TT 45: Correlated Electrons: Poster Session

We recommend to hang up the posters already during the morning sessions.

Time: Thursday 15:00–19:00 Location: Poster B

TT 45.1 Thu 15:00 Poster B

High-field magnetotransport study of $YbRh_2Si_2$ — •Naren HR[1], Sven Friedemann[2], Cornelius Krellner[1], Christoph Geibel[1], Frank Steglich[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 OHE, United Kingdom

Heavy fermion behavior is expected to be suppressed at magnetic fields high enough such that the Zeeman and the Kondo energy scales become comparable. In the prototypical heavy fermion compound $YbRh_2Si_2$, this scale is estimated to be around 10 T where anomalies have been observed in several thermodynamic quantities [1]. With a focus on this issue we present high-field (upto 15 T) magnetoresistance and Hall effect measurements on $YbRh_2Si_2$ down to 50 mK. We study the temperature evolution of the anomalies observed in our magnetotransport measurements. These features can be favourably compared to those seen in thermopower data [2]. Our measurements shed light on whether the localisation of *f*-electrons at such fields is accompanied by topological transformations of the Fermi surface as speculated in the iso-structural heavy fermion metamagnet $CeRu_2Si_2$ [3,4].

[1] P Gegenwart et al, New. J. Phys. **8**, 171 (2006)
[2] R Daou et al, *this conference*
[3] H Pfau et al, arXiv:1110.1160v1 (2011)
[4] R Daou et al, Phys. Rev. Lett., **96**, 026401 (2006)

TT 45.2 Thu 15:00 Poster B

Magnetic properties of $Yb(Rh_{1-x}Co_x)_2Si_2$ with $x = 0.58$ — •A. Haase[1], O. Stockert[1], C. Klingner[1], C. Krellner[1], S. Matas[2], M. Brando[1], C. Geibel[1], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

The heavy-fermion compound $YbRh_2Si_2$ is an ideal model system to study quantum criticality. Due to its very low antiferromagnetic ordering temperature $T_N \approx 70\,\mathrm{mK}$ and the small ordered magnetic moment, the magnetic structure of $YbRh_2Si_2$ is still unknown. Isoelectronic doping with Co leads to an increase of the ordering temperature T_N and of the ordered magnetic moment. The (x - T) - phase diagram of $Yb(Rh_{1-x}Co_x)_2Si_2$ shows a marked dip in the ordering temperature T_N near a Co concentration of about 50%. This may indicate a change of magnetic structure. For $x > 0.58$ the magnetic structure is incommensurate below T_N with a propagation vector $\tau_1 = (0.25\,0.08\,1)$ followed by a change to a commensurate structure at a lower T_L with $\tau_2 = (0.25\,0.25\,1)$. For $x = 0.58$ only the commensurate magnetic order was found below $T \approx 750\,\mathrm{mK}$ up to now. For lower Co-concentrations the magnetic structure is still unknown. To study the change of magnetic structure in more detail, we performed magnetisation, heat capacity and resistivity measurements on $Yb(Rh_{0.42}Co_{0.58})_2Si_2$, which is near the minimum in the (x - T) - phase diagram. While in zero magnetic field heat capacity and resistivity measurements reveal only one phase transition at $T_N \approx 800\,\mathrm{mK}$, a second transition was detected in the magnetisation at $T = 650\,\mathrm{mK}$ and $B < 0.2\,\mathrm{T}$.

TT 45.3 Thu 15:00 Poster B

Thermoelectric transport in $Ce_{1-x}La_xNi_2Ge_2$ — •Ulrike Stockert[1], Adam P. Pikul[2], Nubia Caroca-Canales[1], Stefanie Hartmann[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland

Investigations of the thermoelectric power S provide a sensitive probe of low energy excitations in metallic systems. In Ce-based heavy-fermion systems, Kondo interaction and crystal electric field (CEF) excitations usually give rise to large positive anomalies in $S(T)$.

We performed thermopower and resistivity measurements on the diluted heavy fermion system $Ce_{1-x}La_xNi_2Ge_2$ between 2 K and 300 K. In this temperature range the Kondo interaction as well as CEF excitations of the Ce^{3+} moments play a major role in the transport and scattering processes of the system. Our thermopower measurements reveal a reduction of the Kondo energy scale from about 30 K to 2 K with decreasing Ce concentration x, while the CEF levels remain almost unchanged. Simultaneously, the crossover from coherent to impurity scattering is observed in the resistivity $\rho(T)$. Interestingly, $\rho(T)$ varies smoothly upon Ce-La substitution, while $S(T)$ changes rather abruptly for high Ce concentrations $x \geq 0.9$. We discuss our findings in comparison to recent specific heat measurements on the system.

TT 45.4 Thu 15:00 Poster B

The hidden order transition in URu_2Si_2 investigated by high-resolution angle-resolved photoemission spectroscopy — •Jan Trinckauf[1], Daniel Shai[2], John Harter[2], Torben Hänke[1], Graeme Luke[3], Kyle Shen[2], and Jochen Geck[1] — [1]IFW Dresden, Germany — [2]Cornell University, Ithaca, USA — [3]McMaster University, Hamilton, Canada

We present a study of the hidden order transition in URu_2Si_2 by means of high-resolution angle-resolved photoemission spectroscopy (ARPES). In particular, we find a strong excitation energy dependence of a flat quasi particle band that is associated with and strongly affected by the hidden order transition[1,2]. We compare our ARPES data to density functional theory (DFT) calculations in the local density approximation (LDA)+U to simulate various degrees of 5f localization.

[1] Santander-Syrio et al., Nat. Phys. 2009
[2] Yoshida et al., Phys. Rev. B 2010

TT 45.5 Thu 15:00 Poster B

Quantum Criticality in $Ta(Fe_{1-x}V_x)_2$ Probed by ^{51}V NMR and Magnetization — •Panchanana Khuntia, Michael Baenitz, Manuel Brando, Alexander Kerkau, Guido Kreiner, and Frank Steglich — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Itinerant $3d$ weak ferromagnets like e.g. $NbFe_2$ or MnSi are tunable towards a (quantum) critical regime by doping, external pressure or magnetic field. The vicinity of a QCP leads to non Fermi liquid (NFL) behavior manifested by scaling laws in bulk properties like magnetization $M(T)$, resistivity $\rho(T)$ and specific heat $C(T)$. In NMR, NFL phenomena are associated with non-Korringa like features in spin lattice relaxation rate $(1/T_1)$ for $T \to 0$. We focus on NMR investigations on polycrystalline $Ta(Fe_{1-x}V_x)_2$ ($x = 0.02, 0.05, 0.2,\ 0.3$) samples. For $x = 0.02$, the magnetic properties are reminiscent of itinerant FM at the verge of a FM instability with enhanced $M(T \to 0)$ indicating FM fluctuations. ^{51}V NMR spectra are broadened inhomogeneously at low temperatures with considerable shift which reflects the hyperfine coupling of itinerant $3d$ moments with the ^{51}V nuclei.$^{51}(1/T_1T)$ violates the Korringa law and exhibits a $T^{-0.8}$ dependence for small fields which is a signature of critical fluctuations. The value of the Korringa product(<1) indicates FM correlations between itinerant moments. Further doping the system undergoes AFM ordering up to $x = 0.3$, where a simple paramagnetic behavior is observed. $Ta(Fe_{1-x}V_x)_2$ is of special interest because FM critical fluctuations evolve in the proximity of an AFM state by nominal V doping.

TT 45.6 Thu 15:00 Poster B

Inelastic Neutron Scattering on the heavy-fermion compound $YbNi_4P_2$ — •Zita Huesges[1], Oliver Stockert[1], Cornelius Krellner[1], Micheal Koza[2], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France

It was recently discovered that the strongly correlated electron compound $YbNi_4P_2$ is one of the few heavy-fermion systems exhibiting a ferromagnetic phase transition at very low temperature (T_C=0.17 K) because of strong Kondo screening. It is thus a very promising candidate to study a Kondo system close to ferromagnetic quantum criticality. While nickel is nonmagnetic in $YbNi_4P_2$, the ytterbium moments are located on chains along the *c*-direction of the tetragonal unit cell so that the magnetic interaction is mainly one-dimensional. Together with geometrical frustration in the *ab*-plane , $YbNi_4P_2$ is therefore prone to enhanced quantum fluctuations.

Here, we present time-of-flight neutron spectroscopy measurements on polycrystalline $YbNi_4P_2$ to study the magnetic excitations. This gives insight into the particular magnetic interactions, such as the crys-

talline electric field and the Kondo fluctuations.

TT 45.7 Thu 15:00 Poster B

Annealing effects in the antiferroquadrupolar compound $U(Pd_{1-x}Pt_x)_3$ — •Dirk Schulze Grachtrup[1], Kerstin Westkämper[1], Markus Schäpers[1,2], Matthias Bleckmann[1,3], Stefan Süllow[1], and Keith A. McEwen[4] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden, Germany — [3]Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe, Erding, Germany — [4]University College London, London, United Kingdom

The double hexagonal compound UPd_3 undergoes several successive phase transitions to antiferroquadrupolar (AFQ) ordered phases below 8 K. Measurements of UPd_3 in magnetic fields reveal a complex response of these AFQ phases to the applied field, leading to a rich magnetic phase diagam [1-3].

Doping of UPd_3 with Pt leads to a rapid suppression of the ordered phases in $U(Pd_{1-x}Pt_x)_3$. Recent studies of single crystalline $U(Pd_{1-x}Pt_x)_3$ in the regime $x \leq 0.01$ revealed a strong reduction of the ordering temperatures with doping. At $x = 0.005$ ordering temperatures are reduced to about one half compared to those of pure UPd_3. For $x = 0.01$ the AFQ order is almost completely suppressed. Here, we present the effects of annealing on specific heat and resitivity of single crystalline samples of $U(Pd_{1-x}Pt_x)_3$.

[1] Y. Tokiwa *et al.*, J. Phys. Soc. Jpn. **70** (2001) 1731
[2] D. F. McMorrow *et al.*, Phys. Rev. Lett. **87** (2001) 057201
[3] H. C. Walker *et al.*, Phys. Rev. Lett. **97** (2006) 137203

TT 45.8 Thu 15:00 Poster B

Field-induced Quantum Critical Point in the heavy-fermion superconductor Ce_2PdIn_8 — •Jinkui Dong[1,2], Yoshi Tokiwa[1], Philipp Gegenwart[1], Shiyan Li[2], Daniel Gnida[3], and Dariusz Kaczorowski[3] — [1]I. Physikalisches Institut, Georg-August-Universität Goettingen, 37077 Goettingen, Germany — [2]Department of Physics, State Key Laboratory of Surface Physics, and Laboratory of Advanced Materials, Fudan University, Shanghai 200433, China — [3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wroclaw, Poland

The in-plane resistivity ρ, specific heat C and thermal conductivity κ of the heavy-fermion superconductor Ce_2PdIn_8 single crystals were measured down to 50 mK. A field-induced quantum critical point, occurring at the upper critical field H_{c2}, is demonstrated from the $\rho(T) \sim T$ near H_{c2} and $\rho(T) \sim T^2$ when further increasing the field. In specific heat measurements, the normal-state electronic specific-heat coefficient displays logarithmically divergent behavior, comparable to $CeCoIn_5$ and in agreement with 2D quantum criticality of spin-density-wave type. The large residual linear term κ_0/T at zero field and the rapid increase of $\kappa(H)/T$ at low field give evidence for nodal superconductivity in Ce_2PdIn_8. The jump of $\kappa(H)/T$ near H_{c2} suggests a first-order-like phase transition at low temperature. These results mimic the features of the famous $CeCoIn_5$ superconductor, implying that Ce_2PdIn_8 may be another interesting compound to investigate for the interplay between magnetism and superconductivity.

TT 45.9 Thu 15:00 Poster B

Theory of the Spin Exciton Formation inside the Hidden Order Phase of CeB_6 — •Alireza Akbari and Peter Thalmeier — Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

The heavy fermion metal CeB_6 exhibits hidden order of antiferroquadrupolar (AFQ) type below $T_Q = 3.2$K and subsequent antiferromagnetic (AFM) order at $T_N = 2.3$K. It was interpreted as ordering of the quadrupole and dipole moments of a Γ_8 quartet of localised Ce $4f^1$ electrons. This established picture has been profoundly shaken by recent inelastic neutron scattering [1] that found the evolution of a feedback spin exciton resonance within the hidden order phase at the AFQ wave vector appears and is stabilized by the AFM order. We develop an alternative theory based on a fourfold degenerate Anderson lattice model, including both order parameters as particle-hole condensates of itinerant heavy quasiparticles. This explains in a natural way the appearance of the spin exciton resonance and the momentum dependence of its spectral weight, in particular around the AFQ vector and its rapid disappearance in the disordered phase. Analogies to the feedback effect in unconventional superconductors and Kondo semiconductors are pointed out.

[1] G. Friemel et al., arXiv:1111.4151.

TT 45.10 Thu 15:00 Poster B

Continuous unitary transformation of the single impurity Anderson model — •Jörn Krones and Götz S. Uhrig — TU Dortmund, Theoretische Physik I, 44221 Dortmund, Germany

Quantum impurity systems, such as the considered single impurity Anderson model (SIAM) have been of significant interest throughout the last decades. An efficient way to deal with the exponentially varying energy scales in such models is the numerical renormalization group (NRG). The free orbital regime (FO) at high energies crosses over to the local moment regime (LM) as energies are decreased with a final crossover to the strong coupling regime (SC) at very small energies. The two crossovers are determined by characteristic energies. The crossover from FO to LM is determined by the coulomb interaction U while the crossover from LM to SC is determined by the exponentially small Kondo temperature T_k. Perturbation theory provides a good description for energies $E \gtrsim T_k$ but breaks down for $E \approx T_k$.
It is our aim to use non-perturbative continuous unitary transformations as a new approach to investigate the full energy regime from the conduction electron bandwidth D down to exponentially small energies $E \ll T_k$. We want to construct an effective Hamiltonian in form of a linear chain similar to Wilson's treatment, labeled by single particle energies and interaction terms.

TT 45.11 Thu 15:00 Poster B

Mean-Field Theory of the Time-Dependent Kondo Effect — •Mohammad Sayad and Michael Potthoff — I. Institut für Theoretische Physik, University of Hamburg, Germany

We propose a generalization of the hybridization mean-field theory [1,2] to Kondo systems far from thermal equilibrium. This time-dependent mean-field approach is used to study the formation or breaking of a Kondo singlet on the time axis. To this end we consider a Kondo impurity on a one-dimensional tight-binding chain as well as on two- and three-dimensional clusters after a sudden change of the exchange-coupling strength. We present results for the ground-state and the finite-temperature equilibrium phase diagram of the Kondo Hamiltonian and for the non-equilibrium final-state dynamics after a quench through the phase boundary and discuss the time-dependent competition of the Kondo effect with the RKKY interaction for systems with two magnetic impurities.

