TT 40: Poster Session Correlated Electrons

Time: Wednesday 15:00–19:00 Location: Poster D

TT 40.1 Wed 15:00 Poster D

NRG calculations for Kondo-type models as a way to characterize the magnetic properties of deposited molecules — •Henning-Timm Langwald and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Bielefeld, Deutschland

Magnetic molecules offer a variety of interesting properties which may be used for future technologies. For such applications a molecule might be deposited on a substrate with which it then interacts. Thus in general, when describing the magnetic properties of the deposited molecule, the interaction with the substrate has to be taken into account and needs to be modeled in a suitable way.

We use Numerical Renormalization Group (NRG) calculations for certain single-impurity Kondo models as a way to access the magnetic properties of such deposited molecules. By analyzing simple model systems such as a dimer (an impurity consisting of two spins) coupled to a single site of a substrate lattice we want to gain insight into the specific behavior of deposited molecules and the ways we can describe them. Our focus is on thermodynamic observables such as the magnetization and their dependence on temperature and magnetic field.

TT 40.2 Wed 15:00 Poster D

Bosonic NRG using an Optimised Basis Set of Coherent States — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The bosonic numerical renormalisation group (bNRG) has been developed to investigate the spin-boson model which exhibits a quantum phase transition between a localised and delocalised phase in the subohmic regime.
Since the bNRG must always use a truncated bosonic basis set, we investigate the influence of the different choices of such finite sets onto the NRG level flow and the prediction of the critical exponents. We propose to use a coherent basis set close to the quantum phase transition to estimate the divergent displacements properly. We compare the predictions for the critical coupling α_c with respect to the different basis sets: (1) standard bNRG fock space occupation eigenbase, (2) displaced oscillator occupation eigenbase and (3) coherent base.

TT 40.3 Wed 15:00 Poster D

Time Dynamics of the Two-Impurity Kondo Model — •Benedikt Lechtenberg and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The equilibrium properties of various two-impurity Kondo models (TIKM) have been investigated extensively in the literature. We study the non-equilibrium dynamics of the TIKM employing the time-dependent numerical renormalization-group (TD-NRG). The TD-NRG was developed to treat the real-time dynamics of quantum-impurity systems. We are interested in the real-time response of the the second spin $\vec{S}_2$ as a function of the initial condition of the first spin $\vec{S}_1$ and their distance R. We determine the relevant time scale and relaxation rates. The particle-hole symmetric model exhibits a quantum phase transition at a critical anti-ferromagnetic coupling. We investigate the change in the dynamics as function of the coupling constant close to QPT.

TT 40.4 Wed 15:00 Poster D

Hybrid NRG-DMRG approach to real-time dynamics of quantum impurity systems — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a non-equilibrium hybrid method which uses the numerical renormalization group (NRG) to generate an effective low energy Hamiltonian. This Hamiltonian is then solved with the density-matrix renormalization group (DMRG). By considering systems with two Wilson chains patched together we reduce discretization errors. As the NRG reduces the effective bandwidth of the system the time scales accessible by the DMRG are exponentially increased. We employ the hybrid method to simulate the real-time dynamics of the interacting resonant level model (IRLM) after a sudden local quench. For $U = 0$ the method recovers the exact results. In the limit $U \to \infty$ we compare the hybrid method results to results obtained by a strong coupling treatment of the IRLM. We find an excellent agreement. Furthermore, the hybrid method is capable of treating the IRLM in the whole parameter regime.

TT 40.5 Wed 15:00 Poster D

Real space Correlations of Impurities in a Dissipative Environment — •Etienne Gärtner and Ralf Bulla — Institute for theoretical Physics, University of Cologne, Germany

We investigate a model in which two magnetic impurities couple to a one-dimensional lattice of bosons. Since the system is treated quantum-mechanically there can show up the phenomena of coherence between different states and that of entanglement between e.g. the impurities. It is investigated in which way the entanglement between the impurities varies as the distance between the impurities in real space is altered. The models under investigation cannot be solved analytically and are numerically very demanding. It is treated within the Numerical Renormalization Group (NRG) approach that is adapted to deal with multiple bosonic baths which show up in the transformations performed in the NRG.

TT 40.6 Wed 15:00 Poster D

Towards a Numerical Renormalization Group description of the steady-state nonequilibrium single-impurity Anderson model using Lindblad driving — •Frauke Schwarz[1], Ireneusz Weymann[2], Andreas Weichselbaum[1], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich — [2]Institute of Physics, Adam Mickiewicz University, Poznań

Wilson's Numerical Renormalization Group (NRG) allows to describe the single-impurity Anderson model (SIAM) in equilibrium in a non-perturbative way. However, treating situations of steady-state nonequilibrium, such as transport through a quantum dot at finite source-drain bias, remains a challenge for NRG. To model such situations, we consider two additional baths, which are coupled to the left and right leads, respectively. The effect of these baths on the leads can be described by using Lindblad operators [1] in the Liouville equation for the density matrix of the dot and the leads. The action of these operators can, in principle, be chosen such that the left and right leads are effectively held in separate thermal equilibrium at different chemical potentials or temperatures, despite the flow of current. An efficient way of solving this Liouville equation is to use the stochastic quantum trajectory method [1]. The intermediate time evolution needed to generate such trajectories can be done with time-dependent NRG (tNRG) based on complete basis sets. Here we present our preliminary results illustrating the above ideas.

[1] C.W. Gardiner, P. Zoller, Quantum Noise (Springer, Berlin, 2000)

TT 40.7 Wed 15:00 Poster D

Conductance scaling in Kondo correlated quantum dots: role of level asymmetry — •Lukas Merker[1], Theo Costi[1], Enrique Muñoz[2], and Stefan Kirchner[3] — [1]Forschungszentrum Jülich (PGI-2 / IAS-3), Jülich, Germany — [2]Pontificia Universidad Católica de Chile, Santiago, Chile — [3]MPI PKS & CPfS, Dresden, Germany

The low temperature electrical conductance through correlated quantum dots provides a sensitive probe of the physics (e.g., of Fermi-liquid vs non-Fermi-liquid behavior) of such systems. Here, we investigate the role of level asymmetry (gate voltage) and local Coulomb repulsion (charging energy) on the low temperature and low field scaling properties of the linear conductance of a quantum dot described by the single level Anderson impurity model. We use the numerical renormalization group [1] and renormalized superperturbation theory [2] to quantify the regime of gate voltages and charging energies where universal Kondo scaling may be observed and also quantify the deviations from this universal behavior with increasing gate voltage away from the Kondo regime and with decreasing charging energy. Our results could be a useful guide for detailed experiments on conductance scaling in semiconductor and molecular quantum dots exhibiting the Kondo effect [3,4].

[1] L. Merker, et al., preprint (2012)
[2] E. Muñoz, C. J. Bolech, S. Kirchner, Phys. Rev. Lett. (in press), arXiv:1111.4076

[3] A. V. Kretinin, et al., Phys. Rev. B**84**, 245316 (2012)
[4] G. D. Scott, et al., Phys. Rev. B**79**, 165413 (2009)

TT 40.8 Wed 15:00 Poster D

Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot — •Sebastian Bock[1,2], Denes Sexty[1,2], and Thomas Gasenzer[1,2] — [1]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany — [2]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

We study the Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot. The quantum dot is coupled between two leads forming a chemical-potential gradient and the tunneling to the leads is taken into account exactly. We apply the functional-integral approach based on the Schwinger-Keldysh closed time path integral to derive the Kadanoff-Baym dynamic equations from the two-particle irreducible (2PI) effective action. The dynamic equations are derived in non-perturbative approximation of the resummation of direct, particle-particle, and particle-hole channels. The effect of the resummation leads to the introduction of a frequency-dependent 4-point vertex. The method allows the determination of the transient as well as stationary transport through the quantum dot. We study, in particular, the Kondo regime of strong on-site repulsion and low leads-temperature, focusing on the narrowing of the Kondo resonance.

TT 40.9 Wed 15:00 Poster D

Spin-boson coupling in continuous-time quantum Monte Carlo — •Junya Otsuki — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — Department of Physics, Tohoku University, Sendai, Japan

A vector bosonic field coupled to the electronic spin is treated by means of the continuous-time quantum Monte Carlo method. In the Bose Kondo model with a sub-Ohmic density of states $\rho_{\rm B}(\omega) \sim \omega^{-s}$, two contributions to the spin susceptibility, the Curie term T^{-1} and a bosonic fluctuating term T^{-s}, are observed separately. By including the fermionic bath, a quantum phase transition is identified between the Kondo screened state and the bosonic fluctuating state, at which the effective moment and the local Fermi-liquid energy scale vanish. It is demonstrated that the energy scale of the bosonic fluctuation is not affected by the existence of the quantum phase transition.

[1] J. Otsuki, arXiv:1211.5935.

TT 40.10 Wed 15:00 Poster D

Hybridisierungs-CT-QMC mit großen U — •René John Kerkdyk und Thomas Pruschke — Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Mit dem Hybridisierungs-CT-QMC-Algorithmus wird das Multiorbital-Einstörstellen Anderson Modell im Bereich sehr großer U untersucht. Dabei stößt man auf Ergodizitäts- und Effizienzprobleme, die diskutiert werden. Verbesserte Updates ermöglichen das Umgehen energetisch ungünstiger Zustände und erlauben so eine drastische Reduktion der Autokorrelationszeit. Damit verhindern sie auch ein Einfrieren der Besetzung der verschiedenen Orbitale im Einstörstellen Anderson Modell, was sich in fehlender Ergodizität äußert. Mit den zusätzlichen Updates kann man verläßlich Spektralfunktionen auch für extreme Parameter erzielen.

TT 40.11 Wed 15:00 Poster D

π fluxes near the edge of a quantum spin Hall insulator — •Manuel Weber and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Inserting a π flux into a quantum spin Hall insulator creates four spin-charge separated states in the bandgap - two spin fluxons, which form a Kramers doublet, and two charge fluxons. They lead to a characteristic Curie law in the magnetic susceptibility of both free and interacting systems. We study single π fluxes in close distance to the edge states of the Kane-Mele model on a ribbon. Numerical investigations of the susceptibility in the noninteracting model show the Curie law down to low temperatures even for π fluxes located directly at the edge. This can be interpreted as a consequence of the π fluxes' quantum numbers, which inhibit coupling to the edge mode in the absence of interactions. Using CTQMC simulations we investigate the coupling of the π flux to the edge states, when correlations are taken into account.

TT 40.12 Wed 15:00 Poster D

Preparation chain of single crystal intermetallic compounds under UHV-compatible conditions — Andreas Bauer, •Georg Benka, Marein Rahn, Frederik Goerg, Christian Franz, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

High quality single crystals are perhaps the most important technical requirement for major advances in condensed matter physics. To achieve the highest purity it is crucial to avoid contaminations at any of the preparational steps of the crystal growth process. We report the development of an Ar glove-box with a load-lock system that allows to go from the cutting of the starting elements to the initial synthesis of polycrystals with RF heating or arc-melting in a pure Ar environment. This forms the starting point for single-crystal growth by means of rod casting and optical float-zoning under UHV compatible conditions [1]. The improvements in sample preparation achieved with our glove-box are illustrated in terms of exploratory studies of selected rare-earth compounds.

[1] A. Neubauer et al., RSI **82**, 013902 (2011)

TT 40.13 Wed 15:00 Poster D

A pressure study of $CePt_3B$ — •Daniela Rauch[1], Steffen Hartwig[1,2], Stefan Süllow[1], Hiroyuki Hidaka[3], Seigo Yamazaki[3], Hiroshi Amitsuka[3], and Ernst Bauer[4] — [1]Institute of Condensed Matter Physics, University of Technology Braunschweig, Braunschweig, Germany — [2]BENSC, Helmholtz Zentrum Berlin, Berlin, Germany — [3]Department of Physics, Hokkaido University, Sapporo, Japan — [4]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria

$CePt_3B$ is isostructural to the non-centro symmetric heavy-fermion superconductor $CePt_3Si$. In contrast to the latter system, $CePt_3B$ exhibits a complex magnetically ordered state at low temperatures, with an antiferromagnetic phase below $T_N = 7.8$ K and a weakly ferromagnetic transition below $T_C \approx 5$ K. As demonstrated in Ref. [1] $CePt_3B$ can be understand as a low pressure variant of $CePt_3Si$.

Here we report a study of $CePt_3B$ by means of high pressure magnetization measurements, this way in particular accessing the pressure evolution of the ferromagnetic transition temperature T_C. From our investigation up to about 40 kbar we observe an almost constant transition temperature T_C with pressure. This behavior we will discuss in the context of alloying studies on this material.

[1] D. Rauch *et al.*, Phys. Rev B, in print (2012).

