TT 71: Correlated Electrons: Poster Session

Time: Wednesday 15:00–18:00 Location: Poster B

TT 71.1 Wed 15:00 Poster B

Surface properties of SmB_6 from x-ray photoemission spectroscopy — •Nadine Heming[1], Uwe Treske[1], Martin Knupfer[1], Bernd Büchner[1,2], Dmytro Inosov[2], Natalya Y. Shitsevalova[3], Volodymyr B. Filipov[3], Stephan Kraus[4], and Andreas Koitzsch[1] — [1]Institute for Solid State Research, IFW Dresden — [2]Institut für Festkörperphysik, TU Dresden — [3]Institute for Problems of Material Sciences, Kiev — [4]BESSY II, Berlin

The mixed valence compound SmB_6 has been well known for its anomalous low temperature resistivity behavior for decades: At temperatures below 50 K, SmB_6 transmutes from a metal to an insulator but shows residual resistivity for temperatures less than 5K. Renewed interest in this material comes from theoretical proposals, predicting topological protected surface states making this compound the prime candidate for the new material class of '"Topological Kondo Insulators'". Indeed, elaborate transport experiments have evidenced that the residual conductivity occurs only at the surface. However, it is generally well known that the surface of f-systems undergoes valence changes and reconstructions, which may also influence the surface properties of this material. Applying surface sensitive soft x-ray photoemission spectroscopy, we have investigated the surface properties of freshly cleaved SmB_6 single crystals at 15K monitoring the Sm valance, the chemical state of boron as well as the surface stoichiometry, and also the development of these over time and with increased temperature: We have found that the surface shows an unexpected complexity stemming from both intrinsic and extrinsic changes.

TT 71.2 Wed 15:00 Poster B

Hidden order symmetry and superconductivity in Heavy Fermions investigated by quasiparticle interference — •Alireza Akbari[1,2] and Peter Thalmeier[3] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Gyeongbuk 790-784, Korea — [2]MPI for Solid State Research, Stuttgart, Germany — [3]MPI for the Chemical Physics of Solids, Dresden, Germany

The hidden order (HO) in URu_2Si_2 has been determined as a high rank multipole formed by itinerant 5f-electrons with distinct orbital structure imposed by the crystalline electric field. Because this can lead to a considerable number of different multipoles it is of great importance to use microscopic techniques that are sensitive to their subtle physical differences. Here we investigate whether quasiparticle interference (QPI) method can distinguish between the two most frequently proposed HO parameter models: the even rank-4 hexadecapole and the odd-rank-5 dotriacontapole model. We obtain the quasiparticle dispersion and reconstructed Fermi surface in each HO phase adapting an effective two-orbital model of 5f bands that reproduces the main Fermi surface sheets of the para phase. We show that the resulting QPI spectrum reflects directly the effect of fourfold symmetry breaking in the rank-5 model which is absent in the rank-4 model. Therefore we suggest that QPI method should give a possibility of direct discrimination between the two most investigated models of HO in URu_2Si_2. Furthermore the signature of proposed chiral d-wave superconducting (SC) order parameter in QPI of the coexisting HO+SC phase is investigated.

TT 71.3 Wed 15:00 Poster B

Site dependence of the Kondo scale in $CePd_{1-x}Rh_x$ evidenced by thermopower — •Ulrike Stockert[1], Stefanie Hartmann[1], Micha Deppe[1], Nubia Caroca-Canales[1], Christoph Geibel[1], Julian Sereni[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Division Bajas Temperaturas, Centro Atómico Bariloche, Argentina

$CePd_{1-x}Rh_x$ undergoes a continuous evolution from ferromagnetic order in CePd to an intermediate-valence (IV) ground state for CeRh. Close to the disappearance of magnetic order at $x_{cr} \approx 0.87$ unusual behavior of the ac susceptibility and the specific heat was observed. It was explained with a broad distribution of local Kondo temperatures T_K from below 2 K to above 50 K due to the disorder introduced by Pd-Rh exchange.

The thermopower S is very sensitive to Kondo scattering even for diluted 4f systems. In Ce compounds a large positive maximum in $S(T)$ is usually observed around T_K. We studied $S(T)$ in $CePd_{1-x}Rh_x$ in order to evaluate the presence of Kondo scattering and the involved enery scales. Pure CeRh shows typical IV behavior with a large maximum at 220 K and small values at low T. Already 5 % Pd substitution leads to a strong enhancement of the low-T thermopower. Even larger values are found around x_{cr}, while the high-T maximum shifts only moderately. Our results are in line with the existence of low (local) Kondo scales in the presence of IV behavior at high Rh content $x > x_{cr}$. For lower Rh content a decreasing (average) Kondo scale is found.

TT 71.4 Wed 15:00 Poster B

Electron Spin Resonance of the itinerant ferromagnets $CeCrGe_3$ and $LaCrGe_3$ — •Jörg Sichelschmidt[1], Thomas Gruner[1], Christoph Geibel[1], Debarchan Das[2], and Zakir Hossain[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Department of Physics, Indian Institute of Technology, Kanpur 208016, India

We report Electron Spin Resonance (ESR) of the itinerant ferromagnets $CeCrGe_3$ and $LaCrGe_3$. Both compounds show well defined and very similar spectra of itinerant Cr 3d spins in the paramagnetic temperature region, adding another two examples of a rarely observed conduction electron spin resonance in 3d metals.