[1] C. Lacroix and M. Cyrot, Phys. Rev. B 20, 1969 (1979)
[2] D. Newns and N. Read, Advances in Physics 36, 799 (1987).

TT 45.12 Thu 15:00 Poster B

Kondo Resonance for Orbitally Degenerate Systems — •Arthur Huber, Aljoscha B. J. Wilhelm, Michael Karolak, Tim O. Wehling, and Alexander I. Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

The Kondo effect is usually connected with the interaction between a localized spin moment and itinerant electrons. However, it is also possible that another internal degree of freedom associated with a degeneracy gives rise to a Kondo effect. One example is the so-called orbital Kondo effect [1], where the pseudospin arising from an orbital degeneracy is screened by the conduction electrons. To acquire a better understanding of this specific Kondo effect, we investigate a general two-band Anderson impurity model within continuous time quantum Monte Carlo simulations [2]. To this end we calculate the static charge susceptibility. Furthermore we investigate, the effects of an external "pseudomagnetic" field in detail.

[1] O.Y. Kolesnychenko *et al.*, Nature (London) **415**, 507 (2002).
[2] E. Gull *et al.*, Rev. Mod. Phys. **83**, 349404 (2011).

TT 45.13 Thu 15:00 Poster B

Numerical renormalization group calculation of total energies and specific heats of quantum impurity models — •Lukas Merker and Theo Costi — Peter Grünberg Institut (PGI-2) and Institute for Advanced Simulation (IAS-3), Forschungszentrum Jülich, 52425 Jülich, Germany

The calculation of thermodynamic properties of quantum impurity models within the numerical renormalization group method proceeds via the impurity contribution to the thermodynamic potential $\Omega_{\rm imp} = \Omega_{\rm total} - \Omega_0$, where $\Omega_{\rm total}$, and Ω_0 are the thermodynamic potentials in the presence and absence of the impurity, respectively. Here, we propose a method to obtain specific heats of quantum impurity models via a direct calculation of the internal energy requiring only the evaluation of local static correlation functions. We apply this scheme

to the Anderson impurity model and show by direct comparison with the exact results from Bethe Ansatz [1] that it recovers accurately both the Kondo induced specific heat peak at low temperatures as well as the charge fluctuation induced peak at higher temperatures [2].
[1] A. M. Tsvelick and P. B. Wiegmann, Phys. Lett. **89**A, 368 (1982)
[2] L. Merker and T. A. Costi, preprint (2011).

TT 45.14 Thu 15:00 Poster B

Mechanism for Giant Thermopower in negative-U Molecular Quantum Dots — •Theo Costi[1], Sabine Andergassen[2], and Veljko Zlatic[3] — [1]Peter Grünberg Institut (PGI-2) and Institute for Advanced Simulation (IAS-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, 59056 Aachen, Germany and JARA-Fundamentals for Information Technology — [3]Institute of Physics, 10001 Zagreb, Croatia

We investigate with the aid of numerical renormalization group techniques the thermoelectric properties of a molecular quantum dot described by the negative-U Anderson model. We show that the charge Kondo effect provides a mechanism for enhanced thermoelectric power via a correlation induced asymmetry in the spectral function close to the Fermi level. We show that this effect results in a dramatic enhancement of the Kondo induced peak in the thermopower of negative-U systems with Seebeck coefficients exceeding $50\mu V/K$ over a wide range of gate voltages [1].
[1] S. Andergassen, T. A. Costi and V. Zlatić, Phys. Rev. B (arXiv:1101.4124)

TT 45.15 Thu 15:00 Poster B

Distance dependence of the spin-spin correlation function of two Kondo impurities coupled to a one-dimensional Hubbard chain — •Alexander Tiegel, Piet Dargel, and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany

The distance dependence of the ground state spin-spin correlation function $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle$ of two spin-1/2 Kondo impurities antiferromagnetically attached to a one-dimensional Hubbard chain is studied at half-filling. The results are obtained via the density-matrix renormalization group (DMRG) method. In the case of weak couplings one finds a RKKY dominated behavior for all accessible distances. A crossover into the Kondo regime occurs with increasing coupling and inter-impurity distances R. It is especially studied to which extent there exists a power-law decrease of the inter-impurity correlation function. In the absence of an on-site repulsion a $1/R^2$ behavior of the correlations is observed for large distances and strong couplings. Furthermore the asymptotic properties of the correlation function are discussed if the Coulomb interaction is taken into account. The results are supported by perturbation theory.

TT 45.16 Thu 15:00 Poster B

Hubbard-Holstein Model with Dispersive Phonons — •Patrick Haase, Sebastian Fuchs, and Thomas Pruschke — Georg-August Universität, Göttingen, Deutschland

We investigate the local density-of-states in a Hubbard-Holstein model with dispersive phonons. We solve the model in the dynamical mean field approximation using a continuous-time quantum Monte Carlo solver. We extract the local density of states from the imaginary time Green's function by means of the Maximum Entropy method.

TT 45.17 Thu 15:00 Poster B

Numerical Renormalization Group for dissipative quantum impurity systems — •Etienne Gärtner, Andrew Mitchell, and Ralf Bulla — Institute of Theoretical Physics, University of Cologne, Zuelpicherstr. 77, 50937 Cologne, Germany

The Numerical Renormalization Group (NRG) has been adapted to treat open dissipative quantum systems, but significant challenges remain. Certain models are well-described by this bosonic NRG in certain parameter regimes, but the essential requirement for Hilbert space truncation causes problems in other situations. Here we develop a novel extension of the regular bosonic NRG, employing an optimized basis to capture the important low-temperature physics in the smallest possible Hilbert space. We test the method with the paradigmatic spin-boson model, and go on to apply the method to a two-bath variant where truncation effects are typically more severe.

TT 45.18 Thu 15:00 Poster B

From periodic to dilute Anderson models: evolution of scales — •Lucas Hollender, Andrew Mitchell, and Ralf Bulla — Institut für theoretische Physik, Köln, Deutschland

The periodic Anderson model shows a characteristic energy scale below which the magnetic moments are coherently screened by conduction electrons. We examine within DMFT the behavior of this coherence scale as the number of magnetic impurities is reduced. First, we consider periodic systems comprising inequivalent impurity sublattices, and find a subtle interplay between sublattice scales. Dilute impurity behavior is then obtained on decoupling sublattices completely. Finally, we develop an inhomogeneous DMFT approach to study the extreme non-periodic limit of a few randomly distributed impurities, where single-impurity physics can dominate. The simplest two-impurity system can also be solved directly with NRG, and provides a benchmark.

TT 45.19 Thu 15:00 Poster B

Non-Fermi liquid physics in two-channel Kondo models — •Andrew Mitchell — Institut für Theoretische Physik, Universität zu Köln, Germany

The two-channel Kondo (2CK) model possesses a non-Fermi liquid (NFL) quantum critical point, arising when two conduction channels compete to Kondo-screen a single spin-$\frac{1}{2}$ impurity. The two-impurity Kondo (2IK) model also has a NFL critical point. We establish an exact connection between the models, showing that the 2IK critical fixed point is identical to that of a 2CK model with potential scattering. Furthermore, we demonstrate that the same critical physics arises in chains of impurities, and the spin-S generalization of the 2IK model. But conductance lineshapes measurable in experiment encode the full RG flow. We study the onset of NFL physics, showing that distinctive signatures arise as a function of device asymmetry; and the ultimate recovery of standard Fermi liquid behavior resulting from symmetry-breaking perturbations.
[1] Mitchell, Sela, Logan, `arXiv:1111.6503v1` (2011)
[2] Mitchell, Logan, Krishnamurthy, Phys. Rev. B **84**, 035119 (2011)
[3] Sela, Mitchell, Fritz, Phys. Rev. Lett. **106**, 147202 (2011)

TT 45.20 Thu 15:00 Poster B

Out-of-equilibrium steady state properties of the Bose-Fermi Kondo model — •Pedro Ribeiro and Stefan Kirchner — Max-Planck-Institute for the Physics of Complex Systems

We study the out-of-equilibrium steady state properties of the Bose Fermi Kondo describing a local magnetic moment coupled to two leads supporting bosonic and fermionic low energy excitations. The model describes a single-electron transistor with ferromagnetic leads where the magnetization of the two leads is taken to be antiparallel and the effective magnetic field seen by the local impurity vanishes. In such setup, a Kondo peak in the differential conductance can be observed in the Coulomb-blockade regime. The Bose Fermi Kondo captures the essential physical picture as the Kondo effect is critically destroyed upon increasing the coupling to the magnons in the leads. We explore the different regimes of this model using a dynamical large-N approach and study the response functions when a finite bias voltage or a temperature gradient is imposed across the leads. We report the existence of an effective temperature $T_{\rm eff}$ and show that the local susceptibility, as a function of $T_{\rm eff}$ follows the equilibrium scaling form. We also address the electric and thermal current response.

TT 45.21 Thu 15:00 Poster B

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 the bubble chains to all orders. We analyse the dynamical evolution of the two-point correlation function with respect to the Kondo resonance.

TT 45.22 Thu 15:00 Poster B

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

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

Using THz spectroscopy at frequencies between 5 cm^{-1} and 45 cm^{-1}, we have studied thin-film samples of the $Sr_{1-x}Ca_xRuO_3$ system, which were prepared by metalorganic aerosol deposition. From transmission and phase measurements we have determined the frequency-dependent conductivity for a set of temperatures between 5 K and 300 K, and we discuss it in the framework of the extended Drude model with frequency-dependent relaxation rate and effective mass. While for pure $SrRuO_3$ as well as for doped systems approaching the quantum phase transition we find conventional metallic Drude behavior, $CaRuO_3$ exhibits highly unusual optical properties which we compare to results of dc measurements on these thin films, which also revealed temperature ranges with non-Fermi liquid behavior.

TT 45.23 Thu 15:00 Poster B

Quantum critical field and pressure tuning in the heavy fermion ferromagnet $CeAgSb_2$ — •Peter Logg[1], Zhou Feng[1], Takao Ebihara[2], Patricia Alireza[1], Swee Goh[1], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, Shizuoka University, Shizuoka 422-8529, Japan

Quantum critical phenomena have over the past decade been investigated primarily in ferromagnetic or nearly ferromagnetic d-electron systems and in antiferromagnetic f-electron systems. Here, we present a series of measurements of the ferromagnetic cerium compound $CeAgSb_2$. $CeAgSb_2$ is a Kondo-lattice compound which at ambient pressure undergoes a ferromagnetic transition at T_c = 9.6 K. Ferromagnetism is rapidly suppressed by applied hydrostatic pressure, and at pressures > 3.5 GPa it is replaced by an unidentified ordered phase, presumably antiferromagnetism. Alternatively, the ferromagnetic phase may be suppressed to 0K by the application of a magnetic tuning field, which is applied perpendicular to the easy-axis of magnetisation.

We investigate both the *P-T* and *H-T* phase diagrams of this compound through a series of ac-susceptibility, resistivity and high-pressure magnetisation measurements.

TT 45.24 Thu 15:00 Poster B

Single crystal growth of $Yb(Rh_{1-x}Ni_x)Si_2$: influence of chemical pressure and electron doping — •Elias Blumenröther, Hirale. S Jeevan, Yoshi Tokiwa, Maik Schubert, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany

$YbRh_2Si_2$ is a well-known heavy fermion compound, which has been investigated intensively due to proximity to an antiferromagnetc field induced quantum critical point (QCP). Recent experimental and theoretical investigations propose that this system displays an unconventional QCP driven by localized moments. We report details of the single crystal growth and physical properties of non-isovalent partial substitution of Rh by Ni. We have grown single crystals of $Yb(Rh_{1-x}Ni_x)Si_2$ for x = 0 to 1 using an Indium-flux method in an oxide crucible. The structure of the single crystals and their composition were investigated by Xray-diffraction and microprobe analysis, respectively. We will report resistivity, specific heat and magnetic susceptibility measurements for various doping concentrations. Ni substitution has a twofold effect: chemical pressure and doping with electrons. By comparison with isovalent Co substitution and Fe-(hole)-doping, conclusions concerning the influence of chemical pressure and the change in carrier concentration are drawn.

This work is supported by the DFG Reserach Unit 960 (Quantum Phase Transitions).

TT 45.25 Thu 15:00 Poster B

Effect of hole doping and chemical pressure in $Yb(Rh_{1-x}Fe_x)_2Si_2$ — •Manuel Mchalwat, Hirale S. Jeevan, Yoshi Tokiwa, Maik Schubert, and Philipp Gegenwart — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The heavy fermion compound $YbRh_2Si_2$ shows a quantum critical point when the temperature of antiferromagnetic ordering is suppressed to zero by an external magnetic field. Besides the energy scale defined by the quantum critical fluctuations of the order parameter one finds an additional scale T^* which also merges into the quantum critical point. This scale is connected to a reconstruction of the fermi surface, but it is argued whether a Kondo breakdown or a Zeeman-driven Lifshitz transition is the origin. In order to test both hypothesis we synthesized single crystals of $Yb(Rh_{1-x}Fe_x)_2Si_2$ to introduce holes into the system. Thus the electronic structure is changed, which should have a strong influence on the Lifshitz transition. The measured low temperature properties are discussed with respect to both scenarios.

The work has been supported by the DFG through FOR 960 (Quantum Phase Transitions).

TT 45.26 Thu 15:00 Poster B

Spin structure of Fe- and Co-substituted MnSi and MnGe — •Sven-Arne Siegfried[1], Dirk Menzel[1], Sergey Grigoriev[2], Vadim Dyadkin[2], Nadezhda Potapova[2], Evgeny Moskvin[2], Anatoly V. Tsvyashchenko[3], Mathias Kraken[1], and Jochen Litterst[1] — [1]IPKM, TU Braunschweig, Germany — [2]PNPI, Gatchina, Russia — [3]IHPP, Troitsk, Russia

The intriguing magnetic and transport properties of the transition metal-monosilicides TM-Si (TM = Mn, Fe, Co) have been studied extensively during the last thirty years, whereas the properties of the TM-monogermanides are much less investigated due to the complexity of the synthesis. Both systems order in a helical spin structure which can be transformed by a magnetic field into a conical and even a parallel configuration. Close to the ordering temperature a skyrmionic A-phase exists. SQUID magnetization and Mössbauer-spectroscopic measurements on $Mn_{1-x}Co_xSi$ and $Mn_{1-x}Fe_xSi$ have been performed to determine the magnetic phase diagrams. For a critical substitution of Co ($x_{Co} \approx 0.08$) and Fe ($x_{Fe} \approx 0.15$) the ferromagnetic order in MnSi is suppressed. The intermixing compound $Mn_{1-x}Fe_xGe$ has been magnetically characterized for the first time. A preliminary magnetic phase diagram for different Fe-concentrations has been created. Small angle neutron scattering has been used to determine the spin structure of this compound. The monogermanides show a remarkably huge increase of the helix period from 3 nm for MnGe up to 70 nm for FeGe compared to 18 nm for MnSi, and the critical fields H_{C1} and H_{C2} increase from MnGe towards FeGe by the factor of 10.