TT 40.14 Wed 15:00 Poster D

Momentum dependence of the almost quantum critical spin fluctuations in $CeCu_2Si_2$ — •Zita Huesges[1], Oliver Stockert[1], Hirale S. Jeevan[1], Karin Schmalzl[2], and Frank Steglich[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Jülich Center for Neutron Science, outstation at Institut Laue-Langevin, Grenoble, France

The heavy-fermion superconductor $CeCu_2Si_2$ is located close to a quantum critical point. The spin fluctuations at the nesting wave vector Q_{AF} in the normal state are quasielastic and show considerable slowing down. The magnetic response also exhibits scaling expected for a 3D spin-density-wave quatum critical point. We present here the first measurement of the momentum dependence of these almost quantum critical fluctuations. The temperature dependence of the linewidth of the spin fluctuations in reciprocal space is studied and compared to theoretical expectations, which arise from the connection of momentum width and energy width via the dynamical critical exponent z.

TT 40.15 Wed 15:00 Poster D

Spin-orbit-coupling-induced $j_{\rm eff}$ states in perovskite iridates studied by photoemission spectroscopy — •Atsushi Yamasaki[1,2], Ozan Kirilmaz[2], Michael Sing[2], Akira Sekiyama[3,4], Masaaki Isobe[5], Shigemasa Suga[3,4], and Ralph Claessen[2] — [1]Konan University, Kobe, Japan — [2]Universität Würzburg, Würzburg, Germany — [3]Osaka University, Osaka, Japan — [4]RIKEN SPring-8 Center, Hyogo, Japan — [5]National Institute for Materials Science, Tsukuba, Japan

Novel physics induced by strong spin-orbit coupling has attracted lots of attention from both theory and experiment in recent years. Sr_2IrO_4 has a canted antiferromagnetic insulating state which seems to be driven by the strong spin-orbit coupling and relatively weak Coulomb interaction. The electronic structure near the Fermi level is characterized by $j_{\rm eff} = \frac{1}{2}$ states which have a partially quenched, but still finite angular momentum due to the spin-orbit coupling effect in the O_h crys-

tal field. In order to provide deeper insight into these induced states, we have carried out high energy-resolution photoemission spectroscopy with hν=8.4-8000 eV photons on perovskite iridates. Photoemission spectroscopy in a wide range of excitation energies enables us to identify the bulk and surface electronic structure including their origin in the valence band. Hard-x-ray photoemission spectroscopy reveals genuine bulk j_{eff} states due to the large photoionization cross section of the Ir 5*d*-orbitals and the large photoelectron mean-free path. Our results are compared with LDA+DMFT calculations.

TT 40.16 Wed 15:00 Poster D

Strong Spin-Orbital Coupling and Polarization as origin of the Insulating State in Sr_2IrO_4 — •Markus Aichhorn[1], Cyril Martins[2], Loig Vaugier[2], and Silke Biermann[2] — [1]Institut für theoretische Physik - Computational Physics, TU Graz, Austria — [2]CPHT, Ecole Polytechnique, France

We discuss the notions of spin-orbital polarization and ordering in paramagnetic materials, and address their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory (DMFT) scheme to the case of materials with large spin-orbit interactions, we investigate the electronic excitations of the paramagnetic phases of Sr_2IrO_4 and Sr_2RhO_4. We show that the interplay of spin-orbit interactions, structural distortions and Coulomb interactions suppresses spin-orbital fluctuations. As a result, the room temperature phase of Sr_2IrO_4 is a paramagnetic spin-orbitally ordered Mott insulator. In Sr_2RhO_4, the effective orbital degeneracy is reduced, but the material remains metallic, due to both, smaller spin-orbit and smaller Coulomb interactions. We find excellent agreement of our ab-initio calculations for Sr_2RhO_4 with angle-resolved photoemission.

TT 40.17 Wed 15:00 Poster D

Preparation of $SrIrO_3$ thin films by using metal-organic aerosol deposition technique — •Sebastian Esser, Melanie Schneider, Vasily Moshnyaga, and Philipp Gegenwart — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The interplay between spin-orbit coupling and electronic correlations could lead to interesting novel states in iridium oxide materials. We focus on the perovskite phase of $SrIrO_3$ because Moon et al. [1] showed by using optical spectroscopy and first-principles calculations that the last member of the Ruddlesden-Popper series $Sr_{n+1}Ir_nO_{3n+1}$ ($n = \infty$) is close to the Mott transition. By using metal-organic aerosol deposition technique we have grown $SrIrO_3$ thin films on (111)-oriented $SrTiO_3$ substrates. The cubic symmetry of the $SrTiO_3$ substrate ensured that the $SrIrO_3$ thin film grew in the monoclinic perovskite phase [1,2]. The X-ray diffraction results suggest that $SrIrO_3$ thin films in perovskite structure were obtained and these show out of plane epitaxy with monoclinic $(002)_m$-orientation. The temperature dependence of the electrical resistivity of these $SrIrO_3$ thin films were investigated and metallic behavior was observed down to 50 K.

This work is supported by the German Science foundation through SFB 602, TP A19.

[1] S. J. Moon *et al.*, Phys. Rev. Lett. **101** 226402 (2008)
[2] A. Sumi *et al.*, Thin Solid Films **486**, 182 (2005)

TT 40.18 Wed 15:00 Poster D

Effect of hydrostatic pressure on $Yb(Rh_{1-x}Fe_x)_2Si_2$ — •Sebastian-Horst Hübner, Yoshi Tokiwa, Hirale S. Jeevan, Maik Schubert, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The temperature scale, $T^*(K)$, in undoped $YbRh_2Si_2$ have gathered much attention due to its different interpretations. Substituting Fe on the Rh site in $YbRh_2Si_2$ causes a combined effect of chemical pressure and hole doping. By increasing Fe-doping, both the Kondo temperature and Neél temperature T_N (= 70 mK for x=0) decrease, with a critical concentration of $x \sim$0.08, which suppresses T_N to zero. Since positive pressure enhances T_N in Yb-based materials, the hole doping is most likely responsible for the supression. Along with the suppression of T_N, $T^*(K)$ also decreases with Fe-doping and dissappears around the same critical concentration, x=0.08.

Application of hydrostatic pressure on $Yb(Rh_{1-x}Fe_x)_2Si_2$ with $x >$0.08 may cause a reappearance of antiferromagnetic order and it is highly interesting wheather or not the $T^*(K)$ scale also reappears. Here, we present resistivity of $Yb(Rh_{1-x}Fe_x)_2Si_2$ with x=0.105 under hydrostatic pressure and discuss our results in terms of the proposed interpretations.

TT 40.19 Wed 15:00 Poster D

Magnetic cooling through quantum criticality — •Stefan Doerschug, Bernd Wolf, Natalia van Well, Franz Ritter, Robert Schindler, Wolf Assmus, and Michael Lang — Physikalisches Institut, Goethe-UniversitätFrankfurt (M), Germany

Close to a magnetic field-induced quantum-critical point the entropy at finite temperature exhibit a strong variation upon changing the magnetic field. We demonstrate that this accumulation of entropy can be used for realizing an efficient magnetic cooling. Our proof-of-principle demonstration is based on measurements and theoretical calculations of the magnetothermal properties of low-dimensional antiferromagnets close to their field-induced quantum-critical points. Here we present results of the magnetocaloric effect $\Gamma_B = T^{-1}(\Delta T/\Delta B)_S$ of different xy-antiferromagnets as a function of both field and temperature in the vicinity of the quantum-critical point and discuss various performance characteristics, such as the range of operation, efficiency and hold time. The corresponding figures of the quantum critical systems are compared with those of a state-of-the-art paramagnetic coolant. In addition, we present the experimental set-up, which is used to determine the magnetocaloric effect. The focus is particularly on the construction of a sample-holder for high-resolution measurements in the temperature range 0.02 K $< T <$ 2 K.

TT 40.20 Wed 15:00 Poster D

Candidate for a quantum Griffiths phase in the itinerant ferromagnet $Sr_{1-x}Ca_xRuO_3$ — Dirk Fuchs[1], •Chien-Lung Huang[1,2], Markus Wissinger[1], Rudolf Schneider[1], Jörg Schmalian[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, 76031 Karlsruhe, Germany — [3]Karlsruher Institut für Technologie, Institut für Theorie der Kondensierten Materie, 76031 Karlsruhe, Germany

The magnetization M, susceptibility χ, and the specific heat C of polycrystalline $Sr_{1-x}Ca_xRuO_3$ was investigated as a function of the Ca substitution x. For $x = 0$ a second-order like ferromagnetic (FM) phase transition occurs at T_C = 162 K. T_C decreases with increasing x. Above the critical concentration $x_c \sim 0.7$, i.e., $x \geq x_c$, the FM order is completely suppressed. For $x > 0$ the susceptibility $\chi(T)$ deviates from a Curie-Weiss law below T_C of $SrRuO_3$ which indicates a Griffiths phase (GP) behavior. χ, M, and C are analyzed in detail with respect to the Griffith exponent λ and the GP regime within the phase diagram of $Sr_{1-x}Ca_xRuO_3$.

TT 40.21 Wed 15:00 Poster D

Field-induced quantum criticality in $CeCu_{6-x}Au_x$ — •Kai Grube[1], Sebastian Zaum[1,2], Felix Eilers[1], Diego Zocco[1], Veronika Fritsch[2], Roland Schäfer[1], Oliver Stockert[3], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The heavy-fermion system $CeCu_{6-x}Au_x$ is an archetype for pressure-induced quantum criticality at the onset of antiferromagnetic order. Up to now, investigations focused mainly on the behavior close to the critical concentration $x_c \approx 0.1$. The antiferromagnetic order of samples with higher Au content can, however, be also suppressed by magnetic fields. We studied the field-induced quantum critical behavior of samples with Au contents x = 0.3, 0.5 and 1.0 in fields applied along the magnetic easy axis by using thermal expansion and magnetostriction measurements. Due to their high sensitivities these measurements are especially suited to expose deviations from Fermi-liquid behavior. The measurements have been performed for temperatures ranging between 20 mK and 10 K, and in magnetic fields up to 14 T. With increasing Au content and critical field B_c they show strongly varying critical behavior. We discuss our results taking into account the field-dependent Zeeman splitting of the CEF ground-state doublet, which manifests itself as a Schottky-like anomaly at low temperatures and fields larger than B_c.

TT 40.22 Wed 15:00 Poster D

Spin excitations in CePdAl — •S. Woitschach[1], O. Stockert[1], A. Wildes[2], V. Fritsch[3], H. v. Löhneysen[3], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

Hexagonal CePdAl is a geometrically frustrated heavy-fermion compound that orders antiferromagnetically below $T_N = 2.7$ K in an incommensurate structure. Magnetic order can be continuously suppressed, e.g. by Ni doping on the Pd site. At a Ni content of $\approx 14\%$ the transition is fully suppressed and a quantum critical point is reached. Due to geometrical frustration only 2/3 of the magnetic moments show long-range ordering (LRO), while 1/3 only exhibit short-range order (SRO). In thermodynamic measurements a strong anisotropy between the *c*-axis and the *ab*-plane has been observed. Here we present our neutron diffraction investigations of the (anisotropic) q-space dependence of the LRO and SRO signal in CePdAl below and above T_N.

TT 40.23 Wed 15:00 Poster D

A microscopic study of $Nb_{1-y}Fe_{2+y}$ — •Daniela Rauch[1], Mathias Kraken[1], Jochen Litterst[1], Stefan Süllow[1], and F. Malte Grosche[2] — [1]Institute of Condensed Matter Physics, University of Technology Braunschweig, Braunschweig, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK

The C14 laves phase system $NbFe_2$ represents a very rare case of spin density wave order (SDW) in a 3d metal compound, which can be suppressed by slight changes to the stochiometry in $Nb_{1-y}Fe_{2+y}$. In particular, stoichiometric $NbFe_2$ exhibits a SDW order with a Néel temperature (T_N) around 10K, while slight Fe-excess induces low-moment ferromagnetism, whereas a quantum critical point (QCP) is approached on the Nb-rich side of the composition range. Moreover, samples close to the QCP show non-Fermi liquid behavior ([1]-[4]).

Here we report a microscopic study of the alloying series $Nb_{1-y}Fe_{2+y}$ utilizing μSR and Mössbauer experiments. From our investigation using μSR we verify that all magnetic transitions are bulk transitions. Furthermore, combined with the μSR we present an analysis of the Mössbauer spectroscopy experiments and discuss the nature of the ground state magnetic phase in the light these studies.

[1] D. A. Tompsett *et al.* Phys. Rev B **82**, 155137 (2010)
[2] W. J. Duncan *et al.* Phys. Status Solidi B **247**, 544 (2010)
[3] D. Moroni-Klementowicz *et al.* Phys. Rev B **79**, 224410 (2009)
[4] M. Brando *et al.* Phys. Rev Letter **101**, 026401 (2008).

