements in the paramagnetic phase where temperature sets the scale of the size of dynamic spin clusters fully confirm this picture.

[1] C. Pfleiderer, D. Reznik et al., Nature **427**, 227 (2004)
[2] D. C. Wright and N. D. Mermin, Rev. Mod. Phys. **61**, 385 (1989)
[3] D. Lamago et al., Physica B **385-386**, 385 (2006)

TT 44.81 Thu 10:00 P1

Polarized electron currents in the helical magnet MnSi — •Pascal Krautscheid, Karin Everschor, Markus Garst, and

Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln

The Dzyaloshinskii-Moriya interaction in MnSi results in the formation of helical magnetic phases and even the stabilization of Skyrmion configurations at low temperatures [1]. A polarized electron current couples efficiently to such twisted magnetic structures giving rise to pronounced spin-torques transfer phenomena [2]. We study the interaction of spin currents with the magnetic texture in MnSi in the framework of the Landau-Lifshitz-Gilbert equation. Particular emphasis is put on the influence of spin currents on the pitch of the magnetic helix and its pinning by the underlying crystal structure of MnSi.

[1] S. Mühlbauer et al., Science 323, 915 (2009).
[2] F. Jonietz et al., Science, to be published (2010).

TT 44.82 Thu 10:00 P1

Entanglement spectrum analysis of frustrated Heisenberg antiferromagnets — •Burkhard Scharfenberger[1], Ronny Thomale[2], and Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA

We investigate numerically the entanglement spectra of $S = 1$ chirality - and $S = 1/2$ chiral spin liquids on various lattice geometries ($N = 16, 32$-site square and $N = 18, 36$-site kagome lattices) with cylindrical topology. We compare these spectra to those obtained from groundstates of antiferromagnetic Heisenberg models with either simple nearest neighbour interaction if the lattice geometry already causes frustration (kagome) or next nearest neighbour interaction near the critical coupling strength $J_1 = 2\,J_2$, which introduces frustration via the interaction (square lattice).
On the square lattice we find that both chiral spin liquid and chirality liquid describe the antiferromagnet equally well up to the critical point, despite the fact that the only the chirality liquid has the same symmetries (parity P and time reversal T) as the hamiltonian. In the case of the Kagome lattice, the exponential groundstate degeneracy caused by frustration is mirrored in the exponential freedom we have in writing out our spin liquids for different sublattice configurations. The interesting 'low energy' part of the spectrum proves to be insensitive to this subdivision, which suggests that all these states essentially describe the same phase of the system.

TT 44.83 Thu 10:00 P1

Quantum Phases of the Planar Antiferromagnetic J_1-J_2-J_3 Heisenberg-Model — •Rachid Darradi[1], Johannes Reuther[2], Peter Wölfle[2], Wolfram Brenig[1], Marcelo Arlego[3], and Johannes Richte[4] — [1]Institut für Theoretische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Departamento de Física, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina — [4]Institut für Theoretische Physik, Universität Magdeburg, 39016 Magdeburg, Germany

We present results of a complementary analysis of the frustrated planar J_1-J_2-J_3 spin-1/2 quantum-antiferromagnet. Using dynamical functional renormalization group, high-order coupled cluster calculations, and series expansion based on the flow equation method, we have calculated generalized momentum resolved susceptibilities, the ground state energy, the magnetic order parameter, and the elementary excitation gap. From these we determine a quantum phase diagram which shows a large window of a quantum paramagnetic phase situated between the Neel, spiral and collinear states, which are present already in the classical J_1-J_2-J_3 antiferromagnet. Our findings are consistent with substantial plaquette correlations in the quantum paramagnetic phase. The extent of the quantum paramagnetic region is found to be in satisfying agreement between the three different approaches we have employed.

TT 44.84 Thu 10:00 P1

Generalized Magnetic Impurities in Low-Dimensional Quantum Antiferromagnets — •Björn Willenberg[1,3], Wolfram Brenig[1,3], Holger Frahm[2,3], and Eric Jeckelmann[2,3] — [1]Institute for Theoretical Physics, Technische Universität Braunschweig — [2]Institute for Theoretical Physics, Leibniz Universität Hannover — [3]Niedersächsische Technische Hochschule, NTH

We investigate magnetic impurities with extended multiplet structure in contact with spin-1/2 antiferromagnets. First, and using Quantum Monte-Carlo methods based on the stochastic series expansion, we study a spin-1/2 dimer coupled to the two-dimensional (2D) Heisenberg antiferromagnet (HAFM) at finite temperature. Results will be presented for thermodynamic properties as a function of temperature, exchange-coupling constants, and magnetic field. These include the impurity susceptibilities, magnetization, and the static on- and off-dimer correlation functions. Our findings will be contrasted against those for single spin-1/2 impurities in 2D HAFMs. Moreover we will analyze similar properties for S>1/2 edge-spins coupled to 1D HAFMs with open boundary conditions, where a comparison with results from Bethe ansatz and density-matrix renormalization methods is possible in the limit of zero temperature.