TT 45.27 Thu 15:00 Poster B

Magnetic order and Spin Dynamics in the Heavy Fermion System $YbNi_4P_2$ — •Johannes Spehling[1], Marco Günther[1], Nicholas Yéche[1], Hans-Henning Klauss[1], Hubertus Luetkens[2], Chris Baines[2], Cornelius Krellner[3], Christoph Geibel[3], and Frank Steglich[3] — [1]Institut für Festkörperphysik, TU Dresden,Germany — [2]Laboratory for Muon-Spin Spectroscopy, PaulScherrer Institut, Villigen, Switzerland — [3]Max-Planck-Institutfür Chemische Physik fester Stoffe Dresden, Germany

A longstanding question in the field of quantum criticality relates to the possible existence of a ferromagnetic (FM) quantum critical point (QCP). At a QCP, collective quantum fluctuations tune the system continuously from a magnetically ordered to a non-magnetic ground state. However, so far no 4*f*-material with a FM QCP is found. Recently, in the HF metal $YbNi_4P_2$ with a quasi 1D-electronic structure, FM quantum criticality above a low FM transition temperature of T_C = 170 mK was suggested. Our zero field muon spin relaxation on $YbNi_4P_2$ proves static magnetic order with a strongly reduced ordered Yb^{3+} moment below T_C. Above T_C, the muon asymmetry function $P(t,B)$ is dominated by quasi homogeneous spin fluctuations and exhibits a time-field scaling relation $P(t,B) = P(t/B^{\gamma})$ indicating cooperative critical spin dynamics. At T = 190 mK, slightly above T_C, $\gamma = 0.81(5)$ K suggesting time-scale invariant power-law behavior for the dynamic electronic spin-spin autocorrelation function. The results will be disussed in comparizon with the AFM compound $YbRh_2Si_2$. [1] C. Krellner *et al.*, New J. Phys. **13**, 103014 (2011).

TT 45.28 Thu 15:00 Poster B

Spin-wave excitations in antiferromagnetically ordered

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

Research on quantum phase transitions continue to be in the focus in condensed matter physics, because systems at quantum criticality show quite unusual low temperature properties including unconventional superconductivity in some cases. The heavy-fermion compound $YbRh_2Si_2$ is a model system to study quantum criticality. Isostructural $YbCo_2Si_2$ can be considered as the magnetically well ordered counterpart allowing for the investigation of the spin excitations in the antiferromagnetic state below $T_N \approx 1.7\,K$. The system exhibits well-defined spin waves in the two ordered phases with distinct dispersion. Although the dispersion along several principal directions are almost unchanged between the low temperature commensurate and the high temperature incommensurate phase, some marked differences are observed in the vicinity of (0 0 1). The results help to understand the basic magnetic interactions in this heavy-fermion compound.

TT 45.29 Thu 15:00 Poster B

Towards a complete preparation chain of single crystal intermetallic compounds under UHV compatible conditions — Andreas Bauer, •Ralitsa Bozhanova, Christian Franz, Saskia Gottlieb-Schönmeyer, 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 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 45.30 Thu 15:00 Poster B

Compressible Quantum Critical Metamagnetistm — •Mario Zacharias[1], Indranil Paul[1], and Markus Garst[2] — [1]Institute for Theoretical Physics, University of Cologne — [2]Institut Neel, CNRS/UJF, Grenoble, France

For materials close to quantum criticality the critical degrees of freedom couple generically to the crystal lattice. In case of perturbative couplings, this results e.g. in a divergent Grüneisen parameter allowing to probe critical fluctuations by measuring elastic properties. We argue however that for quantum critical metamagnetism, as discussed in the context of $Sr_3Ru_2O_7$ and $CeRu_2Si_2$, such a coupling is necessarily non-perturbative resulting in a modification of the critical behavior. In particular, we show that the metamagnetic transition is exactly described by mean-field theory without long-range critical fluctuations.

TT 45.31 Thu 15:00 Poster B

Thermal expansion and magnetostriction of CePdAl single crystals — •Kai Grube[1], Sebastian Zaum[1,2], Veronika Fritsch[2], Sarah Woitschach[3], 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 compound CePdAl exhibits long-range antiferromagnetic order below $T_N \approx 2.7\,K$. It adopts a hexagonal ZrNiAl-type crystal structure in which the triangular coordination symmetry of the magnetic Ce ions gives rise to geometrical frustration. Neutron diffraction experiments indicate that below T_N only two thirds of the Cer ions partcipate in the long-range magnetic order [1]. We have performed thermal expansion and magnetostriction measurements in magnetic fields up to $B = 14\,T$ parallel to the c-axis to clarify whether an anisotropic distortion of the unit cell can lift the frustration of the remaining Ce^{3+} moments. The uniaxial pressure dependence of T_N is discussed along with the B-T phase diagram of CePdAl. In addition, the thermal-expansion measurements will be used to look for signs of non-Fermi-liquid behavior induced by the nearby quantum critical point at the onset of magnetic order.

[1] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996)

TT 45.32 Thu 15:00 Poster B

Magnetic anisotropy of the Kondo lattice $CePd_{1-x}Rh_x$ probed with polarized neutrons — •Philipp Schmakat[1,2], Michael Schulz[2], Vladimir Hutanu[2,3], Manuel Brando[4], Christoph Geibel[4], Micha Deppe[4], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik-Department E21, Technische Universität München — [2]Forschungs-Neutronenquelle FRM II, München — [3]RWTH Aachen, Institut für Kristallographie — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the magnetic anisotropy of the Kondo lattice system $CePd_{1-x}Rh_x$ at low temperatures by using polarized neutrons at the instrument POLI-HEIDI where the polarization analysis device CryoPad has been installed recently. The system $CePd_{1-x}Rh_x$ shows significant anisotropy for low Rh concentrations $x < 0.6$. With increasing Rh concentration a ferromagnetic quantum phase transition takes place and the anisotropy reduces. The curvature of the phase boundary $T_C(x)$ changes sign at Rh concentration $x = 0.65$ and a cluster glass phase emerges. Our data are consistent with previous measurements of the magnetisation. The measured polarization matrices will allow us to quantify the average domain size in each direction of space and give us important hints of magnetic stray fields of the sample induced even in zero external magnetic field.

[1] J.G. Sereni, Phys. Rev. B 75, 024432 (2007).
[2] T. Westerkamp, Phys. Rev. Lett. 102, 206404 (2009).

TT 45.33 Thu 15:00 Poster B

Low-Dimensional Chiral Physics: Magnetic Catalysis — •Daniel David Scherer and Holger Gies — Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena, Jena (Germany)

Magnetic catalysis describes the enhancement of symmetry breaking quantum fluctuations in chirally symmetric quantum field theories by the coupling of fermionic degrees of freedom to a magnetic background configuration. We use the functional renormalization group to investigate this phenomenon for interacting Dirac fermions moving in 2+1 dimensional space-time and provide for a clear renormalization-group picture.

TT 45.34 Thu 15:00 Poster B

Effects of dissipation on the phase transition of the disordered O(2) quantum rotor model — •Nicolas Lorscheid and Heiko Rieger — Universität des Saarlandes

Properties of Josephson arrays are conventionally described using the $O(2)$ quantum rotor Hamiltonian. The properties of the occuring quantum phase transition suggest, that the model belongs to the Kosterlitz-Thouless universality class. In order to study the effects of dissipation on this transition, the system is coupled to a dissipative bath of harmonic oscillators. We study the model using an efficient numerical implementation of the real space renormalization group approach, which makes it possible to treat large systems.

TT 45.35 Thu 15:00 Poster B

Quantum Criticality in the pseudogap Kondo model: a dynamical large-N study — •Farzaneh Zamani, Pedro Ribeiro, and Stefan Kirchner — Max Planck Institute for the Physics of Complex Systems

In the pseudogap Kondo model, a continuous zero-temperature phase transition separates a Kondo-screened phase from a Kondo-destroyed local moment phase. This model is a prototype system to study critical Kondo destruction which has been observed in various intermetallic rare earth compounds. It is also the effective low-energy model to describe point-defects in graphene and non-magnetic impurities in d-wave superconductors and can be realized in certain quantum dot systems. We address the critical properties of the SU(N)XSU(M) pseudogap Kondo model in a dynamical large-N limit [1,2]. Applying the scaling ansatz of [1,3], we obtain the leading and critical exponents in the quantum coherent regime ($\hbar\omega \ll k_B T$). Solving the large-N equations, we obtain the full scaling functions in both the quantum coherent and relaxational regime ($k_B T \ll \hbar\omega$). The local critical correlators have the form of a local conformally invariant fixed point although the underlying model lacks conformal symmetry in the bulk.

[1] O.Parcollet et al. PRB 58, 3794 (1998)

[2] M. Vojta, PRL 87, 097202 (2001)
[3] L. Zhu et al., PRL 93, 267201 (2004).

TT 45.36 Thu 15:00 Poster B

Finite size scaling of the typical density of states using the kernel polynomial method — •Daniel Jung[1], Gerd Czycholl[2], and Stefan Kettemann[1,3] — [1]School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany — [2]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [3]Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), San 31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea

We study the metal-insulator transition (MIT) in effective tight binding models (ETBM) by looking at the scaling behaviour of the typical density of states (GDOS) which we obtain by taking the geometrical mean of the local density of states (LDOS) of many different lattice sites and realizations of disorder. The LDOS can be performantly calculated by means of the kernel polynomial method (KPM). Right now we focus on applying this method to the "standard" Anderson model of disorder to check our own implementation and methodical approach and to validate preceding results by others.

TT 45.37 Thu 15:00 Poster B

With DFT and Ewald-summation to realistic parameters in molecular crystals — •Michael M. E. Baumgärtel, Andreas Dolfen, and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany

For the study of strongly correlated molecular crystals the determination of realistic model parameters is an open problem. Rather than fitting to experimental data or semi-empirical approaches, we demonstrate how to determine material-specific parameters for an extended Hubbard model ab-initio. The model can be restricted to HOMO and LUMO by renormalization of the screened Hubbard parameters. While intra-molecular screening is treated within density functional theory, we describe inter-molecular screening by a lattice of distributed polarizabilities. However, the long-range dipole-dipole interaction makes this approach computationally difficult. We can, though, obtain rapidly converging dipole-response matrix elements in reciprocal space using Ewald-summation. We demonstrate this method for TTF-TCNQ.

TT 45.38 Thu 15:00 Poster B

The origin of magnetic and orbital order in K_2CuF_4 — •Guoren Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany

In this work, we investigate the origin of magnetic and orbital order in K_2CuF_4. We first construct Wannier functions from the Bloch states obtained by local-density approximation calculations with the full-potential linearized augmented plane-wave method. Then, by perturbative theory, we calculate magnetic couplings which are in good agreement with experimental results both for the ambient and high pressure structures. To investigate the origin of orbital order, we perform calculations with local-density approximation+dynamical mean-field theory method. We discuss the roles of superexchange[1] and the charge-transfer effects[2] on the orbital ordering.
[1] K. I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].
[2] M.V. Mostovoy and D. I. Khomskii, Phys. Rev. Lett. **92**, 167201 (2004).

TT 45.39 Thu 15:00 Poster B

Energy shifts in pump-probe resonant soft x-ray diffraction experiments — •Christian Schüssler-Langeheine[1], Christoph Trabant[1,2], and Niko Pontius[1] — [1]Helmholtz-Zentrum Berlin — [2]II. Physikalisches Institut, Universität zu Köln

Time resolved pump-probe resonant soft x-ray diffraction is a novel method to study elementary coupling mechanisms in correlated solids or ultrafast magnetism in antiferromagnets. Besides information about the amount of order and its periodicity also spectroscopic information is accessible via the energy dependence of diffraction features in the vicinity of absorption edges. From that the electronic character of a photo-excited state can be determined. For a quantitative analysis of the energy-dependent diffraction data the effect of absorption has to be taken into account. It leads to particularly strong effects, when the pump effect causes a gradient of the density of scatterers in the probed volume. We discuss, how this effect affects the spectral shape in resonant soft x-ray diffraction data.

Supported by the BMBF through contract 05K10PK2

TT 45.40 Thu 15:00 Poster B

X-ray Photon Correlation Spectroscopy Study of Phase Separation in Correlated Oxides — •Marcel Buchholz[1], Bo Shi[2], Christoph Trabant[1,3], Chun-Fu Chang[1,4], Michael Sprung[5], Vasco Tenner[2], Christian Gutt[5], Alexander Komarek[1,4], Enrico Schierle[3], Gerhard Grübel[5], Markus Braden[1], Jeroen B. Goedkoop[2], and Christian Schüssler-Langeheine[3,1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Van der Waals-Zeeman Instituut, Universiteit van Amsterdam — [3]Helmholtz-Zentrum Berlin — [4]MPI Chemische Physik fester Stoffe, Dresden — [5]Deutsches Elektronen-Synchrotron, Hamburg

In systems with complex phase diagrams phase separation and phase coexistence may occur. Such effects lead to an involved relation between local electronic structure and macroscopic properties and may cause a high susceptibility of the latter to external stimuli. Phase separation has in fact been proposed as the mechanism leading to the colossal magnetoresistance effect in manganites. We report results from a study of phase separation effects in correlated oxides with x-ray photon correlation spectroscopy (XPCS). This technique provides a sensitivity to the local structure as well as to the spatial pattern of domains and to their dynamics. We studied the phase separation effect around the metal-to-insulator transition in doped titanates with soft x-ray photons from BESSY II and high energy x-rays from the ESRF and the ultra brilliant x-ray storage ring PETRA III. Supported by the DFG through SFB 608 and the BMBF through contract 05K10PK2.

TT 45.41 Thu 15:00 Poster B

Theoretical investigations on the magnetic properties of strongly correlated transition metal oxides — •J. Minar, S. Mankovsky, S. Bornemann, H. Ebert, and D. Ködderitzsch — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

We present a detailed theoretical investigation on the magnetic properties of the strongly correlated transition metal oxides MnO, FeO, CoO, NiO in their different magnetic structures. The Calculations were performed scalar as well as fully relativistically using the LSDA+U formalism implemented within the full potential Korringa Kohn Rostoker (KKR) Green's function method. We will show results for the spin and orbital magnetic moments, exchange coupling constants as well as the magnetic anisotropy energies in these systems and we will also discuss how these quantities depend on the Hubbard parameter U.