TT 40.24 Wed 15:00 Poster D

Pressure and field tuning in $CeAgSb_2$ and $NbFe_2$ — •Peter Logg[1], Zhuo Feng[1,2], Takao Ebihara[3], William J Duncan[4], Andreas Neubauer[5], Christian Pfleiderer[5], Hong'En Tan[1], Sven Friedemann[1], Patricia Alireza[1], Swee Goh[1], and F Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]London Centre for Nanotechnology, UCL, London, UK — [3]Dept. of Physics, Shizuoka University, Shizuoka, Japan — [4]Dept. of Physics, Royal Holloway, University of London, Egham, UK — [5]Physik Department E21, Technische Universitat Munchen, Garching, Germany

The intermetallic $CeAgSb_2$ and the dilution series $Nb_{1-y}Fe_{2+y}$ both exhibit *uniaxial* magnetic order which is sensitive to both hydrostatic pressure and transverse magnetic fields. $CeAgSb_2$ is a Kondo-lattice compound which at ambient pressure undergoes a ferromagnetic (FM) transition at $T_C = 9.6$ K. FM is suppressed via the application of either hydrostatic pressure or an *in-plane* tuning field, and extrapolates to zero temperature by pressures exceeding 35 kbar or fields greater than 2.8 T. Contrastingly, slightly iron-rich $Nb_{1-y}Fe_{2+y}$ ($y = 0.015$) undergoes a spin-density wave transition at $T_N = 31$ K, before becoming FM at $T_C = 23$ K. The application of pressure rapidly suppresses both phases, driving the system towards the quantum critical point which may be reached via compositional tuning at around $y = -0.015$.

We investigate the HT and PT phase diagrams of both compounds, through a series of high-pressure and field tuned AC and DC susceptibility measurements.

TT 40.25 Wed 15:00 Poster D

Synthesis and characterization of single-layered manganites — •Johannes Engelmayer, Oliver Breunig, Holger Ulbrich, Markus Braden, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Single-layered manganites show a complex interplay between charge, orbital, and magnetic degrees of freedom. For $La_{1-x}Sr_{1+x}MnO_4$ and $Pr_{1-x}Ca_{1+x}MnO_4$ with doping level $x = 0.5$ (half-doping), the Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of Mn^{3+} and Mn^{4+} ions that is accompanied by an orbital order. This charge and orbital order induces a magnetic order with ferromagnetic three-spin zig-zag chains and antiferromagnetic interchain coupling. For $Pr_{1-x}Ca_{1+x}MnO_4$ and $Nd_{1-x}Sr_{1+x}MnO_4$ with $x = 2/3$, four-spin zig-zag chains could be observed due to a 2:1 ratio of Mn^{4+} and Mn^{3+}. In order to study the charge, orbital, and magnetic order in manganites with other dopants, single crystals of $Pr_{1-x}Sr_{1+x}MnO_4$ and $Nd_{1-x}Ca_{1+x}MnO_4$ with $0.5 \leq x \leq 0.75$ were grown and their structural parameters were determined. We present measurements of resistivity, magnetization, and specific heat that show indications for charge order around room temperature. A dopant and doping-level dependence of the ordering temperature is discussed.

Supported by the DFG through SFB 608.

TT 40.26 Wed 15:00 Poster D

Pulsed Laser and THz Induced Charge Carrier Excitations in $Pr_{0.65}Ca_{0.35}MnO_3$ — •Nils Folchert, Stephanie Raabe, Claus Ropers, and Christian Jooss — Institut für Materialphysik, Göttingen

Quite similar to electric and magnetic fields, optical stimulation of manganites like $Pr_{1-x}Ca_xMnO_3$ (PCMO) can induce transitions from insulating to metallic conductivity. Applying a bias smaller than the threshold voltage of the electrically induced colossal resistance effect (CER), a short laser pulse can melt the charge-ordered state of PCMO yielding to-metal like conductive paths in the illuminated region. This state is preserved until the bias is switched off [1]. PCMO reveals strong correlation effects, i.e., strong electron-electron, electron-phonon and magnetic interactions. The change of these correlations during excitation is a still not very well understood phenomena of perovskite manganites. In order to investigate the transition, we performed time-resolved dc-measurements after pulsed laser excitations with frequencies varying from UV to Thz and at temperatures between 80 K to 300 K. The PCMO samples with $x = 0.35$ were prepared by means of ion-beam-sputtering using single-crystalline MgO substrates. In this poster, we will mainly focus on the relaxation dynamics of the optically excited charge carriers.

[1] M. Fiebig et al., Appl. Phys. Lett. 74, 2310 (1999)

TT 40.27 Wed 15:00 Poster D

Spin polarized HSE hybrid functional calculations of VO_2 — •Udo Schwingenschlögl[1], Ricardo Grau-Crespo[2], and Hao Wang[1] — [1]KAUST, PSE Division, Thuwal, Saudi Arabia — [2]University College London, London, United Kingdom

We study the rutile (R) and monoclinic (M1) phases of the prototypical compound VO_2 by first principles calculations based on density functional theory, employing the Heyd-Scuseria-Ernzerhof (HSE) screened hybrid functional. Our results show that the HSE lowest-energy solutions for both the low-temperature M1 phase and the high-temperature R phase, which are obtained upon inclusion of spin polarization, are at odds with experimental observations. For the M1 phase the groundstate is (but should not be) magnetic, while the groundstate of the R phase, which is also spin-polarized, is not (but should be) metallic. The energy difference between the low-temperature and high-temperature phases is also in strong discrepancy with the experimental latent heat [1].

[1] R. Grau-Crespo, H. Wang and U. Schwingenschlögl, Phys. Rev. B **86**, 081101(R) (2012)

TT 40.28 Wed 15:00 Poster D

Orbital order and phase transitions in $KCrF_3$ — •Carmine Autieri[1,2,3] and Eva Pavarini[1] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]CNR-SPIN, I-84084 Fisciano (SA), Italy — [3]Dipartimento di Fisica "E. R. Caianiello", Università di Salerno, I-84084 Fisciano (SA), Italy

We study the tetragonal to monoclinic structural transition and the origin of the orbital order in $KCrF_3$. We discuss similarities with $KCuF_3$ and $LaMnO_3$. We compare the hopping parameters for the cubic, tetragonal and monoclinic structures of $KCrF_3$ using the both projectors and maximally localised Wannier functions. Moreover, we calculate the Coulomb parameters using a linear response approach. Finally, we study the effects of spin-orbit and the origin of low-temperature weak ferromagnetism.

TT 40.29 Wed 15:00 Poster D

Vibrational IR-spectroscopy of charge-ordered α-ET_2I_3 under pressure — •Armin Dengl[1], Rebecca Beyer[1], Tomislav Ivek[1,2], and Martin Dressel[1] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

One of the most important charge-ordered compounds is the quasi-2D organic conductor α-ET_2I_3. Its structure consists of alternating conducting cation (ET-molecules) and insulating anion (I_3) layers. The compound exhibits a first-order metal-insulator phase transition at $T_{MI} = 135$ K which is accompanied by a horizontal striped charge ordering within the ET layer. For ambient pressure the charge distribution has been well investigated, so we turned our attention to pressure-dependent IR-spectroscopy. The asymmetric charge-sensitive vibration $\nu_{27}(B_{1u})$ is the superior mode to determine the molecular charge due to its high sensitivity of resonance frequency on charge.
We performed vibrational reflectance IR measurements under hydrostatic pressure up to 11 kbar for a temperature range from 10 to 300 K. For the insulating charge-ordered phase we determined the molecular charge for the charge rich molecules. By applying pressure, the phase transition gets suppressed to lower temperatures by (9 ± 0.5) K/kbar towards the metallic phase. The charges of the charge rich molecules do not show any dependence on temperature, but by increasing pressure, a linear shift to lower values can be observed.

TT 40.30 Wed 15:00 Poster D

Seebeck measurements on Pt-C FEBID nanostructures — •Heiko Reith[1,3], Roland Sachser[1], Matthias C. Schmitt[2], Friedemann Voelklein[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany — [2]Guenter Effgen GmbH, Herrstein, Germany — [3]IMtech, Hochschule Rhein Main, Ruesselsheim, Germany

We investigated the thermo voltage of Pt-C granular metals fabricated by focused electron beam-induced deposition (FEBID) using trimethyl (methylcyclopentadienyl) platinum (IV) as precursor. The FEBID structures were deposited on specially designed microchips that allow measuring the Seebeck-coefficient of the samples. The electronic intergrain-coupling strength of the samples was tuned by post-growth electron-irradiation. Controlled by in situ measurement of the electrical conductivity of the deposits electrical conducting, insulator-to-metal transition and insulating samples were obtained by post-irradiation. We present the used microchip and results of the electrical conductivity and the Seebeck-coefficient measurements of the Pt-C granular samples in a temperature range from room to liquid 4He temperature and compare our results with theory.

TT 40.31 Wed 15:00 Poster D

Mott correlated states in the underdoped two-dimensional Hubbard model: variational Monte Carlo versus a dynamical cluster approximation — •Luca F. Tocchio, Hunpyo Lee, Harald 0. Jeschke, Roser Valenti, and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Germany

We investigate the properties of the frustrated underdoped Hubbard model on the square lattice using two complementary approaches, the dynamical cluster extension of dynamical mean field theory, and variational Monte Carlo simulations of Gutzwiller-Jastrow wavefunctions with backflow corrections. We compare data for the energy and the double occupancies, as obtained from both approaches. At small dopings, we observe a rapid crossover from a weakly correlated metal at low interaction strength U to a non-Fermi liquid correlated state with strong local spin correlations. Furthermore, we investigate the stability of the correlated state against phase separation. We observe phase separation only for large values of U or very large frustration. No phase separation is present for the parameter range relevant for the cuprates.

TT 40.32 Wed 15:00 Poster D

Multiplets of the full and simplified Coulomb Hamiltonians in bases of spherical and cubic harmonics — •Hermann Ulm and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich, and RWTH Aachen University, 52425 Jülich, Germany

Correctly including electron-electron interactions is crucial for the realistic description of strongly correlated materials. Approaches like LDA+U use simplified Dudarev Hamiltonian [1] or full Hamiltonian [2] which are both solved in the HF(mean-field) approximation and rotationally invariant, i.e. independent of the basis. For the QMC often the Kanamori Hamiltonian [3] or a simplified density-density version which is basis dependent is used to avoid the Fermi sign problem. Here we compare the spectra and eigenstates of the full rotationally invariant electrostatic Hamiltonian and its simplified versions.

[1] S.L. Dudarev et al., Phys. Rev B 57, 1505 (1998)
[2] A.I. Liechtenstein, V.I. Anisimov, J. Zaanen, Phys. Rev. B 52, R5467 (1995)
[3] J. Kanamori, Prog. Theor. Phys., 275 (1963)

TT 40.33 Wed 15:00 Poster D

Ab-initio Hubbard parameters for molecular crystals by a symmetry decomposed Ewald method — •Michael M. E. Baumgärtel and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich, and RWTH Aachen University, 52425 Jülich, Germany

For strongly correlated molecular crystals we determine realistic Hubbard parameters ab-initio. Restricting to electrons in the partially filled bands, screening by the other electrons renormalizes the Hubbard parameters. The intra-molecular screening is treated within DFT, while inter-molecular Coulomb interaction is modeled by a lattice of distributed polarizabilities. Charging of a molecular orbital breaks the periodic symmetry of dipole interactions. By separating the linear response, we obtain a periodic dipole-dipole interaction operator that is independent of the actual polarization pattern. Inverting this operator gives the self-consistent linear screening. In reciprocal space the interaction matrix is low-dimensional, but long-range. However, we obtain rapidly converging matrix elements through an optimized Ewald-summation.

We present eigen-spectra of Fourier transformed dipole interaction matrices. Employed on a Brillouin zone grid our fast diagonalization method yields the Hubbard parameters, both on-site and long-ranged, for any charging of molecular orbitals. We demonstrate our method for Fullerenes as well as TTF-TCNQ crystals.

TT 40.34 Wed 15:00 Poster D

Effective gauge field description for the bilinear-biquadratic spin-one chain — •Shijie Hu[1], Ari M. Turner[2], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]University of Amsterdam, 1090 GL Amsterdam, The Netherlands

We study the one-dimensional bilinear-biquadratic spin-one model. For this model, the possible existence of a nematic phase between the dimerized and the ferromagnetic phase has been debated. An alternative prediction is derived by modeling the nematic as a quantum rotor model with a Berry's phase. This theory predicts that the long-range nematic phase does not strictly exist, but that the dimerized phase is a version of it that has been disordered by quantum fluctuations. We present evidence for the latter theory by using it to predict the scaling of the correlation length and the dimerization strength, and then testing these scaling laws with large scale infinite system density-matrix renormalization group calculations, suggesting that the dimerization persists (albeit very weakly) all the way to the edge of the ferromagnetic state.