Work partially funded by the NTH School for Contacts in Nanosystems.

TT 44.85 Thu 10:00 P1

Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions — Philipp Wissgott[1], Jan Kuneš[2], •Alessandro Toschi[1], Ryotaro Arita[3], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [3]Department of Applied Physics, University of Tokyo, Japan

We present an interface between the full-potential linearized augmented plane wave package wien2k[1] and the wannier90[2] code for the construction of maximally localized Wannier functions (MLWF). The interface wien2wannier (w2w)[3] computes the necessary input data for the use of wannier90 starting from a wien2k `.vector` file. Scripts and FORTRAN90 programs to simplify the workflow are also provided. The original wannier90 program has been adapted to return the Hamiltonian in the basis of the Wannier orbitals and other useful data. As an application of w2w, we consider[3] two examples: $SrVO_3$ and $FeSb_2$. The latter material has a very complicated bandstructure. Here, the use of a basis set of Wannier functions allows for a deeper understanding and a for the proper input of codes for strongly correlated materials, such as LDA+DMFT.

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TT 44.86 Thu 10:00 P1

Optimized basis in continuous unitary transformations for symmetry-broken groundstates — •Nils A. Drescher and Götz S. Uhrig — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund, Germany

Continuous unitary transformations (CUT) [1,2] provide a generic, non-perturbative framework to derive effective low-energy models preserving the system's symmetries. We use them to decouple and study low-lying magnetic excitations [3] of low-dimensional, antiferromagnetic spin $\frac{1}{2}$ models. Our special focus is the quantum phase transition between disordered and long-range ordered phases with spontaneous staggered magnetization in two-dimensional dimerized systems. Introducing a variational parameter, the spin symmetry of the original quasiparticle basis can be broken, thus allowing the CUT to deal with a spontaneously symmetry-broken groundstate. Even in the magnetically disordered one-dimensional system, the optimal choice of the variation parameter allows for a gain of accuracy for magnetic properties.

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TT 44.87 Thu 10:00 P1

Charge self-consistency in an LDA+DMFT framework — •Daniel Grieger, Oleg Peil, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

In recent years, the combination of the local-density approximation (LDA) to density functional theory with the dynamical mean-field theory (DMFT) has proven to be a powerful and reliable tool to describe explicit strong electronic correlations in realistic materials. However in many current implementations thereof, the correlated charge density is not converged within a comprehensive LDA+DMFT interface. Thus the dependence of many observables on self-energy effects connected to the selfconsistent correlated charge density is neglected. We address this problem both within a pseudopotential and a projector-augmented

wave (PAW) [1] implementation of the LDA+DMFT framework. This work first illuminates the crucial parts of the theoretical interfacing structure, such as the extraction of a suitable correlated subspace [2] and the representation of the acquired correlated charge density in a way that it can be processed in the conventional LDA portion as well as the DMFT part of the problem (e.g., Ref. [3]). In addition, concrete materials results from investigations using this charge-selfconsistent scheme in the context of strong correlation problems with relevant charge and spin degrees of freedom will be presented.

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TT 44.88 Thu 10:00 P1

Compression of matrix-product states — •Michael Lee and Michael Potthoff — I. Institut für Theoretische Physik, Jungiusstraße 9, 20355 Hamburg

One-dimensional systems of strongly correlated electrons can efficiently be treated by means of the density-matrix renormalization group (DMRG) [1]. It has been shown [2] that an essentially equivalent formulation of the DMRG is possible using matrix-product states and matrix-product operators.

We propose to employ Krylov-based techniques operating on the space of matrix-product states. This should allow for a calculation of dynamical correlation functions, like the one-particle Green's function, similar to a standard Lanczos calculation without the need for multiple-state targeting. Unlike the correction-vector method this "matrix-product-Lanczos approach" offers the exciting perspective to get the entire frequency dependence of the Green's function from a single calculation.

The iterative algorithm requires a "compression" of matrix-product states of the form $H|\Psi\rangle$ to control the growth of matrix dimensions. Here, we show first results and discuss the accuracy and efficiency of the compression technique.

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TT 44.89 Thu 10:00 P1

Dual-Fermion approach to Non-equilibrium strongly correlated problems — •Alexander Lieder, Christoph Jung, Sergej Brener, Alexander Chudnovskiy, and Alexander Lichtenstein — I. Institut für Theoretische Physik Universität Hamburg

We present a generalization of the recently developed Superperturbation solver for the Anderson impurity model for the non-equilibrium case. We show that the general dual perturbation theory can be formulated on the Keldysh contour. Starting from a reference Hamiltonian system, in which the time-dependent solution is found by exact diagonalization, we make a dual perturbation expansion in order to account for the relaxation effects from the fermionic bath. Test cases for closed as well as open quantum systems in a fermionic bath are presented.