TT 45.42 Thu 15:00 Poster B

Low-temperature high-pressure optical investigation of the Mott-Hubbard insulator TiOCl — •Jihaan Ebad-Allah[1], Matthias Klemm[1], Siegried Horn[1], Michael Sing[2], Ralph Claessen[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (with X=Cl or Br) are Mott-Hubbard insulators with a charge gap of ≈ 2 eV. Our recent pressure-dependent infrared spectroscopic investigations on TiOX at room temperature [1] suggested that the application of external pressure induces an insulator-to-metal transition. As a follow-up, we studied the infrared transmittance and reflectance spectra of TiOCl at temperatures from 300 K down to 50 K and for pressures up to 22 GPa. Above 14 GPa a huge growth of spectral weight is observed in the optical conductivity spectrum. Furthermore, we determined the temperature and pressure dependence of the crystal field splitting via the frequency of the orbital excitation.
[1] C. A. Kuntscher et al., Eur. Phys. J. Special Topics **180**, 29 (2010).

TT 45.43 Thu 15:00 Poster B

Long range order effects in the Mott-Hubbard transition and the Variational Lattice Approach — •Aljoscha Wilhelm[1], Christoph Jung[1], Hartmut Hafermann[2], and Alexander Lichtenstein[1] — [1]I. Institut fur Theoretische Physik, Universitat Hamburg, Jungiusstrae 9 — [2]Centre de Physique Theorique (CPHT), Ecole Polytechnique, 91128 Palaiseau Cedex, France

We introduce an efficient strategy to treat long ranged correlations

in fermionic lattices, the so called variational lattice approach (VLA). The VLA combines the recently developed dual fermion approach for k-dependent problems and the exact diagonalization technique. We present first benchmark results. The phase diagram of the half-filled paramagnetic Mott-Hubbard transition is discussed and results are compared to CDMFT and DCA calculations.

TT 45.44 Thu 15:00 Poster B

Continuous-time quantum Monte Carlo investigation of the metallic state near a Mott insulator — •Junya Otsuki[1,2] and Dieter Vollhardt[1] — [1]Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — [2]Department of Physics, Tohoku University, Sendai, Japan

Motivated by a recently developed theory of extremely correlated Fermi liquids [1], we investigate the t-J model close to half-filling using the extended dynamical mean-field theory in the presence of fermionic and bosonic baths. The effective impurity model is solved by the continuous-time quantum Monte Carlo (CT-QMC) method which we extend to include the spin-boson coupling in the $U = \infty$ Anderson model. Results for the coherence temperature and the single-particle spectra close to the half-filling are presented.

[1] B. S. Shastry, Phys. Rev. Lett. **107**, 056403 (2011).

TT 45.45 Thu 15:00 Poster B

Correlation functions of the spin-1/2 Heisenberg chain at finite temperature via functional equations — •Britta Aufgebauer and Andreas Klümper — Bergische Universität Wuppertal

We present results on static finite temperature correlation functions of the Heisenberg chain on arbitrary successive sites in the thermodynamic limit. The density matrix, encoding all information about the correlation functions on a fixed number of successive sites, is obtained in a suitable limit of the six-vertex model density matrix on a rectangular lattice of unbounded width and finite height with toroidal boundary conditions. We consider an inhomogeneous density matrix. The inhomogeneities enable the derivation of a functional equation of difference type, valid for a finite set of parameter values. This equation in conjunction with the asymptotic behaviour determines the inhomogeneous density operator uniquely.

The functional equation is a discrete version of the so-called reduced quantum Knizhnik-Zamolodchikov equation fulfilled by the density operator at zero temperature. Despite the fundamentally different analytical properties of the correlation functions, it follows that the algebraic structure survives the introduction of a non-zero temperature. In particular the physical input for the calculation of correlation functions on arbitrary successive sites is a finite number of one- and two-point functions.

TT 45.46 Thu 15:00 Poster B

A numerical and an analytical approach to Chalker Coddington type network models — •Win Nuding[1], Michael Brockmann[1], Andreas Klümper[1], and Ara Sedrakyan[2] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Yerevan Physics Institute, Theoretical Department, Yerevan 36, Armenia

Chalker Coddington type network models appear in the context of the Quantum Hall Effect and the Spin Quantum Hall Effect. These network models and corresponding quantum spin chains are investigated to explain plateau - plateau transitions. In the case of integrable $sl(2,1)$ invariant $3 \otimes \bar{3} \ldots$ spin chains, Bethe Ansatz equations were formulated and solved numerically for small systems. For large systems such numerical calculations are not possible. Therefore an alternative approach on the basis of non linear integral equations (NLIE) is presented. The NLIE can be solved for very large systems giving the scaling dimension.

In the non integrable case row transfer matrices can be calculated explicitly yielding for example Lyapunov exponents and the decay length. Since recent high precision numerical simulations of the Lyapunov exponent in the Chalker-Coddington model [1,2] show disagreement with experimental data, we started numerical simulations of the localization length on random networks.

[1] K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304(R) (2009)
[2] M. Amado, A. Malyshev, A. Sedrakyan, F.Dominguez-Adame, Phys.Rev.Lett. 107,066402 (2011)

TT 45.47 Thu 15:00 Poster B

Out of equilibrium energy dynamics in low dimensional quantum magnets — •Stephan Langer[1], Markus Heyl[1], Ian McCulloch[2], and Fabian Heidrich-Meisner[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, LMU München, Germany — [2]School of physical Sciences, The University of Queensland, Brisbane, Australia

We investigate the real-time dynamics of the energy density in spin-1/2 XXZ chains using two types of quenches resulting in initial states which feature an inhomogeneous distribution of local energies. The first involves quenching bonds in the center of the chain from antiferromagnetic to ferromagnetic exchange interactions. The second quench involes an inhomogeneous magnetic field, inducing both, an inhomogeneous magnetization profile and local energy density. The simulations are carried out using the adaptive time-dependent density matrix renormalization group algorithm. We analyze the time-dependence of the spatial variance of the bond energies and the local energy currents which both yield necessary criteria for ballistic or diffusive energy dynamics. For both setups, our results are consistent with ballistic behavior, both in the massless and the massive phase. For the massless regime, we compare our numerical results to bosonization and the non-interacting limit finding very good agreement. The velocity of the energy wave-packets can be understood as average velocity of excitations induced by the quench.

TT 45.48 Thu 15:00 Poster B

Effective quantum dimer models for strongly correlated fermion systems — •Dominik Ixert and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is the standard model for the description of strongly correlated electron systems. Here we focus on single-band Hubbard models at zero temperature and at half filling. Recently, more and more evidences have been found for exotic insulating quantum spin liquid phases close to the metal-insulator transition. We are aiming at a microscopic description of these interesting non-magnetic phases in terms of effective quantum dimer models. To this end we apply graph-based continuous unitary transformations (gCUTs). It is expected that this approach works well as long as the charge and the spin gap is finite which is for example the case for the quantum spin liquid on the honeycomb lattice.

TT 45.49 Thu 15:00 Poster B

Properties of the Heisenberg two-leg Ladder using graph-based Continuous Unitary Transformations — •Johannes-Konstantin Splinter, Kris Cöster, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

Continuous Unitary Transformations (CUTs) have established themselves to handle a variety of strongly correlated quantum many-body systems. The major challenge for the use of CUTs is to find a proper truncation scheme for the flow-equations. Here, we apply a recently developped new truncation scheme which is expected to give reliable effective low-energy models for gapped phases of quantum lattice models. The basic idea is to combine graph theory and CUTs. These intrinsically robust graph-based continuous unitary transformations (gCUTs) are used to calculate zero- and one-triplon properties of the antiferromagnetic S=1/2 Heisenberg ladder. In order to optimize the gCUTs, we implement the full symmetry group of the ladder system.

TT 45.50 Thu 15:00 Poster B

Comparison of TEBD and NRG methods for computing the nonequilibrium dynamics of nanosystems coupled to a bosonic bath — •Malcolm Einhellinger[1], Eric Jeckelmann[1], Sabine Tornow[2], and Gertrud Zwicknagl[2] — [1]Leibniz Universität Hannover — [2]TU Braunschweig

We investigate the applicability of the Time-Dependent Renormalization Group (TEBD) Algorithm to low-dimensional quantum systems coupled to a bosonic bath. For that purpose we compare outcomes from TEBD realtime simulations with results from the Time-Dependent Numerical Renomalization Group (TD-NRG) Algorithm which has been shown to work well for those kind of problems. In this regard, we study the transport from a donor to an acceptor structure, connected via a bridge molecule. Coupling donor and acceptor to a bosonic bath damps the normally occuring oscillations in the particle densities and gives new insights in the physics of transport effects through bridge molecules.

TT 45.51 Thu 15:00 Poster B

Projective approach to transport in weakly interacting 1-d fermionic quantum systems — •Christian Bartsch — Institute

for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig

We investigate transport properties of 1-d fermionic hopping models featuring nearest and next-nearest neighbor hopping, where the fermions are additionally subject to a weak mutual interaction. To this end we employ a pertinent approach which allows for a mapping of the underlying Schrödinger dynamics onto an adequate linear quantum Boltzmann equation. This approach is based on a suitable projection operator method. From this Boltzmann equation we are able to numerically obtain diffusion coefficients for the limit of long times and weak interactions in the case of non-vanishing next-nearest neighbor hopping, whereas the diffusion coefficient diverges without next-nearest neighbor hopping. For the latter case we analytically investigate the decay behavior of the current with the result that parts of the current relax arbitrarily slow which suggests anomalous diffusive transport behavior within the scope of our approach.

TT 45.52 Thu 15:00 Poster B

Possible gapless spin liquid in the Kagome Lattice — •Xue-Feng Zhang and Sebastian Eggert — Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

We studied the Hard-Core Bose-Hubbard Model with nearest neighbor repulsion. In the solid phase, we find a new representation to describe the degeneracy of the ground state. By using the Strong Coupling Expansion and the Quantum Monte Carlo simulation, we got the solid melting critical lines for both positive and negative hopping process. And such phase transitions are induced by the fractional charge excitation.

Considering the superfluid and solid phase respectively break different symmetry, we think such second order melting process would not happen between them and the gapless spin glass intermediate phase may exist there.

TT 45.53 Thu 15:00 Poster B

Supersolid phase transitions for hardcore bosons on a triangular lattice — Xue-Feng Zhang, •Raoul Dillenschneider, and Sebastian Eggert — Physics Dept. and Res. Center OPTIMAS, Univ. of Kaiserslautern, 67663 Kaiserslautern, Germany.

Hard-core bosons on a triangular lattice with nearest neighbor repulsion are a prototypical example for a system with supersolid behavior on a lattice. We show that in this model the physical origin of the supersolid phase can be understood quantitatively and analytically by constructing quasiparticle excitations of defects that are moving on an ordered background.

TT 45.54 Thu 15:00 Poster B

The Density Matrix Renormalization Group for spin-1/2-quantum chains: A demonstration program — •Thomas Köhler, Piet Dargel, and Andreas Honecker — Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

We have implemented a density matrix renormalization group algorithm in the formulation of Matrix-Product-States as Web Applet. This implementation offers direct visualization of the running algorithm including energy, static correlation functions and entropy convergence. It offers the computation of several different Spin-1/2-Hamiltonians and we have explicitly evaluated the Ising-chain in a transversal magnetic field.

TT 45.55 Thu 15:00 Poster B

Lanczos algorithm with Matrix Product States for dynamical correlation functions — •Piet Dargel[1], Anton Wöllert[2], Andreas Honecker[1], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München

The Lanczos algorithm is combined with Matrix Product States to calculate dynamical correlation functions. The use of Matrix Product States allows to handle systems that are larger than those accessible within the standard Lanczos algorithm, for the price of worse convergence of the spectral poles as compared to the original algorithm. In order to achieve a better convergence of the spectral weights and poles we introduce an ex post reorthogonalization method and also test spectral shifts. We present results for the dynamic spin structure factor of the spin-1/2 antiferromagnetic Heisenberg chain. These results are compared to Bethe ansatz results in the thermodynamic limit.

TT 45.56 Thu 15:00 Poster B

cRPA study of a three band one-dimensional Hubbard model — •Michael Seissinger and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Starting from a three band one-dimensional model, we derive an effective one band low energy model using a functional integral formulation of the cRPA approach. The effective model with retarded interactions can be simulated with continuous time weak coupling QMC methods. Our aim is to monitor the variation of the Luttinger liquid exponent as function of the energy scale of the high energy bands which are integrated out in the cRPA approach.

TT 45.57 Thu 15:00 Poster B

QMC impurity solvers for two-particle Green's functions. — •Pavel Augustinský[1,2] and Jan Kuneš[2] — [1]Universitaet Augsburg — [2]Institute of Physics, Academy of Sciences of the Czech Republic

The fundamental observable for QMC impurity solvers, the one-particle Green's function, does not contain a complete information about the studied system. The two-particle Green's function brings additional insight into electronic correlations, response functions and related quantities absent in the one-particle case. However, measurement of 2P Green's functions involves technical difficulties. We present comparison of the Hirsch-Fye and the continuous-time QMC techniques for 2P Green's functions. Namely, we address performance issues and discuss areas of applicability.

TT 45.58 Thu 15:00 Poster B

Band structure engineering and vacancy induced metallicity at the GaAs-AlAs interface — •Mousumi Upadhyay Kahaly, Safdar Nazir, and Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

We study the epitaxial GaAs-AlAs interface of wide gap materials by means of full-potential density functional theory based calculations. We find an insulating state at the interface and a negligible charge transfer. Optimization of the atomic positions results in very small changes in the chemical bonding. We aim to understand how an anionic defect at and near the interface modifies the electronic structure and therefore the physical properties of the GaAs-AlAs heterostructure. Introduction of As vacancies near the interface induces metallicity, which opens great potential for GaAs-AlAs heterostructures in modern electronics. While GaAs and AlAs are known since long to form high quality epitaxial superlattices, the effect of n-doping on the electronic properties of this heterostructure has been ignored so far. The systems under investigation are suitable for disentangling the complex behavior of metallic interface states.

TT 45.59 Thu 15:00 Poster B

Magnetic excitations in the diamond spin system $Cu_3(CO_3)_2(OH)_2$ probed by ESR — •Dmytro Kamenskyi[1], Mykhaylo Ozerov[1], Frederik Wolff-Fabris[1], Joachim Wosnitza[1], Sonia Francoual[2], Vivien Zapf[3], and Sergei Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]Hamburger Synchrotronstrahlungslabor (HASYLAB), Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — [3]National High Magnetic Field Laboratory - Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We report systematic tunable-frequency electron spin resonance (ESR) studies of the natural mineral azurite $Cu_3(CO_3)_2(OH)_2$. This material has a diamond spin-chain structure and exhibits unusual magnetic properties (including a magnetization plateau). ESR experiments have been done at frequencies from 50 to 1000 GHz in magnetic fields up to 51 T. The observed frequency-field dependence of the magnetic excitations clearly indicates the important role of magnetic frustrations in this material, which can be suppressed by high magnetic fields. Our findings are discussed in connection with results of inelastic neutron-scattering experiments. Work was supported by EuroMagNET II (EU contract No. 228043).