TT 40.35 Wed 15:00 Poster D

Thermal form factors of the anisotropic Heisenberg chain — •Maxime Dugave and Frank Göhmann — Bergische Universität Wuppertal

We derive expressions for the form factors of the quantum transfer matrix of the spin-1/2 XXZ chain which allow us to take the infinite Trotter number limit. This solves the longstanding problem of describing analytically the amplitudes in the leading asymptotics of the finite temperature correlation functions of the model. We show how known results for the high-temperature asymptotics are recovered from the form factor expansion. In the zero-temperature limit we derive the 'critical behaviour' of the form factors from our formulae.

TT 40.36 Wed 15:00 Poster D

Factorisation of correlation functions of the integrable spin-1 Heisenberg chain at finite temperature — •Dominic Nawrath and Andreas Klümper — Bergische Universität Wuppertal, Theoretische Physik, Gauss-Strasse 20, 42119 Wuppertal

Based on the reduced quantum Knizhnik-Zamolodchikov equation we derive discrete functional equations for the two site density matrix of

the isotropic spin-1 Heisenberg chain [1, 2, 3]. This set of equations can be solved by a transcendental two point function that satisfy a three point equation. Furthermore by means of the fusion procedure [6] it seems that the factorization of correlation functions in the spin-1/2 case holds for correlation functions of the spin-1 model [4, 5].

[1] B. Aufgebauer and A. Klümper, J. Phys. A Math. Theor. 45 (2012), 20pp.
[2] H. Boos et al., Algebra and Analysis 17 (2005), 115.
[3] H. Boos et al., Comm. Math. Phys. 261 (2006), 245.
[4] H. E. Boos, V. E. Korepin, F. A. Smirnov, Nucl. Phys. B 658 (2003), 417.
[5] H. E. Boos et al., Nucl. Phys. B 712 (2005), 573.

TT 40.37 Wed 15:00 Poster D

Spin dynamics in Azurite: high-field ESR studies — •M. Ozerov[1], D. Kamenskyi[1], J. Wosnitza[1], H. Engelkamp[2], F. Wolff-Fabris[3], S. Francoual[4], M. Jaime[5], and S. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden - Rossendorf, Germany — [2]High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands — [3]European XFEL GmbH, 22607 Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hasylab Petra III, 22607 Hamburg, Germany — [5]MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$), a spin-1/2 chain system with a distorted diamond structure, has been probed by means of electron spin resonance and far-infrared spectroscopy in magnetic fields up to 50 T. The observed spectra revealed a very complex picture of magnetic excitations including the co-existence of monomer and dimer excitations, as well as their high-energy bound states. The observation of the bound monomer-dimer states is of particular importance, illuminating the limitation of the simple *isolated* dimer-monomer chain model employed for the description of magnetic properties of Azurite previously. The peculiarities of the resonance absorption in Azurite are discussed.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043).

TT 40.38 Wed 15:00 Poster D

Exploring the Magnetic Phase Diagram of the Frustrated Chain Cuprate $PbCuSO_4(OH)_2$ - Linarite — •M. Schäpers[1], A. U. B. Wolter[1], F. Lipps[1], V. Kataev[1], S.-L. Drechsler[1], S. Nishimoto[1], R. Beyer[2], M. Uhlarz[2], J. Wosnitza[2], B. Willenberg[3,5], M. Reehuis[3], K. C. Rule[3], B. Ouladdiaf[4], S. Süllow[5], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]HZB, Berlin, Germany — [4]ILL, Grenoble, France — [5]IPKM, TU Braunschweig, Braunschweig, Germany

We present a detailed experimental and theoretical study of the frustrated s = $\frac{1}{2}$ spin-chain compound Linarite, $PbCuSO_4(OH)_2$, with competing nearest-neighbor and next-nearest-neighbor exchange interactions. Our experimental data are described using various theoretical approaches to obtain the magnetic exchange interactions resulting in a frustration ratio $\alpha \approx 0.36$ close to the 1D critical point [1]. ESR and NMR at elevated temperatures indicate a highly frustrated system with the onset of magnetic correlations far above the long range magnetic ordering temperature $T_N = 2.8$ K. Below T_N the ground state was found to be an elliptical, incommensurate spin spiral [2]. Linarite shows a multiplicity of magnetic field induced phases which could be identified by neutron- and NMR-measurements.

This work has partially been supported by the DFG under Contracts No. WO 1532/3-1 and No. SU229/10-1.

[1] A. U. B. Wolter *et al.*, Phys. Rev. B. **85,** 014407 (2012)
[2] B. Willenberg *et al.*, Phys. Rev. Lett. **108,** 117202 (2012)

TT 40.39 Wed 15:00 Poster D

Synthesis and magnetic characterization of $Cu_3(OH)_4SO_4$ — •Jung Hwan Chun[1], Joseph M. Law[2], and Reinhard K. Kremer[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart — [2]Dresden High Magnetic Field Laboratory, Bautzner Landstrasse 400, 01314 Dresden

We report the successful synthesis and magnetic characterization of $Cu_3(OH)_4SO_4$ which contains Cu triple chains of two non-equivalent Cu^{2+} ions, Cu1 and Cu2[1]. Antlerite, $Cu_3(OH)_4SO_4$, was proposed to be a candidate of an idle-spin magnetic system, with long-range ferromagnetic ordering in the Cu2 central chains and AFM ordering between Cu2-Cu1-Cu2 chains[2]. Recently, it was proposed that the central chains of Cu1 also contribute to field-induced phases. Then it is questioning the proposed picture of Antlerite being an idle spin system[3]. We employed hydrothermal synthesis methods to prepare a phase pure microcrystalline Antlerite polycrystalline sample which we characterized by X-ray diffraction, magnetic susceptibility, heat capacity and high field magnetization measurements.

[1] H. J. Koo, *et al.*, J. Phys. Soc. Jap. **81**, 063704 (2012)
[2] S. Vilminot, *et al.*, Inorg. Chem. **46**, 10079 (2007)
[3] S. Hara, *et al.*, J. Phys. Soc. Jap. **30**, 043701 (2011)

TT 40.40 Wed 15:00 Poster D

Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite — •Britta Willenberg[1,2], Markus Schäpers[3], Kirrily Rule[5], Anja Wolter[3], Manfred Reehuis[1], Bachir Ouladdiaf[4], Hanjo Ryll[1], Bastian Klemke[1], Klaus Kiefer[1], and Stefan Süllow[2] — [1]Helmholtz-Zentrum Berlin, Germany — [2]IPKM, TU Braunschweig, Germany — [3]IFW, Dresden, Germany — [4]Institute Laue Langevin, Grenoble, France — [5]ANSTO, Bragg institute, Australia

The natural mineral linarite $PbCuSO_4(OH)_2$ is a realization of a frustrated one dimensional spin chain. Residual interchain coupling leads to a magnetically ordered state for temperatures below T_N=2.8 K with an unusual critical behavior at the transition. A rich magnetic phase diagram for an applied magnetic field along the chain direction was found [1] which we characterized by neutron diffraction and thermodynamic measurements.

This work has partially been supported by the DFG under contracts WO 1532/3-1 and SU229/10-1.

[1] B. Willenberg et al., Phys. Rev. Lett. **108**, 117202 (2012)

TT 40.41 Wed 15:00 Poster D

Spin dynamics in swedenborgites — •Stefan Buhrandt — Universität Köln

Swedenborgites are magnetic systems of stacked Kagome and triangular lattices that exhibit strong geometric frustration due to antiferromagnetic coupling between all ions. In the most simple model, these systems are described with only two distinct antiferromagnetic next neighbor interactions, one inside and one out of the Kagome layers. Depending on their ratio, the groundstate is either unique or highly degenerated. In the latter case, these systems show interesting dynamics in the sense that one finds flat bands in spin-wave calculations as well as zero-mode signatures in the specific heat within classical Monte Carlo simulations. We discuss the appearance of these zero-modes in dependence on the ratio of the antiferromagnetic couplings and compare to experimental findings on the compund $CaBaCo_2Fe_2O_7$.

TT 40.42 Wed 15:00 Poster D

Pulsed-field experiments on the quasi-2d antiferromagnet Cs_2CuBr_4 — •Lars Postulka, Bernd Wolf, Pham Thanh Cong, Natalia van Well, Franz Ritter, Wolf Assmus, and Michael Lang — PhysikalischesInstitut, Goethe-Universität Frankfurt (M), SFB/TR 49, D-60438Frankfurt (M), Germany

We present pulsed-field measurements up to 50 T of the longitudinal elastic constant c_{11} for 1.5 K $< T <$ 4.2 K on single crystalline samples of Cs_2CuBr_4, aiming at identifying the signatures of the proposed spin liquid in the material's elastic properties. A large softening, caused by the coupling of the quasi-2d spin fluctuations to the phonon system, is observed for magnetic fields smaller than the critical field $B_c \sim 31$ T ($B//$a), an effect which is more pronounced for lower temperatures. As expected, in the fully-polarized state the c_{11} mode is field independent for all temperatures. We compare the magnetoelastic properties of Cs_2CuBr_4 with those of Cs_2CuCl_4 which is less frustrated and according to neutron scattering data can be characterized as a spin liquid. In the latter material the quantum-critical point is located at $B_c = 8.5$ T ($B//$a). In addition, we present a set-up for high precision-magnetization measurements in pulsed fields. The results of the experiments on Cs_2CuBr_4 will be discussed in connection with the ultrasonic data.

TT 40.43 Wed 15:00 Poster D

Magnetic susceptibility measurements in the metal-organic spin-dimer system TK91 at very low temperatures — •S. Becker[1], U. Tutsch[1], B. Wolf[1], Y. Tsui[1], A. Brühl[1], T. Kretz[2], H.-W. Lerner[2], M. Wagner[2], S. Wessel[3], T. Saha-Dasgupta[4], H. Jeschke[5], R. Valentí[5], and M. Lang[1] — [1]Phys.

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Low-dimensional quantum spin systems show interesting properties at very low temperatures and sufficiently high magnetic fields. According to first principle Density Functional Theory calculations, the compound $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91) is expected to be a 2-dimensionally (2d) coupled spin-1/2 dimer system with an intradimer interaction of $J_1/k_B \sim 10$ K and interdimer couplings of $J_i/k_B \sim 1$ K. We report on high-resolution ac-susceptibility measurements on TK91 as function of magnetic field $B \leq 8$ T and temperature 0.04 K $\leq T \leq$ 1 K. Quantum Monte Carlo simulations for various interdimer coupling schemes fit the data very well for the 2d model whereas significant deviations are observed for all other cases thus confirming TK91 as a 2d spin-dimer system. In particular, we identify a range in the B-T phase diagram where the system shows distinct 2dXY behaviour accompanied by the formation of vortices and antivortices in the effective spin configuration.

TT 40.44 Wed 15:00 Poster D

Local probe studies (ESR and NMR) on the $BaAg_2Cu[VO_4]_2$ quantum magnet — •Y. Krupskaya[1], M. Schäpers[1], E. Vavilova[1,2], A.U.B. Wolter-Giraud[1], H.-J. Grafe[1], V. Kataev[1], A. Möller[3], and B. Büchner[1] — [1]IFW Dresden, Germany — [2]ZPhTI, Kazan, Russia — [3]University of Houston, USA

$BaAg_2Cu[VO_4]_2$ contains Cu(II) $S = 1/2$ on a distorted triangular lattice. DFT band structure calculations, quantum Monte-Carlo simulations, and high-field magnetization measurements show that the physics of this compound is determined by a superposition of ferromagnetic and antiferromagnetic uniform spin chains with nearest neighbour exchange couplings of $J_{\mathrm{FM}} = -19$ K and $J_{\mathrm{AFM}} = 9.5$ K [1]. Here we report the study of $BaAg_2Cu[VO_4]_2$ by High-Field/Frequency Electron Spin Resonance (HF-ESR) and Nuclear Magnetic Resonance (NMR) spectroscopies, which probe the local magnetic properties. In the HF-ESR measurements, we observe an anisotropic ESR spectrum typical for the Cu(II) ions and determine the g-tensor, $g_{\mathrm{paral}} = 2.38$ and $g_{\mathrm{perp}} = 2.06$. Moreover, we see a substantial shift of the ESR lines at temperatures below 40 K indicating the presence of short range magnetic correlations. NMR methods allowed for the investigation of local magnetic fields, the T_1 and T_2 relaxation times of the ^{51}V sites. A pronounced broadening of the NMR line is observed at temperatures below 60 K which is consistent with the ESR results. We discuss the local probe results with relation to the thermodynamic studies and theory calculations.

[1] A.A. Tsirlin et al. *Phys. Rev. B* **85**, 014401 (2012)

TT 40.45 Wed 15:00 Poster D

Superconducting energy gap of the organic charge-transfer salts κ-$(ET)_2Cu[N(CN)_2]Br$ and κ-$(ET)_2Cu(NCS)_2$ studied by point-contact spectroscopy — •Severin Schad, Benedikt Hartmann, and Jens Müller — Physikalisches Institut, Goethe Universität, Frankfurt, Germany

The organic charge transfer salts $(BEDT\text{-}TTF)_2X$ form crystalline structures with alternating conducting and insulating layers serving as model systems for two-dimensional metals with strong electronic correlations. Different electronic phases are realised for example by varying the anion X. Compounds with $X{=}Cu[N(CN)_2]Br$ and $Cu(NCS)_2$ show metallic behaviour with a superconducting transition at temperatures of 11.5 K and 9.5 K, respectively.
Although intensively studied, both the anomalous normal conducting state and the nature of superconductivity (regarding the order parameter symetry and the mechanism of cooper pairing) remain unresolved [1]. We use the technique of soft point contact spectroscopy for investigating the superconducting gap structure. Meaningful results require the creation of small interfaces between the superconductor and a normal metal in order to obtain $\frac{\mathrm{d}I}{\mathrm{d}V}$ vs. V curves. The poster will provide information about measurement and various fabrication techniques. Experimental results of both temperature and magnetic-field dependences are presented as well as the discussion of zero-bias conductance curves.

[1] N. Toyota, M. Lang and J. Müller, *Low-Dimensional Molecular Metals*, Solid State Science, Springer-Verlag Berlin Heidelberg (2007)

TT 40.46 Wed 15:00 Poster D

Thin films of the organic charge transfer compounds TMP-F_4TCNQ and TMP-DTF — •Kai Ackermann[1], Milan Rudloff[1], Michael Bolte[2], Harald Jeschke[3], Matthias Wagner[2], Roser Valenti[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue-Straße 7, 60438 Frankfurt am Main — [3]Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We present results of our investigations on thin films of the organic charge transfer compounds TMP-F_4TCNQ [(4,5,9,10-Tetramethoxypyrene)-(2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane)] and TMP-DTF [(4,5,9,10-Tetramethoxypyrene)-(9-Dicyanomethylene-2,4,7-trinitrofluorene)]. The films were grown on silicon dioxide, silicon nitride, sodium chloride and gold substrates by using organic molecular beam deposition (OMBD). The growth properties were investigated by atomic force microscopy (AFM), scanning electron microscopy (SEM) and X-ray diffractometry. The structure analysis of TMP-F_4TCNQ shows a triclinic symmetry with a mixed stack configuration and a layered structure of donor and acceptor molecules. First X-ray diffractograms of TMP-F_4TCNQ films suggest preferential growth perpendicular to the stacking direction on silicon dioxide. Capacitance, conductivity and field effect measurements of both materials are presented and discussed in conjunction with band structure calculations within the framework of density functional theory.

TT 40.47 Wed 15:00 Poster D

Scanning Tunneling Spectroscopy at Surfaces of Superconducting Charge-Transfer Salts — •Sandra Diehl[1,2,3], Torsten Methfessel[2,3], Jens Müller[2,4], Michael Lang[2,4], and Hans-Joachim Elmers[2,3] — [1]Graduate School Materials Science in Mainz, 55099 Mainz — [2]SFB/TR 49 — [3]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [4]Physikalisches Institut, Goethe-Universität, 60438 Frankfurt am Main

Superconducting materials based on organic charge-transfer salts are regarded as candidates for unconventional superconductors because their properties strongly deviate from the BCS theory, similar to the high-temperature superconductors. We study κ-$[ET]_2Cu[N(CN)_2]Br$-crystals. Previous measurements showed a surface contamination of the crystals. Because of that we developed an in-situ cleaving mechanism for the preparation of clean surfaces. Measurements on these cleaved crystals show an improved signal-to-noise ratio in the measured $I(U)$ spectra and atomic flat surfaces in the topographic images (nanometer scale in the height profile). All investigations were done under UHV-conditions ($5 \cdot 10^{-11}$ mbar) using a scanning tunneling microscope at 5 K.

TT 40.48 Wed 15:00 Poster D

New insight in the glass-like dynamics of the organic charge-transfer salts κ-$(BEDT\text{-}TTF)_2X$ from fluctuation spectroscopy — •Benedikt Hartmann[1], Robert Rommel[1], Jens Brandenburg[1], John Schlueter[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt (M) — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

The organic molecular conductors κ-$(BEDT\text{-}TTF)_2X$ are model systems for studying the physics of correlated electrons in reduced dimensions. Recently, the influence of intrinsic disorder on the Mott metal-to-insulator transition (MIT) has been in the focus of experimental and theoretical studies. Fortunately, the degree of intrinsic disorder can be systematically studied through a structural glass-like transition related to the ethylen-endgroups of the BEDT-TTF molecules.
The common method of choice to study the fundamentals of this transition would be dielectric spectroscopy, which due to the materials' high conductivity, however, is not applicable.
In this contribution we demonstrate that fluctuation (noise) spectroscopy is a suitable technique to access the intrinsic properties of the glass-like transition. The temperature dependence of $1/f$-type fluctuations around this transition can be described by a Vogel-Fulcher-Tamman law. Thereby new insight in the glass-like transition is gained and enables one to classify the κ-$(BEDT\text{-}TTF)_2X$-salts as highly fragile glasses.

TT 40.49 Wed 15:00 Poster D

Exploring the full phase diagram of TTF-CA under pressure — •Armin Dengl[1], Tobias Knoblauch[1], Rebecca Beyer[1],

Tomislav Ivek[1,2], Gabriele Untereiner[1], and Martin Dressel[1] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

Tetrathiafulvalene-p-chloranil (TTF-CA) is a 1D organic charge-transfer complex exhibiting a neutral-to-ionic phase transition (NIT), which can be induced both by temperature and pressure. At ambient pressure the phase transition occurs at the critical temperature $T_{\mathrm{NIT}} = 81$ K. It is a first order transition with a jump in ionicity from $\mathrm{CA}^{-0.3}$ to $\mathrm{CA}^{-0.6}$. For a long time the pressure induced NIT was assumed to be continuous, but subsequent studies were able to show a small jump in ionicity. Above a pressure of about 8 kbar, a second sort of CA with a slightly different ionization evolves, an effect which is not yet well investigated.
Most studies on this compound were done either with a dependance on temperature or pressure. We performed vibrational reflectance IR-spectroscopy under hydrostatic pressure up to 11 kbar for a temperature range from 10 to 300 K. To determine the average ionicity per CA molecule we took advantage of the b_{1u} C=O stretching vibration which has a strong dependence of resonance frequency on ionicity. By applying pressure, the NIT shifts to higher temperatures by (25.2 ± 1) K/kbar and the transition becomes broader. For the first time we show the ionicity of CA as a function of both temperature and pressure throughout the whole phase diagram.

TT 40.50 Wed 15:00 Poster D

Thin film growth and characterization of the neutral-ionic phase transition system tetrathiafulvalene-p-chloranil — •Achim Rippert, Milan Rudloff, Kai Ackermann, Lukas Keller, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

Tetrathiafulvalene-p-chloranil (TTF-QCl4) thin films have been prepared by physical vapor deposition of the pre-reacted source material on the substrate materials NaCl, SiO2 and Au. We studied the growth characteristics and electronic transport properties with a view to the influence of substrate-induced effects, such as clamping and strain, on the electronic properties of the layers. TTF-QCl4 is a mixed-stack organic charge transfer compound that shows a temperature-driven paraelectric-to-ferroelectric phase transition associated with a charge of the charge transfer degree at 81 K. This phase transition could be observed in our thin films during electronic transport measurements, as well as in frequency dependent capacity measurements. Furthermore, a color change of the materials could be noticed at the transition temperature. Our research aims for taking advantage of thin-film specific control mechanisms, such as induced biaxial strain and electrostatic field effects, and thus providing a new perspective on the neutral-ionic phase transition in the one-dimensional, mixed-stack organic charge transfer compounds.

TT 40.51 Wed 15:00 Poster D

Resistivity and Hall-Effect Measurements on $LaAlO_3/SrTiO_{3-\delta}$ Heterostructures — •Ahmed Sleem[1,2], Dirk Fuchs[1], Philipp Müller[3], Rudolf Schneider[1], Dagmar Gerthsen[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany — [3]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany

The influence of the oxygen partial pressure $p(O_2)$ during film deposition on the transport properties of $LaAlO_3/SrTiO_{3-\delta}$ heterostructures was analyzed by resistivity and Hall-effect measurements. To this end, thin films of $LaAlO_3$ were grown epitaxially by pulsed laser deposition on TiO_2 terminated <001> oriented $SrTiO_3$ substrates at different oxygen partial pressure $p(O_2)$, i. e., 10^{-3} mbar $\geq p(O_2) \geq 10^{-5}$ mbar. Electrical contacts to the interface were prepared by argon ion-etching and subsequent filling by sputtering of Pt pads. Resistivity measurements were carried out in Van-der-Pauw geometry for 4.2 K $\leq$ T $\leq$ 300 K. The charge carrier concentration, n_e, and mobility, μ_e, were deduced from the Hall-constant, R_H, and conductivity, σ , at room temperature and 4.2K. With decreasing $p(O_2)$ the resistivity changes from an insulating/semi-conductive to a metallic behavior. Experimental results with respect to the sheet resistance R_S, n_e, and μ_e versus $p(O_2)$ will be presented and discussed.

TT 40.52 Wed 15:00 Poster D

Wetting an oxide heterostructure: influence of surface water adsorbates on the electronic properties of $LaAlO_3/SrTiO_3$ studied by in situ photoelectron spectroscopy — •Philipp Scheiderer[1], Florian Pfaff[1], Judith Gabel[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Universität Würzburg, Physikalisches Institut — [2]BESSY II., Albert-Einstein-Strasse 15, Berlin

Oxide heterostructures display many interesting phenomena, one example being the formation of a two-dimensional electron system (2DES) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface beyond a critical thickness of 4 monolayers (ML) of the polar LAO [1,2]. An explanation for this behavior is the so-called electronic reconstruction. In this context it was recently shown that polar adsorbates can enhance the conductivity of the 2DES [3]. Besides their electrostatic influence it was discussed that surface defects/adsorbates can also act as a charge reservoir [4]. To examine the impact of surface adsorbates on the 2DES we performed in situ photoelectron spectroscopy on 6ML thick LAO/STO heterostructures exposed to a defined amount of water vapor. In response to the adsorbed water we observe an increase of charge carriers at titanium sites. Furthermore a comparison between bulk and interface sensitive measurements indicates that the additional charge carriers are located at the interface.

[1] Ohtomo et al., Nature **427**, 423 (2004)
[2] Thiel et al., Science **313**, 1942 (2006)
[3] Xie et al., Nature Comm. **2**, 494 (2011)
[4] Bristowe et al., Phys. Rev. B **83**, 205405 (2011)

TT 40.53 Wed 15:00 Poster D

Localized and delocalized interface states in $LaAlO_3/SrTiO_3$ heterostructures as probed by resonant inelastic x-ray scattering — •Florian Pfaff[1], Hidenori Fujiwara[2], Yoshito Nishitani[3], Yoshihisa Harada[4], Shigemasa Suga[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Graduate School of Engineering Science, Osaka University — [3]Department of Physics, Konan University — [4]Institute for Solid State Physics, University of Tokyo

The interface between the two band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) hosts a two-dimensional electron system of *itinerant* charge carriers above a critical LAO overlayer thickness of 3 monolayers. Interface ferromagnetism coexisting with superconductivity has been found and attributed to *local* moments. Recently, two peaks in resonant inelastic x-ray scattering (RIXS) indeed have been correlated with *delocalized* and *localized* charge carriers [1]. To shed light on the coexistence of the two types of Ti 3d carriers we performed RIXS on LAO/STO heterostructures with different overlayer thicknesses and different concentrations of oxygen vacancies. While there is an increase of the total charge seen in RIXS with increasing film thickness for samples showing the critical thickness behavior, surprisingly, the spectrum remains unchanged for samples that have been intentionally doped with oxygen vacancies. We discuss this in terms of the electronic reconstruction scenario and a possible non equilibrium situation due to the generation of electron-hole pairs during irradiation.

[1] Ke-Jin Zhou et al., Phys. Rev. B 83, 201402(R) (2011)

TT 40.54 Wed 15:00 Poster D

Growth and physical properties of $La_8Cu_7O_{19}$ single crystals — •Ashwin Mohan[1], Surjeet Singh[2], Wolf Schottenhamel[1], Giacomo Prando[1], Sven Partzsch[1], Valentina Bisogni[1], Abdel-Hafez Mahmoud[1], Jochen Geck[1], Sabine Wurmehl[1], Christian Hess[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]IISER Pune, India

Spin ladder compounds are valuable in understanding the physics of crossover from one dimensional to the two dimensional nature of spin systems. They have been known to show interesting magnetic ground states and even superconductivity upon doping. Gapped and ungapped spin excitation spectra have been predicted and experimentally verified for spin ladders with even and odd number of ladder-legs respectively. Therefore, this class of materials has been of particular interest in the field of low dimensional quantum magnets. It is known that in the thermodynamic phase diagram of La_2O_3-CuO there exists a compound whose spin structure resembles that of a five leg ladder, though there has not been much progress towards understanding its magnetism as it is challenging to grow it as a single crystal. Here, we have used the travelling floating zone method to grow single crystals of $La_8Cu_7O_{19}$ and measured some of its physical properties. This compound magnetically orders below 103K and shows anisotropic magnetic behavior, the nature of which is not yet clear.