TT 45.60 Thu 15:00 Poster B

NMR on the quasi two-dimensional antiferromagnet $Ba(Ni_{1-x}Mg_x)_2V_2O_8$ — •Dirk Waibel[1], Thomas Wolf[2], Hilbert v. Löhneysen[1,2], and Bernd Pilawa[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — [2]Karlsruher Institut für Technologie, Institut für Festkörperphysik,

76021 Karlsruhe

Magnetic-field dependent NMR measurements in the quasi two-dimensional (2D) antiferromagnet (AF) $Ba(Ni_{1-x}Mg_x)_2V_2O_8$ have been performed for $\mathbf{B} \perp \mathbf{c}$ and $\mathbf{B} \parallel \mathbf{c}$ at 2 K and 79 MHz. The spin echo signal of the ^{51}V nuclei in the undoped sample consists of one distinct peak for $\mathbf{B} \parallel \mathbf{c}$ which is split into three lines for $\mathbf{B} \perp \mathbf{c}$. The signals of the ^{51}V nuclei significantly broaden upon doping. Futhermore, the ^{51}V nuclear spin-lattice relaxation rate T_1^{-1} has been measured over a temperature range from 6 K to 300 K at 7 T and 79 MHz revealing a strong increase of the T_1^{-1} rate at $T_N = 47.4$ K. This divergent behavior has been analyzed for $\mathbf{B} \perp \mathbf{c}$ and $\mathbf{B} \parallel \mathbf{c}$ in the context of the 2D topological Berezinskii-Kosterlitz-Thouless (BKT) phase transition. Also, the oscillatory decay of the spin echo due to the quadrupole interaction of the ^{51}V $\left(I = \frac{7}{2}\right)$ nuclei is clearly visible in the temperature range from 50 K to 300 K.

TT 45.61 Thu 15:00 Poster B

Atomically resolved images of lithium purple bronze — •Melanie Klinke[1], Robert Bienert[1], Michael Waelsch[1], Tatjana Podlich[1], Rongying Jin[2], and René Matzdorf[1] — [1]Experimentalphysik II, Universität Kassel, Deutschland — [2]Department of Physics and Astronomy, Lousiana State University, USA

The lithium molybdenum purple bronze $Li_{0.9}Mo_6O_{17}$ is a quasi 1D metal at room temperature showing Luttinger liquid physics. The highly anisotropic conductivity runs along the crystallographic b axis where Mo-O chains, formed by the shared edges of the MoO_6 octahedra, provide the electrical transport. $Li_{0.9}Mo_6O_{17}$ samples were investigated with low-temperature scanning tunneling microscopy and spectroscopy. By cleaving the samples at low temperatures (60 K) we obtained atomically resolved images of the surface. In these images the Mo-O chains are visible, which are covered by layers of MoO_6 octahedra and MoO_4 tetrahedra.

TT 45.62 Thu 15:00 Poster B

Non-linear transport properties of pure, Rb- and W-doped blue bronze $K_{0.3}MoO_3$ — •Ali Khairi Al-Hadeethi[1], Dominik Grund[1], Song Yue[2], Martin Dressel[2], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The temperature dependence of the dc resistivity and the non-linear transport properties of pure, Rb-doped, and W-doped blue bronze $K_{0.3}MoO_3$ single crystals are presented. These are prototypical charge-density-wave (CDW) compounds. Nonlinear conductivity due to the sliding of the CDW is observed, when the applied electric field exceeds the first threshold field (E_T). Furthermore, above a second threshold field ($E_T{}^* > E_T$) coherent CDW-sliding sets in. For all studied materials E_T and $E_T{}^*$ increase monotonically with decreasing temperature . This finding is discussed in terms of the incommensurate-commensurate transition of the CDW and within the frame of the Fukuyama-Lee-Rice model.

TT 45.63 Thu 15:00 Poster B

Thermal conductivity of the $S = 1/2$ two-leg spin-ladder compound bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY) — •Gerhard Kolland[1], Johannes Engelmayer[1], Mark M. Turnbull[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Carlson School of Chemistry and Department of Physics, Clark University, Worcester, Massachusetts, USA

Bis(2,3-dimethylpyridinium) tetrabromocuprate (DIMPY) is a model material for a Heisenberg $S = 1/2$ two-leg spin-ladder with antiferromagnetic couplings $J_{\mathrm{rung}} \simeq 4.3\,\mathrm{K}$ (along the rungs of the spin-ladder) and $J_{\mathrm{leg}} \simeq 8.4\,\mathrm{K}$ (along the legs) in the strong-leg regime, i.e. $J_{\mathrm{leg}} > J_{\mathrm{rung}}$. In zero magnetic field, the spin ladder has a finite excitation gap, which is closed at a lower critical field $B_{C1} \simeq 3\,\mathrm{T}$, where the system enters a gapless Luttinger-liquid (LL) phase. At the saturation field $B_{C2} \simeq 30\,\mathrm{T}$ the system leaves the LL phase and a gap opens. We present measurements of the magnetic-field dependent thermal conductivity κ. The field was applied along the b direction. To investigate a magnetic contribution to κ, we measured the thermal conductivity parallel $\kappa_{||}$ and perpendicular $\kappa_\perp$ to the ladder direction. At higher temperatures around 2 K, the magnetic-field influence is rather similar for both directions. We observe a broad minimum around 5 T, which sharpens and approaches B_{C1} with decreasing temperature. In addition, the magnetic-field dependent thermal conductivity gets anisotropic. Below 1 K, $\kappa_{||}$ is strongly enhanced, whereas $\kappa_\perp$ stays almost constant. *Supported by the DFG through SFB 608.*

TT 45.64 Thu 15:00 Poster B

Magnetic ordering transitions of the effective XY-spin-$\frac{1}{2}$ compound Cs_2CoCl_4 in transverse magnetic fields — •Oliver Breunig[1], Eran Sela[2], Benjamin Buldmann[2], Markus Garst[2], Petra Becker[3], Ladislav Bohatý[3], Christian Dax[1], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 is a model system for studying the magnetism of one-dimensional spin chains. It contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The groundstate doublet is separated from the first excited doublet state by approximately 15 K, such that at temperatures between 0.3 and 4 K the compound is well described by the one-dimensional XXZ model. Decreasing temperature further, magnetic order arises at field-dependent temperatures $T_C(H)$. According to [1] spins are confined to the bc-plane in the ordered phase. Measuring thermal expansion with a magnetic field applied along the crystallographic b-axis, we observe a series of magnetic transitions within the ordered state. We discuss thermodynamic properties of the magnetically ordered state.

This work was supported by the DFG through SFB 608.

[1] M. Kenzelmann et al., Phys. Rev. B **65** (2002).

TT 45.65 Thu 15:00 Poster B

Phase diagram of the Ising chain compound Nb_2O_6 in transverse magnetic field — •Simon Scharffe, Oliver Breunig, Johanna Frielingsdorf, Martin Valldor, Michael Seher, and Thomas Lorenz — II. Physikalisches Insitut, Universität zu Köln

$CoNb_2O_6$ is a model system to investigate a quantum phase transition in magnetic fields. The structure consists of layers of CoO_6 octahedrons separated by non-magnetic NbO_6 layers. Within each layer the Co^{2+}spins are linked through superexchange and form 1D ferromagnetic zigzag chains along the c axis. Due to crystal field effects (compression of the CoO_6 octahedrons) an easy-axis anisotropy of the Co^{2+}moments is present, which leads to an effective spin-1/2 system described by the Ising model. The easy axis is in the a c plane, and alternates by $\pm$ 31° with respect to the c axis for neighboring chains. Due to small inter-chain couplings $J_{||} \approx 0.01 \cdot J_\perp$ the system shows long-range antiferromagnetic order, which is insommensurate below T_{N1}=2.9K and becomes commensurate at T_{N2}=1.9K. A magnetic field parallel to the b axis is normal to the easy axis and allows to study the quantum phase transition of an Ising-spin chain in tranverse field. The system is driven to its quantum critical point between a quasi 1D ferromagnet to a quantum paramagnet. Only few studies of the transverse field case are available so far. We present measurements of specific heat and magnetization in a temperature range from about 0.3 to up to 10 K and discuss the phase diagram.

This work was supported by the DFG through SFB 608.

TT 45.66 Thu 15:00 Poster B

Quasi one-dimensional spin chain materials $AM_2V_2O_8$ — •Michael Seher, Sandra Niesen, Gerhard Kolland, Oliver Heyer, Simon Scharffe, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

Compounds with the general formula $AM_2V_2O_8$ with an alkaline-earth on the A-site and a transition-metal on the M-site show a lot of interesting properties. This class of compounds is mainly isostructural with tetragonal symmetry and provides spin chain structures. The magnetic properties are vitally influenced by the chosen transition metal with its partially filled 3d shell. Thus, these compounds are suitable to study spin systems from $S = 1/2$ to 5/2 and spin quantum number anisotropy can be studied from Ising- to Heisenberg behavior. Here, we present a detailed study on the magnetic phase diagram of the effective $S = 1/2$ Ising system $BaCo_2V_2O_8$. Moreover, we have grown large single crystals of the nearly isotropic Heisenberg systems $BaMn_2V_2O_8$ and the new compound $SrMn_2V_2O_8$. At higher temperatures both compounds behave like 1D magnetic systems. But due to finite interchain couplings both systems show long-range antiferromagnetic order with T_N = 37 K (A= Ba) [1] and T_N = 43 K (A= Sr) [2].

This work is supported by the DFG through SFB 608.

[1] Z. He *et al.* Solid State Comm. **141** (2007) 22
[2] S.K. Niesen *et al.* J. Mag. Mag. Mat. **323** (2011) 2575

TT 45.67 Thu 15:00 Poster B

NMR evidence for peculiar spin gaps in a doped S=1/2 Heisenberg spin chain — •Yannic Utz[1], Christian Rudisch[1], Franziska Hammerath[1], Hans-Joachim Grafe[1], Ashwin Mohan[1], Surjeet Singh[2], Romuald Saint-Martin[3], Alexandre Revcolevschi[3], Patrick Ribeiro[1], Christian Hess[1], Anja Wolter[1], Vladislav Kataev[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]Indian Institute of Science Education and Research, Pune, India — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris-Sud, Orsay, France

We present ^{63}Cu Nuclear Magnetic Resonance (NMR) measurements on undoped, Ca-doped and Ni-doped $SrCuO_2$ single crystals. $SrCuO_2$ is a good realization of a one-dimensional S=1/2 Heisenberg spin chain. This is manifested by the theoretically-expected temperature-independent NMR spin-lattice relaxation rate T_1^{-1}. In $Sr_{0.9}Ca_{0.1}CuO_2$ an exponential decrease of T_1^{-1} below 90 K evidences the opening of a gap in the spin excitation spectrum, which amounts to $\Delta = 50$ K [1]. DMRG calculations are presented to discuss the origin of this spin gap. New results on $SrCu_{0.99}Ni_{0.01}O_2$ also indicate the presence of a spin gap, which is twice as large as in $Sr_{0.9}Ca_{0.1}CuO_2$, despite the minor doping level of Ni compared to Ca. We discuss different possible impacts of Ca (S=0) and Ni (S=1) doping on structural and magnetic properties of the parent compound.
[1] F. Hammerath et al., Phys. Rev. Lett. **107**, 017203 (2011).

TT 45.68 Thu 15:00 Poster B

Thin film growth and characterization of the neutral-ionic phase transition system tetrathiafulvalene-p-chloranil — •Achim Rippert, Milan Rudloff, Kai Ackermann, 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 different substrate materials. 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 brings about a distinct change of the electrical conductivity, an anomaly of the frequency dependent dielectric function, as well as a color change of the material. Via partial Br-Cl-substitution the phase transition can be shifted to 0 K resulting in a quantum critical state. 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 45.69 Thu 15:00 Poster B

ESR studies of the quasi-2D antiferromagnet $Cu(Pz)_2(ClO_4)_2$ — •M. Ozerov[1], J. Wosnitza[1], E. Čižmár[2], F. Xiao[3], M.M. Turnbull[3], C. P. Landee[4], and S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD),Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]Centre of Low Temperature Physics, P.J. Šafárik University, SK-041 54 Košice, Slovakia — [3]Carlson School of Chemistry and Biochemistry, Clark University, Worcester, Massachusetts 01610, USA — [4]Department of Physics, Clark University, Worcester, Massachusetts 01610, USA

We report systematic high-field electron spin resonance (ESR) studies of the quasi-two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet $Cu(pz)_2(ClO_4)_2$ (pz denotes pyrazine or $C_4H_4N_2$). The linewidth and resonance-field temperature dependences of the ESR absorptions in this compound were investigated in the frequency range from 85 to 416 GHz in magnetic fields up to 16 T. A pronounced ESR linewidth anomaly was revealed in the vicinity of T_N. This anomaly reflects enhanced critical fluctuations in this compound at the 3D ordering. The experiment revealed a significant change in the linewidth behavior for magnetic fields above 7 T, whose origin will be discussed.

The work was supported in part by DFG and EuroMagNET II (EU Contract No. 228043).

TT 45.70 Thu 15:00 Poster B

$Cs_2CuCl_{4-x}Br_x$: perspectives of experimentally tunable frustration in a triangular lattice — •Kateryna Foyevtsova, Ingo Opahle, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Frustrated antiferromagnets Cs_2CuCl_4 and Cs_2CuBr_4 with an underlying triangular lattice demonstrate rich magnetic phase diagrams, where one finds a spin-liquid phase for Cs_2CuCl_4 and quantum fluctuation stabilized magnetization plateaux for Cs_2CuBr_4. The magnetism of Cs_2CuCl_4 and Cs_2CuBr_4 might be understood in terms of the triangular Heisenberg model with different degrees of frustration: $J'/J \sim 0.3$ for Cs_2CuCl_4 and $J'/J \sim 0.7$ for Cs_2CuBr_4. Recently, mixed systems $Cs_2CuCl_{4-x}Br_x$ have been synthesized for a dense mesh of x values from 0 to 4, which suggests that it might be possible to tune the J'/J ratio by varying x. We apply the density functional theory to study the crystal and electronic structures of some members of the $Cs_2CuCl_{4-x}Br_x$ series. In particular, we are interested in the microscopic equilibrium distribution of the substituted halogen atoms which affects the spin exchange couplings J and J'. We also discuss the two structural phases – orthorhombic and tetragonal – that might emerge during crystal growth, depending on the growth conditions.

TT 45.71 Thu 15:00 Poster B

Searching for the Power-Law Conductivity Inside the Mott Gap in κ-$(ET)_2Cu_2(CN)_3$ — •Sebastian Elsässer[1], John A. Schlueter[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Argonne Nat. Lab., U.S.A.