TT 40.55 Wed 15:00 Poster D

Phase diagram of the effective Ising spin-1/2 chain compound $CoNb_2O_6$ in transverse magnetic field — •Simon Scharffe, Oliver Breunig, Johanna Frielingsdorf, Martin Valldor, Markus Garst, Eran Sela, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

$CoNb_2O_6$ is a model system to investigate the quantum phase transition of Ising spins in a transverse magnetic field. The interesting physics exclusively takes place within the magnetic CoO_6 layers, separated by non-magnetic NbO_6 layers. The edge-sharing oxygen octahedrons link the Co^{2+}spins and form 1D ferromagnetic chains along the c axis. Due to crystal field effects an easy-axis anisotropy is present, which leads to an effective spin-1/2 system described by the Ising model. Small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$ cause long-range antiferromagnetic order, which is incommensurate below T_{N1}=2.95 K and becomes commensurate at T_{N2}=1.97 K. A magnetic field parallel to the b axis is normal to the easy axis and allows to study the quantum phase transition in transverse field. Above 5 T the system is driven through its quantum critical point to a quantum paramagnet. Only few studies of the transverse field case are available. We present measurements of specific heat and magnetization in a temperature range from about 0.3 up to 10 K and discuss the phase diagram. We compare our measurements with the theoretical predictions of the 1D Ising model in a transverse field.

This work was supported by the DFG through SFB 608.

TT 40.56 Wed 15:00 Poster D

Coexistence of anomalous and normal diffusion in integrable Mott insulators — •Robin Steinigeweg[1,2], Jacek Herbrych[2], Peter Prelovšek[2], and Marcin Mierzejewski[3] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig — [2]Department of Theoretical Physics, Jožef Stefan Institute, SI-1000 Ljubljana — [3]Institute of Physics, University of Silesia, PL-40-007 Katowice

We study the finite-momentum spin dynamics in the one-dimensional XXZ spin chain within the Ising-type regime at high temperatures using density autocorrelations within linear response theory and real-time propagation of nonequilibrium densities. While for the nonintegrable model results are well consistent with normal diffusion, the finite-size integrable model unveils the coexistence of anomalous and normal diffusion in different regimes of time. In particular, numerical results show a Gaussian relaxation at smallest nonzero momenta which we relate to nonzero stiffness in a grand canonical ensemble. For larger but still small momenta normal-like diffusion is recovered. Similar results for the model of impenetrable particles also help to resolve rather conflicting conclusions on transport in integrable Mott insulators.

TT 40.57 Wed 15:00 Poster D

Quantum phases of a frustrated four-leg spin tube — Marcelo Arlego[1], Wolfram Brenig[2,3], •Yousef Rahnavard[2,3], Björn Willenberg[2,3], Hector Rosales[1], and Gerardo Rossini[1] — [1]Departamento de Fisica, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina — [2]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [3]Niedersächsische Technische Hochschule, NTH

We study the ground state phase diagram of a frustrated spin-1/2 four-leg tube. Using a variety of complementary techniques, namely density matrix renormalization group, exact diagonalization, Schwinger boson mean field theory, quantum Monte-Carlo and series expansion, we explore the parameter space of this model in the regime of all-antiferromagnetic exchange. In contrast to unfrustrated four-leg tubes we uncover a rich phase diagram. Apart from the Luttinger liquid fixed point in the limit of decoupled legs, this comprises several gapped ground states, namely a plaquette, an incommensurate, and an antiferromagnetic quasi spin-2 chain phase. The transitions between these phases are analyzed in terms of total energy and static structure factor calculations and are found to be of (weak) first order. Despite the absence of long range order in the quantum case, remarkable similarities to the classical phase diagram are uncovered, with the exception of the icommensurate regime, which is strongly renormalized by quantum fluctuations. In the limit of large leg exchange the tube exhibits a deconfinement cross-over from gapped magnon like excitations to spinons.

TT 40.58 Wed 15:00 Poster D

Tuning frustrated antiferromagnetism in intermetallic AFe_4X_2 systems — •Katharina Weber[1,2], Nandang Mufti[1], Til Goltz[2], Theo Woike[3], Hans-Henning Klauss[2], Christoph Bergmann[1], Inga Kraft[1], Helge Rosner[1], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Solid State Physics, Dresden University of Technology, Dresden, Germany — [3]Institute for Structural Physics, Dresden University of Technology, Dresden, Germany

Magnetic systems with reduced dimensionality or frustration are attracting strong interest because these features lead to an increase of quantum fluctuations which often results in unusual, very interesting properties. Here we present a detailed study of the intermetallic AFe_4X_2 compounds (A = Sc, Y, Lu, Zr; X = Si, Ge) crystallizing in the $ZrFe_4Si_2$ structure type in which the Fe-sublattice is formed by chains of edge-linked tetrahedra. We synthesized polycrystalline samples of all these compounds and investigated their magnetic, thermodynamic, structural and transport properties. Our results indeed evidence this family of compounds to cover the whole regime from frustrated antiferromagnetic (AFM) order up to the quantum critical point separating the AFM ground state from the paramagnetic ground state. All compounds with trivalent A elements show frustrated AFM order. Replacement of trivalent A by tetravalent Zr shifts the system towards an unstable magnetic state. Since YFe_4Si_2 and $ZrFe_4Si_2$ present peculiar features, we also studied the influence of different annealing conditions and slight off-stoichiometry on their unusual properties.

TT 40.59 Wed 15:00 Poster D

Phase Space Berry Phases and Electronic Transport in Magnetic Whirl Structures — •Robert Bamler and Achim Rosch — Universität zu Köln, Cologne, Germany

We present a semi-classical theory of electronic transport in magnetic whirl structures with spin-orbit coupling. Our theory predicts that the magnetic whirls carry an electric charge due to a non-vanishing Berry phase curvature in phase space.

In magnetic materials without inversion symmetry (e.g. MnSi), the spin-orbit coupling can lead to smooth whirls (skyrmions) in the magnetization. The magnetic whirls give rise to an emergent magnetic field that can be measured as a so-called "topological" contribution to the Hall signal. The emergent magnetic field is usually explained with the picture that conduction electrons that transverse the system pick up a Berry phase because their spin follows adiabatically the direction of the local magnetization. This explanation neglects the influence of spin-orbit coupling. However, the anomalous Hall effect in MnSi is known to be large, indicating that spin-orbit coupling may be relevant in this material.

In our work, we develop a semi-classical theory of electronic transport in magnetic whirl structures under the influence of spin-orbit coupling. In addition to the emergent magnetic field and the anomalous velocity known from the anomalous Hall effect, new cross-terms arise in the equations of motion and the skyrmions acquire an electric charge due to Berry phases picked up on closed trajectories in mixed coordinate and momentum space.

TT 40.60 Wed 15:00 Poster D

Transverse susceptibility of high-quality single crystal MnSi — •Felix Rucker[1], Andreas Bauer[1], Alfonso Chacón[1], Maximilian Hirschberger[2,1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Department of Physics, Princeton University, Jadwin Hall, Princeton, USA

We have developed a bespoke ac susceptometer which is mounted to a computer controlled rotator. Our susceptometer permits low temperature measurements in applied magnetic fields as a function of angle ranging from a purely longitudinal to a purely transverse set up, i.e., the excitation field may be varied from a parallel to a perpendicular orientation with respect to the applied field, respectively. To demonstrate the operation of our susceptometer we have measured the ac susceptibility of high-quality single crystal MnSi, which reveals several unexpected features of the transverse susceptibility across the magnetic phase diagram. We discuss our results in the context of the comprehensive theoretical framework developed for the helical order and field-induced phases in B20 compounds.

TT 40.61 Wed 15:00 Poster D

Linear magnetoelectric effects in the cubic ferrimagnetic helimagnet Cu_2OSeO_3: phenomenological theory — Maria Eleni Belesi[1,2], •Ioannis Rousochatzakis[2], Mohamed Abid[1,3], Ulrich Rössler[2], Helmut Berger[1], and Jean-Philippe Ansermet[1] — [1]Institut de Physique de la Matiére Condensée, Ecole Polytechnique

Fédérale de Lausanne, Station 3, CH-1015 Lausanne-EPFL, Switzerland — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [3]King Saud University, Riyadh 11451, Saudi Arabia

We present a phenomenological Landau-Ginzburg theory for the linear magnetoelectric (ME) effect in the spin 1/2 compound Cu_2OSeO_3. Single-crystal ME data show two additional phases below the 3up-1down ferrimagnetic state. We demonstrate that these are related to the field-driven evolution of a long-period helical phase, which is stabilized by the chiral Dzyaloshinskii-Moriya term $D\mathbf{M}\cdot(\nabla\times\mathbf{M})$ that is present in this noncentrosymmetric compound. The theory is in excellent agreement with experiment, and shows three main features: (i) the polarization P has a uniform as well as a long-wavelength component that follows the magnetic twisting; (ii) the uniform component points along (H_yH_z, H_zH_x, H_xH_y); and (iii) its strength is proportional to $\eta_\parallel^2-\eta_\perp^2/2$, where $\eta_\parallel$ and $\eta_\perp$ are the longitudinal and transverse components of the magnetic order. Hence, the field dependence of P provides a clear signature of the evolution of a conical helix under a magnetic field. A similar theory is discussed for the magnetocapacitance.

TT 40.62 Wed 15:00 Poster D

Skyrmionic exictations in magnetoelectric Cu_2OSeO_3 — •Steffen Harms[1], Maria Belesi[2], Helmuth Berger[3], Jean-Philippe Ansermet[3], Christoph Grams[1], Daniel Niermann[1] und Joachim Hemberger[1] — [1]2. Physikalisches Institut, University of Cologne, Germany — [2]Leibniz Institute for Solid State and Material Research, Dresden, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Skyrmions are topologically protected spin textures that can be characterized by their winding number. Since their discovery in MnSi, skyrmions are of special interest because of their high potential for applications in spintronics [1]. The magnetoelectric helimagnetic insulator Cu_2OSeO_3 undergoes a phase transition from the helical magnetic phase into the skyrmion phase at 57.5 K around 200 Oe. It was recently shown, that the excitation of these phases can be seen in the microwave absorption spectra where an AC magnetic field was coupled to the sample [2]. We present the results of our broadband dielectric spectroscopy measurements up to 4 GHz, in which we measured the excitiations created by coupling an AC electric field to the sample for different magnetic fields at fixed temperatures of 57.5 K and 40 K.

Work supported by the DFG through SFB 608.

[1] C. Pfleiderer and A. Rosch., Nature 465, 880 (2010)
[2] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012)

TT 40.63 Wed 15:00 Poster D

Vibrating-coil magnetometry in rare-earth pyrochlore compounds — •Christopher Krey[1], Stefan Legl[1], Sarah R. Dunsiger[1], Jason S. Gardner[2], Jennifer M. Roper[3], Hanna A. Dabkowska[4], Jose A. Rodriguez[5], Graeme M. Luke[5], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, Garching — [2]Department of Physics, Indiana University, Bloomington, USA — [3]Los Alamos National Laboratory, New Mexico, USA — [4]Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — [5]Department of Physics and Astronomy, McMaster University, Hamilton, Canada

An important characteristic of the spin ice systems $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ as well as the spin liquid system $Tb_2Ti_2O_7$ is the observation of spin freezing below a few hundred mK. We report vibrating coil magnetometry down to mK temperatures of these systems, addressing the evidence for field-induced transitions [1,2]. Of particular interest is evidence of putative magnetisation avalanches in the spin-frozen state, which for the case of $Dy_2Ti_2O_7$ have been interpreted as magnetic monopole avalanches [3].

[1] C. Krey *et al.*, Phys. Rev. Lett. **108**, 257204 (2012)
[2] S. Legl *et al.*, Phys. Rev. Lett. **109**, 047201 (2012))
[3] D. Slobinsky *et al.*, Phys. Rev. Lett. **105**, 267205 (2010)

TT 40.64 Wed 15:00 Poster D

Versatile module for fast experiments with focussing neutron guides — •Tim Adams[1], Georg Brandl[1], Alfonso Chacon[1], Marein Rahn[1], Sebastian Mühlbauer[2], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, 85748 Garching — [2]ZWE FRM II, Technische Universität München, 85748 Garching

We report the development of a versatile module that permits fast and reliably the use of focussing neutron guides. We report the procedure of setting up the instrument and typical artefacts under non-ideal conditions. Exploiting gain factors of intensity by an order of magnitude we demonstrate the functionality of the module in a study of the effects of uniaxial stress on the spin-flip transition in single crystal Cr.

TT 40.65 Wed 15:00 Poster D

Preparation and characterization of doped spin ice — •Peter Laschitzky, Martin Hiertz, Oliver Breunig, Gerhard Kolland, Johanna Frielingsdorf, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

The magnetic Dy sites in $Dy_2Ti_2O_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. A strong crystal field results in an Ising anisotropy of the magnetic moments of the Dy site which align along their local easy axes in the {111} directions pointing either into or out of the tetrahedra. As a consequence, the spin system is geometrically frustrated even in the groundstate. The magnetic excitations in spin ice are discussed as magnetic monopoles. We synthesized the mother compound $Dy_2Ti_2O_7$ and the doped compounds $Dy_{2-x}Y_xTi_2O_7$ with $x = 0.1, 0.2, 1, 2$ and $Dy_2Ti_{1.8}Zr_{0.2}O_7$. Large, high-quality single crystals were grown by the floating-zone method. To characterize the grown crystals, we measured the magnetization, the specific heat and the thermal conductivity for various magnetic-field directions. Doping with non-magnetic Y has a strong influence on the magnetic subsystem. For example, the magnetic contribution κ_{mag} to the thermal conductivity[1] can be completly suppressed by Y doping. Substitution of the non-magnetic Ti by larger Zr ions reduces the phononic thermal conductivity, whereas the magnetic contribution is essentially conserved.

Supported by the DFG through SFB 608

[1] Kolland *et. al.*, Phys. Rev. B **86**, 060402 (2012)

TT 40.66 Wed 15:00 Poster D

Investigations of the Magnetic Properties in the Pyrochlore $Ho_2Ti_2O_7$ — •Rico Schönemann[1], Thomas Herrmannsdörfer[1], Elizabeth Lauren Green[1], Richard Skrotzki[1,2], Zhaosheng Wang[1], Hiroshi Kaneko[3], Haruhiko Suzuki[3], and Joachim Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, Dresden, Germany — [3]Faculty of Mathematics and Physics, Kanazawa University, Kanazawa, Japan

Pyrochlore compounds such as $R_2Ti_2O_7$ (where R is Ho or Dy) have an highly degenerate ground state where the R^{3+} moments obey the "ice rules". This provides access to study extraordinary physical phenomena, like the formation of magnetic monopoles. Recent publications evidence monopoles which can be probed using high frequency (adiabatic) susceptibility measurements [1]. We performed ac susceptibility measurements on a single-crystal $Ho_2Ti_2O_7$ sample at low temperatures down to 30 mK and magnetic fields up to 14 T. Based on isothermal frequency sweeps we were able to determine spin relaxation rates. Both the real and imaginary parts of the temperature-dependent magnetic susceptibility measurements show the spins freezing below 1 K and provide insight into the magnetic-monopole density.

This research has been funded in part by EuroMagNET II (EU contract No. 228043).

[1] L. Bovo et al., arXiv:1210.0106v1 (2012)

TT 40.67 Wed 15:00 Poster D

Thermodynamic properties of spin-S boundary defects in antiferromagnetic Heisenberg chains — •Björn Willenberg[1,3], Jan Grelik[2,3], Wolfram Brenig[1,3], and Holger Frahm[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 spin-S impurities in contact to isotropic and anisotropic S=1/2 Heisenberg chains with open boundary conditions and an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo methods based on Stochastic Series Expansion. Results will be presented for thermodynamic properties as functions of temperature, exchange-coupling constants, anisotropy, magnetic fields, and system size. For particular choices of parameters the models we investigate are exactly solvable by means of Bethe Ansatz techniques which will be used to obtain quantities like energy, magnetization, and susceptibility at zero temperature. In this limit we will compare our findings from both methods.

TT 40.68 Wed 15:00 Poster D

Optical phonons in multiferroic $CuCrO_2$, studied by Raman and Far-Infrared spectroscopy — •Michael Eichberger[1], Jean Geurts[1], Michael Schmidt[2], Vladimir Tsurkan[2,3], and Joachim Deisenhofer[2] — [1]Institute of Physics, University of Würzburg, Germany — [2]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

$CuCrO_2$ is an example for a multiferroic material, in which the ferroelectric order is driven by a proper-screw type magnetic order, occurring below $T_N \sim 24$ K. While the magnetic order and its coupling with the ferroelectricity has been in the focus of most research activities on this system, we investigated the optical phonons and the possible effect of spin ordering, employing Raman and FIR spectroscopy. As the $CuCrO_2$ crystal structure (space group $R\bar{3}m$) has an inversion centre, Raman spectroscopy gives access to the g-modes, while FIR probes the u-modes. All expected optical modes (A_{1g}, E_g, $2A_{2u}$, $2E_u$) were observed. No mode splitting or emergence of new modes occurs when entering the magnetically ordered state. The E_g mode shows a slight softening in the low temperature range, which may indicate a weak spin-phonon coupling. This mode is modulating the Cr-O bonding and thereby affecting the overlap of the participating wavefunctions. At the same time, this overlap is responsible for the antiferromagnetic interaction between the Cr-atoms and hence establishing the magnetic order within the Cr-plane.

TT 40.69 Wed 15:00 Poster D

The spin Drude weight in the spin-1/2 XXZ chain: a combined exact diagonalization and time-dependent DMRG study — •Johannes Hauschild[1], Christoph Karrasch[2], Stephan Langer[1,3], and Fabian Heidrich-Meisner[1,4] — [1]LMU Munich — [2]University of California, Berkley — [3]University of Pittsburgh, USA — [4]FAU Erlangen-Nuremberg

Various theoretical approaches predict a finite Drude weight D for spin transport in the gapless phase of the spin-1/2 XXZ chain, suggesting ballistic transport properties. Here we address two open questions: first, the temperature dependence of the Drude weight and second, the particular point of an SU(2) symmetric exchange, for which there is no agreement as to whether D is finite or not. We compute the Drude weight at finite temperatures with two approaches [1]: time-dependent density matrix renormalization group simulations using purification [2] and exact diagonalization. For the latter, we compare finite-size data obtained in either the grand-canonical or the canonical ensemble. We argue that the grand-canonical data, obtained from averaging over all subspaces with different magnetizations, have a more systematic finite-size dependence than the canonical one. The results for D(T) from exact diagonalization and tDMRG are in good quantitative agreement in the massless phase.

We acknowledge support from the DFG through FOR 912.

[1] C. Karrasch, J. Hauschild, S. Langer, F. Heidrich-Meisner, in preparation
[2] C. Karrasch, J. H. Bardarson, and J. E. Moore, Phys. Rev. Lett. 108, 227206 (2012)

TT 40.70 Wed 15:00 Poster D

Kinetic description of the thermalization dynamics of weakly interacting quantum systems — •Michael Stark and Marcus Kollar — Theoretical Physics III, Center for electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

After a sudden disruption, weakly interacting quantum systems first relax to a prethermalized state [1] that can be described by perturbation theory and a generalized Gibbs ensemble [2]. Using these properties of the prethermalized state we perturbatively derive a kinetic equation which becomes a quantum Boltzmann equation in the scaling limit of vanishing interaction [3]. Applying this to interaction quenches in the fermionic Hubbard model [4] we find that the momentum distribution relaxes to the thermal prediction of statistical mechanics. For not too large interaction, this two-stage scenario can thus provide a quantitative understanding of the time evolution leading from a pure initial state to the thermal state.

[1] M. Moeckel and S. Kehrein, PRL **100**, 175702 (2008); Ann. Phys. (New York) **324**, 2146 (2009)
[2] M. Kollar, F. A. Wolf, and M. Eckstein, PRB **84**, 054304 (2011)
[3] L. Erdös, M. Salmhofer, H.-T. Yau, J. Stat. Phys. **116**, 367 (2004)
[4] M. Eckstein, M. Kollar, and P. Werner, PRL **103**, 056403 (2009); PRB **81**, 115131 (2010)

TT 40.71 Wed 15:00 Poster D

Quasiparticle parameterization of meanfields, Galilean invariance and universal conserving response function — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The form of meanfield and density functional parameterization in terms of current, energy and density are examined by the restriction of Galilean invariance. It is found that besides a density functional only one parameter remains which is usually condensed in the effective mass. The universal response with respect to density, momentum and energy is found in the sense that the response becomes independent on actual parameterization of the local equilibrium provided the conservation laws are enforced. The sum rules by frequency moments and the compressibility sum rule impose further restrictions which determines the last parameter.

TT 40.72 Wed 15:00 Poster D

Electronic structure of Cu: An LDA+DMFT approach — •Kathrin Garb[1], Wilhelm Appelt[1], Joseph-Andreas Weber[2], Michael Leitner[3], Christoph Hugenschmidt[2,4], Peter Böni[2], Igor Di Marco[5], and Liviu Chioncel[6,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [3]Technische Universität München, Physik Department E13, D-85748 Garching, Germany — [4]Technische Universität München, FRM II, 85747 Garching, Germany — [5]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden — [6]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

Although DFT calculations predict the overall band structure of Cu correctly, the entire d-bands' manifold is experimentally found at energies about 0.5 eV lower than the calculated ones. We apply state-of-the-art LDA+DMFT calculations and discuss several technical aspects of the implementation that can be used to explain the picture of weak correlation provided by the Fermi surface results with the intrinsic in-band shift of 0.5 eV.

TT 40.73 Wed 15:00 Poster D

Electronic correlations in FeAl: an LDA+DMFT study — •Anna Galler[1], Ciro Taranto[1], Merzuk Kaltak[2], Giorgio Sangiovanni[3], Alessandro Toschi[1], Georg Kresse[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Vienna, Austria — [2]Department of Computational Materials Physics, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We applied the local density approximation combined with dynamical mean-field theory (LDA+DMFT) to the intermetallic compound FeAl. This material shows unexpected magnetic properties. In fact, experimentally it is known to be nonmagnetic while conventional LDA calculations give a ferromagnetic solution.

We claim that this feature is an effect of nontrivial electronic correlations due to the presence of narrow Fe d bands at the Fermi level. The low energy part of the Hamiltonian was projected onto a set of 9 maximally localized Wannier orbitals, and the interaction parameters were computed using the constrained random-phase approximation (cRPA) approach. A continuous-time quantum Monte Carlo in the hybridization expansion was used as impurity solver for the DMFT. In analogy with the iron pnictides, our results show the important role played by the Hund's coupling, that places FeAl in the class of the so called Hund's metals.

TT 40.74 Wed 15:00 Poster D

The LDA+RISB and LDA+DMFT method: A juxtaposition — •Christoph Piefke[1], Daniel Grieger[1,2], and Frank Lechermann[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]SISSA, via Bonomea 265, 34136 Trieste, Italy

The LDA+RISB (Rotationally Invariant Slave Bosons) and LDA+DMFT (Dynamical Mean-Field Theory) methods are nowadays well established tools describing effects of strong electronic correlations in realistic materials from first principles. Their general concept is to add many-body physics to effective one-particle band structure

calculations. Both of them have specific advantages and disadvantages concerning accuracy, numerical efficiency and types of physical effects that can be described. This presentation aims at giving an overview of the theoretical and technical details of both LDA+methods in question, as well as showing the respective strengths and problems via comparing results for a selection of materials. Special attention is given to charge self-consistency[1], which allows for a direct feedback of the respective many-body method onto the LDA part.

[1] D. Grieger, C. Piefke, O. E. Peil and F. Lechermann, Phys. Rev. B 86, 155121 (2012)

TT 40.75 Wed 15:00 Poster D

Variational Cluster Approximation for broken symmetry phases in strongly correlated electron systems — •Benjamin Lenz, Piet Dargel, and Thomas Pruschke — Institut für theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany

The variational cluster approximation (VCA) allows to study broken symmetry phases of various lattice models at zero temperature. We present results for s-type superconductivity of the attractive two-dimensional Hubbard model in the infinite-cluster size limit of VCA. They are discussed in comparison to results from dynamical mean-field theory in combination with the numerical renormalization group method. As a second example, we give an outlook to the investigation of antiferromagnetism and superconductivity in a paradigmatic model for heavy fermions – the Kondo lattice model.

TT 40.76 Wed 15:00 Poster D

Quantification of correlations in an exactly solvable model of harmonically interacting particles — Jan Skolimowski[1], •Krzysztof Byczuk[1], and Dieter Vollhardt[2] — [1]Faculty of Physics, University of Warsaw, Hoza 69, 00-681 Wrszawa, Poland — [2]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We employ the relative von Neumann entropy to quantify correlations in a system of interacting particles. The interaction between the particles is harmonic potential-like, making the model exactly solvable. The exact expression for the relative entropy is expanded in the coupling constant, which allows us to classify the different contributions to correlations in terms of Feynman diagrams or correlation functions.