The organic charge-transfer salt κ-$(ET)_2Cu_2(CN)_3$, which is a Mott insulator, has recently gained interest as possible realisation of the spin-liquid state in two dimensions. This phenomenon is due to spin frustration in the nearly isotropic triangular lattice where spin fluctuations are enhanced and do not order even at the lowest temperatures despite comparable strong antiferromagnetic interactions [1]. Also, spin-liquids support exotic excitations like spinons. Although spinons do not carry charge and thus can not interact with the electromagnetic field directly, they couple to the induced gauge field, leading to a contribution to optical conductivity inside the charge gap. For low frequencies a power-law conductivity $\sigma_1 \propto \omega^{3.33}$ for $\hbar\omega > k_BT$ and $\sigma_1 \propto \omega^2$ for $\hbar\omega < k_BT$ is predicted [2]. To verify this on a quantitative basis, we performed polarisation dependent optical investigations ranging from 23 - 8000 cm^{-1} at temperatures from 300 K - 12.6 K. We find that a power-law is applicable over a wide range inside the Mott gap, however, the exponent clearly deviates from the proposed values as it is actually much lower. The temperature-dependent crossover could not be observed as well. Upon cooling, a saturation of the power-law is observed.
[1] Y. Shimizu *et al.*, Phys. Rev. Lett. **91**, 107001 (2003)
[2] T.-K. Ng and P. A. Lee, Phys. Rev. Lett. **99**, 156402 (2007)

TT 45.72 Thu 15:00 Poster B

Pressure-dependent resistivity measurements on the novel charge-transfer salt $(BEDT\text{-}TTF)_2Cu_2Br_3$ — •Sebastian Köhler[1], Ulrich Tutsch[1], Friedhelm Isselbächer[1], Michael Lang[1], Frauke Schödel[2], Hans-Wolfram Lerner[2], and Matthias Wagner[2] — [1]Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TRR49, D-60438 Frankfurt (M) — [2]Institut für Anorganische Chemie, Goethe-Universität Frankfurt (M), D-60438 Frankfurt (M)

During the course of optimizing parameters for the synthesis of the known charge-transfer salt $(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$, a novel salt, $(BEDT\text{-}TTF)_2Cu_2Br_3$ has been obtained [1]. It is known that other compounds from this family of materials exhibit a variety of electronic properties such as (Mott-)insulating, semiconducting, metallic or even superconducting behaviour, accessible by either chemical or hydrostatic pressure. Resistivity measurements have been performed at ambient pressure on single crystals of $(BEDT\text{-}TTF)_2Cu_2Br_3$ in a temperature range from 300 K down to 10 K, yielding a semiconductor-like behaviour with a small gap of about 30 meV. Our aim is to study the possibility of closing the semiconducting gap by applying hydrostatic pressure and thereby to induce metallic or even superconducting behaviour. We present measurements of the resistance under hydrostatic pressure on $(BEDT\text{-}TTF)_2Cu_2Br_3$ in a temperature range from 300 K to 4 K at various pressure values.
[1] Eur. J. Inorg. Chem. 2011, 1205-1211

TT 45.73 Thu 15:00 Poster B

Critical behavior at the antiferromagnetic phase transition

of Azurite — •P. T. Cong, B. Wolf, R. S. Manna, A. Brühl, S. Köhler, and M. Lang — Physikalisches Institut, J.W. Goethe-Universität Frankfurt, SFB/TR49, 60438 Frankfurt(M)

The natural mineral azurite has been considered as a model substance for a 1D spin 1/2 Heisenberg diamond chain [1]. However, early studies of this material indicate the presence of 3D long-range antiferromagnetic (AF) order below $T_N \sim 1.88$ K [2]. Clear signatures of the transition into the ordered phase have been observed in ultrasound, thermal expansion and specific heat measurement at T_N. Here we present a detailed investigation of the critical behavior of the sound velocity and ultrasonic attenuation in the vicinity of T_N. While the critical velocity changes exhibit a uniform behavior for various magnetic fields, the critical attenuation shows a sudden change as the system moves from the ordered AF to the spin-flop state. We compare the critical behavior derived from the ultrasonic studies with that observed in the specific heat and thermal expansion.

[1] H. Kikuchi *et. al.*, Phys. Rev. Lett. **94**, 227201 (2005).
[2] H. Forstat *et. al.*, J. Chem. Phys. **31**, 929 (1959).

TT 45.74 Thu 15:00 Poster B

Surface Topology and Electronic Structure of Layered Strontium Ruthenates — •Robert Bienert[1], Melanie Klinke[1], Michael Waelsch[1], Sebastian Mietke[1], Jin Peng[2], Zhiqiang Mao[2], and René Matzdorf[1] — [1]Experimentalphysik II, Universität Kassel, Deutschland — [2]Department of Physics, Tulane University, New Orleans, USA

In complex materials the interplay of properties like crystal structure, electronic structure and magnetism results in very interesting physical phenomena. The Ruddlesden-Popper series of layered Strontium Ruthenates $Sr_{n+1}Ru_nO_{3n+1}$ describes one class of these materials.

The double and triple layer systems behave like a Fermi liquid up to the transition temperature of 15 K and 24 K, respectively. In both compounds the local density of states (LDOS) shows a peak within the dip-like feature around the Fermi energy E_F. Using low-temperature (LT) STM and STS we studied the temperature dependence of the LDOS in the range from 4.7 to 35 K. By increasing the temperature the peak within the dip in the LDOS at E_F is only affected by thermal broadening.

The surface unit cell of the Strontium Ruthenates exhibits a $c(2\times2)$ super structure, which is stable from 4.7 K up to room temperature as shown by our atomically resolved LT STM images and room temperature LEED experiments.

TT 45.75 Thu 15:00 Poster B

^{139}La-NMR in the T'-La_2CuO_4 antiferromagnetic phase — •Marco Günther[1], Katharina Weber[1], Hubertus Luetkens[2], Gwendolyne Pascua[2], Roland Hord[3], Barbara Albert[3], Lambert Alff[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon Spin Spectroscopy, PSI — [3]Eduard-Zintl-Institut, TU Darmstadt — [4]Institute of Materials Science, TU Darmstadt

We study the antiferromagnetic ordered phase of T'-La_2CuO_4, a recently synthesized parent compound of electron doped cuprate superconductors by means of I= $\frac{7}{2}$ ^{139}La-NMR spectroscopy and powder spectra simulation.

The observed field sweep spectra at temperatures range between 10-240 K are compared with simulations of the combined nuclear Zeeman- and quadrupole-hamiltonian. In this approach the experimentally found line broadening arises from a local hyperfine field parallel to the copper-oxygen planes and is interpreted as the order parameter showing magnetic order below 207 K. We construct the hyperfine fields in a local electronic antiferromagnetic dipole model. Our results are compared to other local probe experiments on parent compounds of cuprate superconductors.

TT 45.76 Thu 15:00 Poster B

Magnetic Impurity with Generalized Couplings to 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 S=1/2 Heisenberg chains with open boundary conditions and an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo based on Stochastic Series Expansion. Results will be presented for thermodynamic properties as a function of temperature, exchange-coupling constants, anisotropy, magnetic fields, and system size. These include the energy, susceptibilities, magnetization and static correlation functions. For particular settings the models we investigate are integrable by Bethe Ansatz and we will compare findings from both methods in the limit of zero temperature.

TT 45.77 Thu 15:00 Poster B

Spin diffusion in the Heisenberg Chain: a quantum Monte-Carlo study — •Yousef Rahnavard[1,2], Björn Willenberg[1,2], and Wolfram Brenig[1,2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Niedersächsische Technische Hochschule, NTH

We study the long-wavelength, finite frequency spectrum of the spin density response of the antiferromagnetic Heisenberg chain. Current proposals for this, based on results from bosonization, transfer-matrix renormalization group, and quantum Monte-Carlo (QMC), suggest a diffusive spectrum in the isotropic case with a diffusion kernel independent of frequency and momentum which is diverging in the low temperature limit. Here we extend on the previous QMC work, which has been restricted to a single system size only. Results will be presented for the low frequency current relaxation rate versus momentum and temperature, for various system sizes from N=64 to 256. Moreover signatures of anomalous diffusion will be checked for by considering potential power-law frequency dependence of the diffusion kernel.

TT 45.78 Thu 15:00 Poster B

Helimagnets studied with neutron spin echo at RESEDA — •Jonas Kindervater[1,2], Wolfgang Häussler[1,2], Alexander Tischendorf[1,2], Andreas Bauer[1], Christian Pfleiderer[1], and Peter Böni[1] — [1]Technische Universität München, Physik Department E21, 85748 Garching, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRMII), 85748 Garching, Germany

Using RESEDA (FRM II, Munich), several studies on magnetic fluctuations in ferro- and helimagnetic compounds have been performed. RESEDA uses the Neutron Resonance Spin Echo (NRSE) technique, being a variant of conventional Neutron Spin Echo (NSE). In NRSE as in NSE, the beam polarization is the measured quantity. It provides the intermediate scattering function yielding information on the slow dynamics of the sample. However, NRSE experiments on magnetic systems, which affect the beam polarization, are difficult or even not feasible at all. In this contribution, we present the results of elastic and quasi-elastic scattering experiments on manganese silicide. We summarize the data analysis, proofing the polarizing effect of the sample, and taking into account this feature in the normalization of the results from quasi-elastic measurements.

TT 45.79 Thu 15:00 Poster B

Orbitons and bi-orbitons in $GdVO_3$ and YVO_3 — •Luis Fels[1], Michael Voigt[1], Komalavalli Thirunavukkuarasu[1], Eva Benckiser[2,1], Giacomo Ghiringhelli[3], Marco Moretti Sala[3], Graeme R. Blake[4], Nandang Mufti[4], Agung A. Nugroho[4,5], Thomas T. M. Palstra[4], Pasquale Marra[6], Krzysztof Wohlfeld[6], Jeroen. van den Brink[6], Maurits Haverkort[2], Thorsten Schmitt[7], and Markus Grüninger[1] — [1]Universität zu Köln — [2]MPI-FKF Stuttgart — [3]Politecnico di Milano — [4]University of Groningen — [5]Institut Teknologi Bandung — [6]IFWDresden — [7]Paul Scherrer Institut, Villigen

Here we report on optical measurements and high-resolution RIXS on $GdVO_3$ and YVO_3 single crystals. The goal of the measurements is the observation of so called orbitons which are, in analogy to magnons, collective orbital excitations on top of an orbitally ordered state. In both investigated compounds a G-type orbital ordered (OO) phase occurs, but only in YVO_3 an additional low temperature phase with C-type OO exists.

In the optical conductivity $\sigma(w)$ of $GdVO_3$, a striking feature is seen at 0.4 eV in the OO phase which is interpreted as bi-orbiton in agreement with further investigations on YVO_3 and $HoVO_3$ [1]. With the RIXS measurements it was possible to observe a significant dispersion of the intra-t_{2g} excitations at roughly 0.2 eV. However, the origin of this dispersion, whether it is due to a collective character of the excitations or a local effect, is still unclear.

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TT 45.80 Thu 15:00 Poster B

Ground state properties of antiferromatgnetic anisotropic S=1 Heisenberg spin chains — •David Peters — Institut für

Theoretische Physik, RWTH Aachen, 52064 Aachen

Using (infinite) density matrix renormalization group techniques, ground state properties of antiferromagnetic S=1 Heisenberg spin chains with exchange and single–site anisotropies in an external field are studied. The phase diagram is known to display a plenitude of interesting phases. We elucidate quantum phase transitions between the supersolid and spin–liquid as well as the spin–liquid and the ferromagnetic phases. Analyzing spin correlation functions in the spin–liquid phase, commensurate and (two distinct) incommensurate regions are identified.

TT 45.81 Thu 15:00 Poster B

Transport of an electron through a spin structure inside a quantum wire — •Christoph Hübner and Daniela Pfannkuche — I. Institut für Theoretische Physik, Hamburg, Germany

Transport properties of a quantum wire with embedded impurities is investigated in the framework of a numerically exact scattering formalism. The itinerant electrons are considered to interact with the impurities via a finite range exchange interaction. This leads to scattering of an initial wave package into different modes and spin states. We can map the integral Lippmann-Schwinger equation onto a system of linear equations. The solution of this equations is called the T-matrix. This matrix is directly related to the time dependent spacial and spin probability distribution of the itinerant electrons. The conductance of the quantum wire is associated with the transmission coefficients via the Landauer-Buettiker formula. It can be shown that the coefficients linearly depend on the elements of the T-matrix. Focus of our investigation lies on the cooperative dynamics of the impurities mediated by the conduction electrons. Screening effects of impurity momenta by localization of electrons are also of interest.

TT 45.82 Thu 15:00 Poster B

Thermal expansion investigation on EuB_6 — •Rudra Sekhar Manna[1], Frank Schnelle[1], Mariano de Souza[1], Michael Lang[1], Pintu Das[1], Adham Amyan[1], Jens Müller[1], Stephan von Molnár[2], Peng Xiong[2], and Zachary Fisk[3] — [1]Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Department of Physics, Florida State University, Tallahassee, Florida 32306, USA — [3]Dept. of Physics, University of California, Irvine, California 92697, USA

EuB_6 is a semimetallic correlated electron system, which exhibits a complex sequence of electronic and magnetic phase transitions at $\sim$ 15.5 K (T_1) and 12.5 K (T_2). The material also shows a colossal magnetoresistance effect which is largest at T_1. The paramagnetic to ferromagnetic transition in this system is suggested to take place via the formation of magnetic polarons. In this work, we investigate by means of thermal expansion and magnetostriction measurements to which extent lattice degrees of freedom are involved in these phase transitions. We find two corresponding anomalies in the thermal expansion, the one occurring at T_2 being much larger than that at T_1. The anomalies are very sensitive to magnetic fields. By applying a small magnetic field of less than 50 mT the anomaly at T_1 is fully suppressed, while the lower-temperature anomaly at T_2 shifts to higher temperature as the field is increased and finally fades out at a field $B > 5$ T. These measurements are complemented by measurements of the magnetostriction at various temperatures from below T_2 to above T_1 which highlight the extraordinarily large magnetoelastic effects in this material.

TT 45.83 Thu 15:00 Poster B

Realization of a Setup for Ultrasonic Experiments under He-Gas Pressure and Test Measurements on MnF_2 — •Sebastian Becker, Pham Thanh Cong, Bernd Wolf, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

Ultrasonic measurements are a powerful tool for investigating strongly correlated materials. The extension of these experiments to hydrostatic pressures, which opens up interesting possibilities for a detailed thermodynamic characterization, is challenging and has been rarely documented in the literature. Here we discuss the realization of an experimental setup, where ultrasonic measurements can be performed in a temperature range 1.2 - 300 K, at hydrostatic (He-gas) pressure values up to 10 kbar, and magnetic fields up to 16 T. The setup has been tested by measuring the ultrasonic attenuation and sound velocity on single crystalline MnF_2 in the temperature range 50 K $\leq$ T $\leq$ 300 K at various pressures. From these measurements the pressure dependence of the Néel temperature was derived to (380 $\pm$ 165) mK/kbar which compares favourably with literature results.

TT 45.84 Thu 15:00 Poster B

ESR spectrum of the spin-1/2 Heisenberg-Ising chain — •Michael Brockmann[1], Frank Göhmann[1], Michael Karbach[1], Andreas Klümper[1], and Alexander Weisse[2] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Max-Planck-Institut für Mathematik, 53072 Bonn, Germany

We analyze the ESR absorption spectrum of the spin-1/2 Heisenberg-Ising chain, also known as XXZ chain. The moments of the absorbed intensity can be calculated exactly due to the integrability of this model. They can be used to define the shift of the resonance as well as the width of the spectral line, both induced by the anisotropy of the interactions. If the frequency of the incident microwave is varied for fixed Zeeman field, the first four moments are sufficient to explore the exact resonance shift and line width at arbitrary temperatures and Zeeman fields in the full range of anisotropy parameters. In current ESR experiments, however, the Zeeman field is varied for fixed frequency. For this case we can still present results for the shift at small anisotropies and a high-temperature expansion for the line width.

We performed numerical calculations which agree well with exact data. Additionally, we are able to extract an empirical parameter-free model for the line shape at high temperatures which is extremely accurate over a wide range of anisotropy parameters and is exact at the free-fermion point and at the isotropic point. The anisotropic model shows strong absorption even in the zero-field limit. We derive the exact two-spinon ground-state contribution to the spectral line which accounts for more than 96% of the spectral weight at moderate anisotropy.

TT 45.85 Thu 15:00 Poster B

Interplay of structural and electronic properties in itinerant $A\mathbf{Fe}_4X_2$ systems — •Til Goltz[1], Nandang Mufti[2], Christoph Geibel[2], Theo Woike[3], Hubertus Luetkens[4], Johannes Spehling[1], and Hans-Henning Klauss[1] — [1]Institute of Solid State Physics, TU Dresden, Germany — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Institute of Structural Physics, TU Dresden, Germany — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland

The $A\mathrm{Fe}_4X_2$ (A=Y, Lu, Zr; X=Ge, Si) family of transition metal tetrels has shown to be a promising candidate for studying the change of the electronic ground state under chemical substitution [1]. Within the $ZrFe_4Si_2$-type structure ($P4_2/mnm$), the iron atoms are arranged in chains of edge-linked tetrahedra [2]. Their structure is prone for reduced dimensionality or frustration and is thus expected to lead to emergent phenomena near a quantum critical point. Since neutron scattering data on YFe_4Ge_2 show a simultaneous structural and magnetic transition [3], electronic and structural properties seem intimately connected within the whole $A\mathrm{Fe}_4X_2$ family. On the poster, we discuss the electronic and structural properties, extracted from our μSR, Mössbauer, X-Ray and thermodynamic data in the context of a structural driven magnetic phase transition.

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TT 45.86 Thu 15:00 Poster B

Strong evidence against orbital fluctuations in $R\mathbf{VO}_3$ — •Julia Reul[1], Agung Nugroho[2], Thomas Palstra[2], and Markus Grüninger[1] — [1]Universität zu Köln — [2]Rijksuniversiteit Groningen

Spin and orbital degrees of freedom play a decisive role for the low-energy physics of strongly correlated transition-metal oxides. Whereas the spin is a true low-energy degree of freedom with propagating low-energy excitations, it is still questionable if the same holds true for the orbital degree of freedom. In a typical situation the orbitals are strongly coupled to the lattice, which makes it sufficient to consider classical orbitals with rigid orbital order. However, different groups have pointed out that orbital fluctuations may be strong in the $3d^2$ Mott-Hubbard insulators $R\mathrm{VO}_3$ (R =rare earth ion or Y).

Optical spectroscopy offers an efficient method to study the nature of the orbital degree of freedom, because the spectral weight of excitations across the Mott-Hubbard gap depends sensitively on nearest-neighbor spin-spin and orbital-orbital correlations. We study the temperature dependence of the optical spectral weight by means of ellipsometry in the frequency range 0.75 - 5.5 eV. A comparison of our experimental results for R = Y, Gd and Ce with a theory based on a low-energy spin

orbital superexchange Hamiltonian [1,2] leads us as to the conclusion of rigid orbital order in $R\mathrm{VO}_3$.
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TT 45.87 Thu 15:00 Poster B

Skyrmions in two and three dimensional Dzyaloshinskii-Moriya magnets — •Stefan Buhrandt and Lars Fritz — Universität zu Köln, Institut für theoretische Physik, Zülpicher Strasse 77, 50937 Köln

Using classical Monte Carlo we study the phase diagram of ferromagnetic O(3) spin models with Dzyaloshinskii-Moriya interaction and spin anisotropies in applied magnetic fields. We determine the phase diagram for the two dimensional problem by simulated annealing upon investigation of the spin structure factor. We also study the evolution of the phase diagram upon becoming increasingly three dimensional. We especially focus on the evolution of the skyrmion crystal phase upon increasing the dimensionality.

TT 45.88 Thu 15:00 Poster B

Magnetic structures and magnon dispersion of $\mathbf{LaSrFeO_4}$ — •N. Qureshi[1], H. Ulbrich[1], Y. Sidis[2], A. Cousson[2], and M. Braden[1] — [1]University of Cologne — [2]LLB, Saclay (France)

We have conducted an extensive study on the single-layered perovskite $LaSrFeO_4$, a transition metal oxide of the Ruddelsden-Poppers series. This system orders antiferromagnetically at T_N=380 K and undergoes two further magnetic phase transitions at 90 K and 30 K [1,2] whose nature is still unclear. Our neutron diffraction experiments shed some light on this open issue: We have observed that there is no significant difference between the three magnetic structures. Although, the presence of four magnetic domains renders it impossible to determine the Fe moment direction within the basal plane using unpolarized neutrons. Hence, we conclude that the transitions must be connected to a spin reorientation within the basal plane. Additionally, we have investigated the magnon dispersion along two main symmetry directions. We find that the dispersions are well described by a Heisenberg antiferromagnet Hamiltonian including isotropic nearest and next-nearest neighbour interaction as well as an effective magnetic anisotropy field. The resulting values fit well into the series of the isostructural homologues. In $LaSrFeO_4$ the Fe ions nominally present a three-valent $3d^5$ state yielding S=2.5 and L=0. However, the results of our neutron study give rise to the assumption of a non-quenched orbital moment.
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TT 45.89 Thu 15:00 Poster B

Mott-Hubbard excitations in hole doped $R\mathbf{TiO_3}$ (R = rare earth ion or Y) studied via spectroscopic ellipsometry — •Ignacio Vergara, Julia Reul, Alexander Gössling, Alexander Komarek, and Markus Grüninger — Universität zu Köln

Hole doping of the $3d^1$ Mott-Hubbard insulators $R\mathrm{TiO}_3$ (R = rare earth ion or Y) leads to an interesting phase diagram including spin, charge and orbital order. Temperature dependent (20 K<T<500 K) spectroscopic ellipsometry (0.75 - 5.5 eV) offers a very sensitive method to study these phenomena as the Mott-Hubbard excitations from the lower to the upper Hubbard-Band $|d^n\rangle\,|d^n\rangle \rightarrow |d^{n+1}\rangle\,|d^{n-1}\rangle$ are sensitively dependent on nearest-neighbor spin-spin and orbital-orbital correlations.

The optical spectra of the undoped $3d^1$ compounds $R\mathrm{TiO}_3$ show a complex multipeak structure which has been attributed to the Mott-Hubbard excitations into the different $3d^2$ multiplets, while the temperature dependence has been analyzed on the basis of nearest-neighbor spin-spin correlations [1]. We now study the impact of hole doping on the optical spectra. In a perfect charge ordered scenario of a half doped compound, the hopping of an electron to the neighboring lattice site should not result in a double occupancy. Thus, instead of the Hubbard energy U the excitation should only cost the nearest-neighbor repulsion V.
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TT 45.90 Thu 15:00 Poster B

High-precision magnetisation measurements in pulsed fields — •Lars Postulka, Lukas Hinz, Bernd Wolf, and Michael Lang — Physikalisches Institut Goethe-Universität, SFB/TR 49; Frankfurt

To determine the magnetic behaviour of materials at magnetic fields as high as 50 T, pulsed fields are required. This implies the handling of huge changes of magnetic flux during the magnetic field pulse. For ac-susceptibility measurements, the typical realisation of the experimental setup is done with a pair of compensated coils. In one of these coils a sample is positioned which leads to a change of the inductance and therefore to an induced voltage. However, the large changes of magnetic flux produce a non-negligible background signal if these coils are not identical. Therefore, a modification of the typical sample holder has been constructed which enables reference measurement without a sample to be performed in a convenient way. In addition, we have added an electronic circuit to the experimental setup with which we can adjust the signal of the empty sample holder to zero voltage. The calibration and testing has been done at different temperatures by using a well-characterized material, the paramagnet $CuSO_4 \cdot 5H_2O$.

TT 45.91 Thu 15:00 Poster B

Ground-state energy and beyond: High-accuracy results for the Hubbard model on the Bethe lattice in the strong-coupling limit — •Martin Paech[1,2], Eva Kalinowski[2], Walter Apel[3,1], Gunther Gruber[4], Rita Loogen[4], and Eric Jeckelmann[1] — [1]Leibniz Universität, Hannover, Germany — [2]Academy of Computer Science and Management, Bielsko-Biała, Poland — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Philipps-Universität, Marburg, Germany

We present critical parameters for the Mott-Hubbard transition on the half-filled Bethe lattice with infinite coordination number with unprecedented accuracy of order 15 in $1/U$. This became possible by an essentially improved C implementation of our parallelized diagrammatic-combinatorial computer algorithm for the strong-coupling expansion [1].

Furthermore, we give insight into an on-going graph-theoretical analysis, which is related to an implementation of the algorithm kernel in the functional programming language Haskell [2]. This analysis is a technical prerequisite e. g. for the calculation of the band gap, for precise information about the density of states, or for investigations in finite dimensions and of systems away from half filling.
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TT 45.92 Thu 15:00 Poster B

Strong dynamic correlations and Korringa Ratio of $\mathbf{Na_xCoO_2}$ — •Lewin Boehnke and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The Korringa Ratio forms a valuable link between experimental and theoretical investigations of strongly correlated materials systems as it links the Knight shift and nuclear relaxiation time to dynamical spin properties of the conduction electrons of an itinerant magnet system.

While it has been studied phenomenologically [1] or for weakly interacting systems [2], rigorous calculations for strongly correlated systems are hindered by the need for accurate dynamical lattice susceptibilities which used to be numerically prohibitive in memory usage and runtime.

We employ the recently introduced Orthogonal Polynomial basis for one- and two-Particle Green's functions [3] to obtain reliable dynamic lattice correlation functions within the Dynamical Mean Field Theory [4] for the layered triangular system Na_xCoO_2. This system exhibits a vast variety of charge- and spin-instability tendencies, which is very well confirmed by our calculations. Most of these can not be reproduced without explicitly including vertex contributions.
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TT 45.93 Thu 15:00 Poster B

Perspectives of LDA+Slave-boson mean-field theory for realistic low-energy physics — •Christoph Piefke, Malte Behrmann, Sergej Schuwalow, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) is used to investigate large parameter spaces of arbitrary strongly interacting

systems [1,2,3] based on realistic LDA calculations [4,5]. The multiorbital Hubbard-Hamiltonian is mapped onto an itinerant quasiparticle part and localized bosonic degrees of freedom. This decouples complex interactions, quartic in the original electron-operators, at the cost of a set of constraints. At saddle-point, a self-consistent mean-field solution is obtained. Practical computations using RISB are limited by the fact that the degrees of freedom of the modelation grow exponentially with the number of correlated orbitals. To circumvent this limitation, one reduces the number of variational parameters using symmetries. We demonstrate some of the recently implemented techniques and improvements in the context of itinerant systems with magnetic degrees of freedom and/or geometric frustration.

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TT 45.94 Thu 15:00 Poster B

Bosonization approach to singular low-energy contributions in the thermodynamics of Fermi liquids — •Hendrik Meier[1], Catherine Pépin[2,3], and Konstantin Efetov[1,3] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Institut de Physique Théorique, CEA-Saclay, France — [3]International Institute of Physics, Universidade Federal do Rio Grande do Norte, Brazil

Applying a recently suggested method of bosonization in an arbitrary dimension [2] to the two-dimensional Fermi liquid, we derive an effective supersymmetric field theory for the low-energy spin and charge excitations emerging in the vicinity of the non-flat Fermi surface. Using this field theory to study the anomalous contribution δc to the specific heat in the limit $T \to 0$, we find the leading logarithmic corrections to $\delta c/T^2$ by means of a one-loop renormalization group analysis. The final result is represented as the sum of two separate terms that can be interpreted as coming from singlet and triplet superconducting excitations.

Last, it is discussed how the bosonization method may become a useful analytical tool to study different problems in the field of strongly correlated systems.

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TT 45.95 Thu 15:00 Poster B

Two-stage thermalization of weakly interacting quantum systems — •Michael Stark and Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

An isolated quantum many-body system, which is suddenly forced out of equilibrium, is said to thermalize if it relaxes to a new equilibrium state and if this is the thermal state predicted by statistical mechanics. Weakly interacting systems are usually first trapped in a prethermalized state and can thermalize only at a later stage [1]. The prethermalization stage can be described by a generalized Gibbs ensemble built from approximate constants of motion in the vicinity of the noninteracting point [2]. In a subsequent stage the crossover from the prethermalized to the thermal state occurs. This two-stage scenario provides an understanding of thermalization from a pure initial state to a final thermal ensemble state for not too large interaction.

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TT 45.96 Thu 15:00 Poster B

Merging *GW* and dyanmical mean-field theory — •Ciro Taranto[1], Alessandro Toschi[1], Merzuk Kaltak[2], Martijn Marsman[2], Georg Kresse[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Computational Materials Physics, University of Vienna, Sensengasse 8/12 A-1090 Vienna, Austria

The combined approach of local density approximation (LDA) and dynamical mean-field theory (DMFT) is the tool of choice for the study of strongly correlated materials. Nevertheless the predictive power of this approach is hampered by two principal difficulties: the extimate of the screened Coulomb interaction and the so called double-counting correction. Both of these problems are rooted in the conceptual difficulty of formulating the DMFT and the LDA in a common (diagrammatic) context. For this reasons we believe that the *GW*+DMFT [1] approach, which can be formulated also diagramatically [2], can represent a major improvement to the LDA+DMFT one. Specifically we show how one can interface the *GW* approach with the DMFT in a possibly self-consistent cycle. We also present our preliminary *GW*+DMFT results on the test-material $SrVO_3$.