TT 40.77 Wed 15:00 Poster D

A slave rotor approach to the dynamical screening of Coulomb interactions — •Igor Krivenko[1,2], Silke Biermann[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]Centre de Physique Théorique (CPHT), École Polytechnique, 91128 Palaiseau Cedex, France

We present a new theoretical approach to lattice and impurity models of strongly correlated electrons with the dynamically screened Coulomb interactions. The method is based on a slave rotors decoupling of the screened interaction and provides a consistent description of quantum impurities with both fermionic and bosonic bath. It is shown, that the simplest meaningful approximation within this method coincides with the dynamic atomic limit approximation (DALA). More refined approximations beyond DALA are constructible in a regular way using a saddle-point or perturbative treatment of the rotor degrees of freedom. The proposed method gives a computationally cheap way to apply existing quantum impurity solvers for unscreened static interactions to the cases of frequency-dependent interactions. It allows to calculate thermal Green's functions and higher-order correlation functions of the impurity models. These functions then can be used as building blocks of modern perturbative approaches to lattice models involving phonons, magnons and other bosonic excitations.

TT 40.78 Wed 15:00 Poster D

Functional RG study of Goldstone fluctuations in the ground state of a fermionic superfluid — •Benjamin Obert, Christoph Husemann, and Walter Metzner — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

We analyse the effect of Goldstone fluctuations in the superfluid ground state of the attractive Hubbard model. We apply a coupled bosonic-fermionic functional renormalization group approach to investigate the infrared behaviour in the symmetry-broken state. Bosonic fluctuations, especially Goldstone fluctuations lead to several divergencies in the infrared, which partially cancel due to symmetry. Our results capture the exact infrared behaviour of the interacting Bose gas.

TT 40.79 Wed 15:00 Poster D

Two-particle Green functions calculated by continuous time quantum Monte Carlo simulations — •Markus Wallerberger[1], Emanuel Gull[2], Nico Parragh[3], Giorgio Sangiovanni[3], Alessandro Toschi[1], and Karsten Held[1] — [1]Technische Universität Wien, Austria — [2]University of Michigan, Ann Arbor MI, USA — [3]Universität Würzburg, Germany

While dynamical mean field theory (DMFT) has provided fundamental insights into the physics of strongly correlated materials, its approximations break down in low dimensional systems and near second-order phase transitions. Diagrammatic extensions of DMFT like the dynamical vertex approximation (DΓA) and the dual fermion approach which attempt to tackle this problem have the local two-particle Green function as central ingredient. Besides, this quantity is also needed for vertex corrections to response functions.

A state-of-the-art method for solving the DMFT impurity problem is the continuous-time quantum Monte Carlo (CT-QMC) method in its hybridization expansion formulation (CT-HYB). The sheer amount of information encoded in two-particle quantities, however, makes their computation very demanding in this framework. We improve on the naïve measurement by using fast Fourier transformations as well as symmetries of the Hamiltonian and of the vertex. We have implemented this method into the CT-HYB solver [1] using the Krylov method and provide benchmarks and examples for up to seven correlated orbitals.

[1] N Parragh et al., arXiv:1209.0915v1

TT 40.80 Wed 15:00 Poster D

Reduced Density Matrix Functional Theory- A suitable vehicle to import explicit correlations — •Ebad Kamil[1], Thomas Pruschke[1], and Peter E. Bloechl[2] — [1]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany — [2]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany

A variational formulation for the calculation of interacting fermions system based on density matrix functional theory is presented. This formulation allows importing explicit many particle effects into standard density functional theory based calculations and also avoids ambiguities of double counting terms inherent to other approaches. Local approximation for explicit correlations is introduced and the resulting local density matrix functional is calculated using resolvent expansion/Quantum Master equation technique developed in the field of Open quantum system.

TT 40.81 Wed 15:00 Poster D

Measurement of the full three-dimensional Fermi surface at room temperature by angular correlation of positron annihilation radiation — •Josef Andreas Weber[1], Hubert Ceeh[1], Liviu Chioncel[4], Kathrin Anna Garb[4], Christoph Hugenschmidt[1,3], Michael Leitner[2], and Peter Böni[1] — [1]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [2]Technische Universität München, Physik Department E13, D-85748 Garching, Germany — [3]FRM II, Technische Universität München, D-85747 Garching, Germany — [4]University of Augsburg, Theoretical Physics III, D-86135 Augsburg, Germany

The two-dimensional measurement of the angular correlation of the positron annihilation radiation (2D-ACAR) is a powerful tool to investigate the electronic structure of materials. Here we present the full three-dimensional Fermi surface obtained by temperature dependent 2D-ACAR measurements in combination with common reconstruction algorithms. Although copper is believed to be a well understood system we find discrepancies between measurement and recent ab-initio calculations.

TT 40.82 Wed 15:00 Poster D

Development of high frequency measurement methods for Fermi surface studies under high pressure — •Hui Chang, Sven Friedemann, and Malte Grosche — Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK

The observation of quantum oscillatory phenomena in high magnetic field, for example of the electrical resistivity (Shubnikov-de Haas), can help resolve the electronic structure of challenging materials. Important progress is expected in a number of areas of current interest, when the Fermi surface can be tracked near to or across pressure and field-induced quantum phase transitions. These include Mott metal-insulator transitions, magnetic or charge density wave transitions and

the orbitally selective Mott transition - or Kondo volume collapse - discussed in f-electron metals.

High sensitivity measurements at elevated pressures in anvil cells are hindered by the need to make reliable and robust high quality contacts to submillimetre samples. Radio frequency tank oscillator methods based on tunnel diode or proximity detector based circuits offer an attractive alternative, because they avoid the need to make contacts and at the same time offer supreme relative sensitivity. Further simplification is possible by patterning the detection coil onto the high pressure anvils[1]. We present recent progress in developing such contactless methods for use in high pressure cells and illustrate this by test measurements of quantum oscillations in low carrier density materials.

[1] O. P. Welzel and F. M. Grosche, Rev. Sci. Instrum. 82, 033901 (2011)

TT 40.83 Wed 15:00 Poster D

Electron-hole pair condensation at the semimetal-semiconductor transition: a BCS-BEC crossover scenario — •Holger Fehske[1], Bernd Zenker[1], Franz Xaver Bronold[1], Dieter Ihle[2], Van-Nham Phan[3], and Klaus Becker[4] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, D-17487 Greifswald — [2]Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig — [3]Institute of Physics, Vietnamese Academy of Science and Technology, PO Box 429, 10000 Hanoi — [4]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden

We act on the suggestion that an excitonic insulator state might separate - at very low temperatures - a semimetal from a semiconductor and ask for the nature of these transitions. Based on a detailed analysis of electron-hole pairing in the extended Falicov-Kimball model, we show that tuning the Coulomb attraction between both species, a continuous crossover between a BCS-like transition of Cooper-type pairs and a Bose-Einstein condensation of preformed tightly-bound excitons might be achieved in a solid-state system. The precursor of this crossover in the normal state might cause the transport anomalies observed in several strongly correlated mixed-valence compounds.

TT 40.84 Wed 15:00 Poster D

Coexistance of phase transition and hysteresis near BEC — •Michael Maennel[1], Klaus Morawetz[1,2,3], and Pavel Lipavsky[4] — [1]Muenster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Federal University of Rio Grande do Norte, Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

Multiple phases occurring in a Bose gas with finite-range interaction are investigated. In the vicinity of the onset of Bose-Einstein condensation (BEC) the chemical potential and the pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore the equation of state becomes multivalued near the BEC transition. For weak interactions described by a hard-sphere (Hartree-Fock) or Popov (Hartree-Fock-Bogoliubov) approximation such a multivalued region can be avoided by the Maxwell construction. However, for strong interaction described by the many-body T-matrix there remains a multivalued region even after a Maxwell construction which is interpreted as a density hysteresis. This unified treatment becomes possible due to the recently found scheme to eliminate self-interaction in the T-matrix approximation which allows to calculate properties below and above the critical temperature.

TT 40.85 Wed 15:00 Poster D

Anisotropic superfluidity of bosons in optical Kagome superlattice — •Xuefeng Zhang[1], Tao Wang[1], Axel Pelster[2], and Sebastian Eggert[1] — [1]Department of the Physics,Univ. Kaiserslautern, Kaiserslautern, Germany — [2]Hanse-Wissenschaftskolleg, Germany

We study the quantum phase transitions for the extended Bose-Hubbard model with bosons on a Kagome superlattice which can be implemented by enhancing the long wavelength laser in one direction of the optical lattice. To this end we combine the virtues of a Mean-Field theory with the Laudau theory and work out of a decoupled effective potential method by comparing the corresponding analytic results with extensive quantum Monte Carlo simulations, we find that several striped solids emerge in this system. Due to the blockade effect of such a striped order, the resulting superfluid density turns out to be anisotropic and thus, reveal its tensional property. Finally, we discuss the complete quantum phase diagram.

TT 40.86 Wed 15:00 Poster D

Controlled manipulations of fermionic doublon states in the Hubbard model — •Karsten Balzer and Martin Eckstein — Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany

External fields can cause interesting phases and phase transitions in strongly correlated quantum systems [1-3].

In this contribution, we study the dynamics of the Hubbard model at strong coupling and show that a specifically tailored time-dependent electric field can separate a localized doublon into two electrons with a given lattice spacing and also to gradually move one or more doublons through the lattice without destroying the spaciotemporal coherence.

Furthermore, we demonstrate that the same mechanism can be used to create a charge-ordered state (of doublons) starting from a band insulator. This may be of importance for initial state preparations, manipulations and measurements in cold-atom experiments involving optical lattices.

[1] S. Sachdev, K. Sengupta and S.M. Girvin, Phys. Rev. B **66**, 075128 (2002)
[2] J. Simon, W.S. Bakr, R. Ma, M.E. Tai, P.M. Preiss and M. Greiner, Nature **472**, 307 (2011)
[3] Ph. Werner, N. Tsuji and M. Eckstein, Phys. Rev. B **86**, 205101 (2012).

TT 40.87 Wed 15:00 Poster D

Cooperative phenomena in superconducting atom-chips — •Sebastian Fuchs, Björn Kubala, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

We theoretically investigate the physics of hybrid quantum systems, where a cloud of cold atoms is coupled to superconducting microstructures, so called superconducting atom-chips. Coherent enhancement, due to the large number of atoms in the cloud, opens a path to the study of strong coupling effects, like superradiance/Dicke-physics in a decohering environment [1]. A structured environment can be designed by embedding a Cooper pair box within the cavity. Moreover, in such a system the transfer of quantum information between the atomic cloud and the superconducting solid state system can be studied.

[1] K. Henschel, J., J. Schmiedmayer, and H. Ritsch, Phys. Rev. A **82**, 033810 (2010)

TT 40.88 Wed 15:00 Poster D

localization-delocalization transition in double-well optical lattices — •gang wang — Max Planck Institute for the Physics of Complex Systems

Ultracold atoms in optical lattices allow for the study of localization of quantum waves. Within the framework of 1D incommensurate optical lattice, a sharp transition from all eigenstates being extended to all being localized occurs in one dimension, so-called self-duality in the Harper model. This transition has been observed with ultracold atoms loaded in optical lattices. We investigated the localization properties of ultracold atoms loaded in double-well optical lattices, perturbed by a secondary incommensurate lattice to induce the deterministic disorder potential. We found the localization-delocalization transition qualitatively different from those of the Harper model, signaled by the appearance of energy-dependent mobility edges and broken duality.

TT 40.89 Wed 15:00 Poster D

Negative absolute temperature for motional degrees of freedom and expansion of interacting bosons in optical lattices — •Simon Braun[1,2], Philipp Ronzheimer[1,2], Michael Schreiber[1,2], Sean Hodgman[1,2], Daniel Garbe[1,2], Immanuel Bloch[1,2], and Ulrich Schneider[1,2] — [1]Ludwig-Maximilians-Universität München — [2]Max-Planck-Institut für Quantenoptik, Garching

Absolute temperature is usually bound to be strictly positive. However, in systems with an upper energy bound, negative absolute temperature states are possible, where the occupation probability of states increases with their energy. We realized a negative absolute temperature state for motional degrees of freedom with ultracold bosonic ^{39}K atoms in an optical lattice, by implementing the attractive Bose-

Hubbard Hamiltonian. This new state strikingly revealed itself by strong occupation peaks at maximum kinetic energy. We found that the negative absolute temperature state is close to degeneracy and as stable as the corresponding positive temperature state.

Additionally, we investigated the out-of-equilibrium expansion dynamics of interacting bosons in one- and two-dimensional Hubbard systems. We found that the fastest, ballistic expansions occur in the integrable limits. In 1D, these are both the non-interacting and the strongly interacting limit where the system enters into the hard-core boson regime. For intermediate interactions, the expansion slows down significantly. In 2D, the system expands ballistically only in the non-interacting case, and even small interactions lead to strongly diffusive behavior. We also mapped out the transition between 1D and 2D.