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TT 45.97 Thu 15:00 Poster B

Symmetry properties of the U-matrix — •Hermann Ulm and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich

We present a simple method of calculating Gaunt coefficients in the basis of spherical harmonics. Considering these coefficients as a 3-dimensional tensor gives us flexibility in choosing basis. We tabulate the Gaunt coefficients in spherical, semi cubic, cubic bases for *d*- and *f*-electrons. Moreover, it allows us to study the symmetry properties of the full $\hat{U}$-matrix easily. We finally present an elegant way of calculating relations between U and J parameters and Slater integrals and give a proof of their invariance.

TT 45.98 Thu 15:00 Poster B

Response functions of correlated materials — •Amin Kiani Sheikhabadi[1] and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation (IAS), Forschungszentrum Jülich, Jülich, Germany — [2]Peter Grünberg Institut (PGI), Forschungszentrum Jülich, Jülich, Germany

Two-particle correlation functions provide a bridge between experimentals and theory. For strongly correlated systems, response functions can be determined with the LDA+DMFT method. In this approach the response functions are extracted from the local two-particle vertex and the local Green's functions. Here we use such method and a Hirsch-Fye QMC impurity solver to calculate the response functions of correlated transition-metal oxides. As representative case, we present results for $KCuF_3$.

TT 45.99 Thu 15:00 Poster B

Reduced Density Matrix Functional Theory- A suitable vehicle to import explicit correlations — •Ebad Kamil — Institute for Theoretical Physics, University of Goettingen, Goettingen, 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 impurity problem is solved using techniques of open quantum system.

TT 45.100 Thu 15:00 Poster B

Vortex arrays in two-species Bose–Einstein condensates with interspecies attraction — •Pekko Kuopanportti[1], Jukka A. M. Huhtamäki[1], and Mikko Möttönen[1,2] — [1]Department of Applied Physics/COMP, Aalto University, P.O. Box 14100, FI-00076 AALTO, Finland — [2]Low Temperature Laboratory, Aalto University, P.O. Box 13500, FI-00076 AALTO, Finland

One of the defining properties of superfluids is that they respond to rotation by forming quantized vortices. A convenient environment to controllably study vortices is dilute Bose–Einstein condensates (BECs) of alkali-metal atoms. To date, numerous experiments have shown that when a BEC is set into quick rotation, a triangular vortex lattice is typically formed. The density of vortices in the lattice, n_v, is governed by the Feynman relation $n_\mathrm{v} = m\Omega/(\pi\hbar)$, where m is the mass of the constituent boson and Ω is the rotation frequency.

In this theoretical work, we investigate vortex lattices in a rotating two-component BEC where the components have unequal atomic masses and interact attractively with each other. Because the atomic masses are unequal, the Feynman relation implies that the vortex densities in the two components should also differ from one another. On the other hand, the intercomponent attraction results in an effective attraction between vortices in different components. We show that to-

gether these two effects lead to exotic ground-state vortex structures such as square vortex lattices and arrays of two-quantum vortices. The obtained states invariably obey the Feynman relation, and they should be experimentally realizable with the current state of the art.

TT 45.101 Thu 15:00 Poster B

Quantum dynamics of few ultra-cold atoms in a periodically shaken double-well superlattice — •Martin Esmann[1,4], Niklas Teichmann[1], Jon Pritchard[3], and Christoph Weiss[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität, 26111 Oldenburg, Germany — [2]Department of Physics, Durham University, Durham, DH1 3LE, UK — [3]Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK — [4]Physics Department, Harvard University, Cambridge, MA 02138, USA

An analog of fractional photon-assisted tunneling (PAT) is investigated both numerically and analytically. The system under consideration is a periodically shaken optical superlattice of effectively decoupled double wells with few interacting ultra-cold Bosons per well. While previous results based on a perturbative approach suggest that the coherent transfer between the individual wells induced by PAT is a small effect [1], we introduced a resonance approximation [2] to show that for the right choice of parameters fractional PAT resonances yield major contributions to the transfer of particles. Our technique is particularly useful to investigate conditions for perfect transfer employing PAT resonances and first experimental results were recently obtained [3] in good agreement with our predictions [2,4].

[1] N. Teichmann et. al., Phys. Rev. A, 79:063620, 2009.
[2] M. Esmann et al., Phys. Rev. A, 83:063634, 2011.
[3] Y.-O. Chen et al., Phys. Rev. Lett., 107:210405, 2011.
[4] M. Esmann et al., Laser Phys. Lett., doi: 10.1002/lapl.201110109.

TT 45.102 Thu 15:00 Poster B

Viscosity of a two dimensional Fermi gas at strong coupling — •Carolin Küppersbusch[1], Lars Fritz[1], and Tilman Enss[2] — [1]Universität zu Köln, Institut für theoretische Physik, Zülpicher Strasse 77, 50937 Köln — [2]Physik Department, Technische Universität München, 85747 Garching, Germany

We consider a two dimensional Fermi gas which is experimentally realized in balanced and imbalanced fermionic ultra cold atom systems. An experimentally accessible quantity that has received a lot of interest recently as a measure of the interaction strength is the shear viscosity. This quantity describes the resistance of the system towards establishing a flow gradient. Using a Boltzmann equation we calculate the viscosity in all temperature and interaction ranges from a full numerical solution. In the high temperature limit we compare our results with the analytic solution of the non-degenerate Fermi gas.

TT 45.103 Thu 15:00 Poster B

Search for Floquet states in many-body quantum systems — •Armin Seibert, Sergey Denisov, and Peter Hänggi — Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg

Even under equilibrium conditions, a typical many-body system is hard to handle due to the exponential growth of the number of system states with the number of particles – spins, cold atoms, qubits, etc –it contains. Recent advances on the front of computational many-body quantum physics, marked by the development of the density matrix renormalization group (DMRG) methods, allowed to get insight into the Hilbert space of 'big' time-independent systems. In order to study the same, but now driven, systems, one must use more sophisticated methods, which should combine existing know-how with specific algorithms developed for periodically driven quantum systems. We present a brief overview of our recent attempts to advance in the corresponding direction, which attempts have involved the combination of the DMRG algorithms, the Floquet theory and a newest computational facility such as a graphic-processing unit (GPU) supercomputer.

TT 45.104 Thu 15:00 Poster B

Collective Excitations of Quantum Solid Phases — •Guenther Meissner and Uwe Schmitt — Department of Physics, Saarland University, P.O.B. 151150, D-66041 Saarbruecken, Germany

For collective excitations of quantum solid phases at low temperatures as, e.g., sound propagation in solid helium or in magnetic field-induced 2D Wigner solids, Born's classical theory of lattice dynamics breaks down. This happens due to large zero-point motions of the helium atoms with low mass and the cyclotron motions of the electrons with electrical charge. These deficiencies have been removed in our general quantum many-body approach, where the collective excitations are obtained quite generally from correlation functions allowing, e.g., also to include the balance between single-particle and collective excitations [1]. In the presence of random disorder the dispersion of the modes of these collective excitations is no longer gapless in zero wave vector limit. The gap has been considered in recent microwave resonance experiments being a confirmation of a disorder-pinned 2D Wigner quantum solid phase [2]. It will be shown, that from a theoretical point of view this interpretation in terms of quasi-particles of magnetic flux quanta and fractional charge is feasible, particularly, since the resonances observed near the fractional filling factor one third are very similar to those, found near the integer filling factor one.

[1] G. Meissner, Phys. Rev. Lett. 21, 435 (1968); Physica B 184, 66 (1993).
[2] Hahn Zhu, Yong P. Chen, P. Jiang, L.W. Engel, D.C. Tsui, L.N. Pfeiffer and K.W. West, Phys. Rev. Lett. 105, 126803 (2010) and references therein.

TT 45.105 Thu 15:00 Poster B

Statistical properties of interacting Rydberg gases — •David Breyel and Andreas Komnik — Institut für theoretische Physik, Universität Heidelberg

The main goal of our work is answering the question whether it is possible to detect the formation of a crystal in a gas of interacting Rydberg atoms by purely statistical means. We model the cycles of cloud formation and subsequent Rydberg atom number measurement using exact diagonalisation technique and plot the probability to produce N Rydberg atoms in a histogram. The resulting distribution is sub-Poissonian with distinct features due to interaction effects. We extract the density correlation function, which unambiguously points towards a condensed phase formation in the Rydberg cloud.

TT 45.106 Thu 15:00 Poster B

Embedded cluster approach for strongly correlated systems out of equilibrium — Michael Knap, Anna Fulterer, Martin Nuss, Wolfgang von der Linden, and •Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We present a numerical approach to compute nonequilibrium properties of strongly-correlated quantum many-body systems. The method is based on the nonequilibrium Green's function formalism combined with a treatment of strong correlations via cluster perturbation theory and its variational extensions. Upon including appropriate virtual bath parameters the method bridges to nonequilibrium dynamical mean-field theory.

We present results for steady-state transport across different spatially extended strongly-correlated regions, such as (i) a quantum wire, and (ii) a Hubbard layer displaying d-wave superconductivity. In the latter case, we discuss the effect of the bias voltage on superconducting properties. Time transient behavior is also discussed.

TT 45.107 Thu 15:00 Poster B

Variational cluster approach for strongly correlated bosonic systems in and out of equilibrium — •Enrico Arrigoni, Benjamin Kollmitzer, Michael Knap, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

We present a variational cluster approach to treat strongly-correlated lattice bosons in the superfluid phase. To this end, we reformulate the method within a pseudoparticle formalism, whereby cluster excited states are described in terms of particle-like excitations. The approximation amounts to solving a multi-component noninteracting bosonic system by means of a multi-mode Bogoliubov transformation. A criterion for the stability of the solution is discussed.

For the two-dimensional Bose-Hubbard model the method provides excellent agreement with Quantum Monte Carlo results even in the vicinity of the tip of the Mott lobe, both on the insulating as well as in the superfluid phase.

We illustrate the application of the method to strongly-correlated bosonic systems out of equilibrium within a Keldysh Green's function formulation.

TT 45.108 Thu 15:00 Poster B

Characterization of Mott-insulating and superfluid phases in the one-dimensional Bose-Hubbard model — •S. Ejima[1], H. Fehske[1], F. Gebhard[2], K. zu Münster[2], M. Knap[3], E.

Arrigoni[3], and W. von den Linden[3] — [1]University Greifswald, Germany — [2]University Marburg, Germany — [3]TU Graz, Austria

We study the one-dimensional Bose-Hubbard model, the generic model for ultracold Bose gases, by means of various analytical and numerical techniques. Firstly, we determine the Kosterlitz-Thouless transition between the Mott insulator and the superfluid phase for the lowest two Mott lobes by analyzing the von Neumann entanglement entropy within a density matrix renormalization group (DMRG) approach. The phase boundaries are found to be in excellent agreement with those extracted from the scaling of the Luttinger liquid parameter. Secondly, we investigate the dynamical properties of the Bose-Hubberd model in both phases using analytical (strong-coupling expansion) and numerical (variational cluster approximation (VCA) and dynamical DMRG) methods. The results obtained for the single-particle photoemission spectra and the density of states agree very well in the strong-coupling regime. But even for intermediate couplings and within the superfluid phase, VCA reproduces the unbiased dynamical DMRG data surprisingly well, albeit the former one is based on a dynamical mean-field approach. Thirdly, including higher-order corrections in the strong coupling approach for the dynamical density-density correlation function, we discuss how the properties of the Mott insulator change in passing from the strong to the intermediate coupling regime.

TT 45.109 Thu 15:00 Poster B

Instability of a repulsive Bose gas near the BEC transition — •Michael Maennel[1], Klaus Morawetz[1,2], and Pavel Lipavsky[3,4] — [1]Department Physical Engineering, Münster University of Applied Science, 48565 Steinfurt, Germany — [2]International Institute of Physics, Universidade Federal do Rio grande do Norte, 59.072-970 Natal-RN, Brazil — [3]Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

We investigate a Bose gas with finite-range interaction using a scheme to eliminate self-interaction in the T-matrix approximation. In this way the corrected T-matrix becomes suitable to calculate properties below the critical temperature, without the use of anomalous functions. In the vicinity of the onset of Bose-Einstein condensation (BEC) chemical potential and pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore for sufficiently strong interaction the equation of state becomes multivalued near the BEC transition. For a Hatree-Fock or Hartree-Fock-Bogoliubov approximation such a multivalued region can be avoided by a Maxwell construction. However, for the T-matrix approximation there remains a multivalued region even after a Maxwell construction.

TT 45.110 Thu 15:00 Poster B

One-dimensional many-body quantum transport of Bose-Einstein condensates — •Julien Dujardin, Arturo Argüelles, and Peter Schlagheck — Département de Physique, Université de Liège, 4000 Liège, Belgium

We calculate the transport properties of an ultracold gas of Bose-Einstein condensed atoms that is coupled from a magnetic trap into a one-dimensional waveguide [1,2]. A central aim of such guided atom lasers [1] is to study the role of atom-atom interaction in many-body transport processes across finite scattering regions within the waveguide resembling tunnel junctions or quantum dots. Our theoretical approach to solve this problem is based on a scattering formalism for which we consider the system to consist of two semi-infinite non-interacting leads and a finite interacting scattering region. We calulate the atom density, the current, and the transmission in the steady-state regime and compare these observables to the mean-field regime where the dynamics of the Bose gas is described by a Gross-Pitaevskii equation [2].

[1] W. Guerin et al., PRL 97, 200402 (2006).
[2] T. Ernst et al., PRA 81, 013631 (2010).

TT 45.111 Thu 15:00 Poster B

Crystal Structure and Magnetic Properties of $NaCu[(Cu_3O)(PO_4)_2Cl]$ — Teng-Teng Jin[1], Wei Liu[2], Shuang Chen[3], Yurii Prots[3], Walter Schnelle[3], Jing-Tai Zhao[1], Rüdiger Kniep[3], and •Stefan Hoffmann[3] — [1]Shanghai Institute of Ceramics, Shanghai, P. R. China — [2]Ocean University of China, Qingdao, P. R. China — [3]MPI CPfS, Dresden, Germany

A new copper(II) phosphate chloride, $NaCu[(Cu_3O)(PO_4)_2Cl]$, has been synthesized and structurally characterized. Complex chains of copper-centered polyhedra give rise to a low-dimensional magnetic behavior similar to $Cu_3O(MoO_4)_2$ [1,2]. Field and temperature dependent measurements of the specific heat and the magnetic susceptibility revealed two transitions $T_{N1} = 11.3(3)$ K and $T_{N2} = 6.5(2)$ K. T_{N1} signals the long-range ordering of the Cu spins in the chains. The phase transition at T_{N2} is accompanied by the formation of a weak ferromagnetic moment typical for basically anti-ferromagnetic structures with spin canting.

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[2] S. Vilminot; G. Andre; M. Kurmoo Inorg. Chem. 2009, 48, 2687-2692.