Upon cooling and crossing the Cr-FM ordering (below around 90 K) strong spectral structures start to dominate the resonance spectra in a quite different manner in $CeCrGe_3$ and $LaCrGe_3$. In the Ce-compound the resonance is visible in the paramagnetic region only whereas in the La-compound the resonance can be followed far below the FM ordering temperature. This behavior will be discussed in terms of the specific interplay between Ce and Cr magnetism which appears quite remarkable since $CeCrGe_3$ displays Kondo lattice behavior with a heavy fermion specific heat even in the magnetically ordered state [1].

[1] D. Das, T. Gruner, H. Pfau, U. B. Paramanik, U. Burkhardt, C. Geibel, and Z. Hossain, J. Phys. Condens. Matter 26, 106001 (2014).

TT 71.5 Wed 15:00 Poster B

de Haas-van Alphen oscillations in (La,Ce)$TiGe_3$ — •J. Grasemann[1,2], M. Uhlarz[1], W. Kittler[3], V. Fritsch[3,4], O. Stockert[5], T. Förster[1], J. Wosnitza[1,2], and H. v. Löhneysen[3] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Karlsruhe Institute of Technology, 76049 Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg — [5]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

$CeTiGe_3$ is one of the few Kondo-lattice compounds which order ferromagnetically ($T_C \approx 14$ K); $LaTiGe_3$ may be used as its nonmagnetic reference, since both compounds crystallize in the same hexagonal perovskite structure [1, 2]. We report on angular-resolved de Haas-van Alphen oscillations in single crystals of $CeTiGe_3$, $LaTiGe_3$, and $Ce_{0.1}La_{0.9}TiGe_3$ grown from Ge flux, measured in magnetic fields up to 13 T in a cantilever-type torque magnetometer. We found several dHvA frequencies, ranging in $CeTiGe_3$ from 100 to 530 T and with effective masses around $0.7\,m_0$, featuring a comparably weak angular dependence. Further, we give an interpretation of our results on the basis of DFT calculations of the electronic band structure of $CeTiGe_3$ and $LaTiGe_3$.

[1] P. Manfrinetti et al., Solid State Commun. **135** (2005) 444-448.
[2] W. Kittler et al., Phys. Rev. B **88** (2013) 165123

TT 71.6 Wed 15:00 Poster B

DFT Study on (La,Ce)$TiGe_3$ — •Tobias Förster[1], Helge Rosner[2], Jacob Grasemann[1], Marc Uhlarz[1], Wolfram Kittler[3], Veronika Fritsch[3,4], Oliver Stockert[2], Jochen Wosnitza[1], and Hilbert v. Löhneysen[3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

$CeTiGe_3$ presents the rare case of a ferromagnetically ($T_C \approx 14$ K) ordered Kondo-lattice compound and is probably the first known example of an intermetallic hexagonal perovskite of the $BaNiO_3$ structure type. $LaTiGe_3$ is the nonmagnetic analogue. To clarify the interplay

between structural, localized, and itinerant degrees of freedom an accurate knowledge of the electronic band structure is necessary. Here, we present detailed comparative electronic structure calculations for both compounds. Applying full potential density functional calculations in different approximations, we attempt to separate the influence of different parameters of the crystal structure on the topology and character of the respective Fermi surfaces. We compare our calculated results with de Haas-van Alphen measurements.

TT 71.7 Wed 15:00 Poster B

Heavy fermion behaviour in the high pressure structure of $CeSb_2$ — •Vitaly Fedoseev[1], Zhuo Feng[1], Yang Zou[1], Terence Giles[2], Philipp Niklowitz[2], Heribert Wilhelm[3], Giulio Lampronti[4], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK — [3]Beamline I15, Diamond Light Source, Didcot OX11 0DE — [4]Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK

The Kondo lattice system $CeSb_2$ crystallises in the orthorhombic $SmSb_2$ structure and exhibits a series of magnetic phase transitions at low temperature. It has been reported to become ferromagnetic below 15 K, with the ordered moment oriented within the basal plane, and to undergo two further transitions at 9K and 12K [1]. These transition are suppressed above a hydrostatic pressure $p_c \simeq 16$ kbar. We present high pressure transport and x-ray diffraction results, which examine the high pressure state of $CeSb_2$. Our findings suggest that $CeSb_2$ undergoes a drastic structural change at p_c into a new and now fully resolved crystal structure. Whereas in the low pressure structure, $CeSb_2$ is a local moment magnet, in the high pressure structure it exhibits transport properties characteristic of a heavy fermion material with a low Kondo temperature scale of the order of 10 K.

[1] Bud'ko et al. PRB **57**, 21 (1998)

TT 71.8 Wed 15:00 Poster B

Crystal field splitting in $CePt_5$: magnetic analysis and Raman spectroscopy — •Martin Zinner[1], Benedikt Halbig[2], Utz Bass[2], Christian Praetorius[1], Jean Geurts[2], and Kai Fauth[1] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg, Germany — [2]Universität Würzburg, Experimentelle Physik III, 97074 Würzburg, Germany

The crystal electric field (CF) is an essential factor determining the paramagnetic response of rare earth ions in solids. In Ce intermetallics, Kondo screening can additionally modify the magnetic behavior and it may then prove difficult to disentangle the two. In the hexagonal surface intermetallic $CePt_5$, grown on Pt(111) [1], we find two distinct sets of CF parameters which both account rather well for the anisotropic magnetic susceptibility and its temperature dependence. Different strengths of Kondo screening have to be assumed in the two cases in order to obtain quantitative agreement with experimental results.

Discriminating between the two solutions requires an independent determination of the CF splitting. We shall report on our attempts to obtain this information from electronic Raman scattering. Raman signal is indeed even obtained from $CePt_5$ specimens with a thickness of just two unit cells. We shall discuss the identification of electronic Raman losses by comparison with $LaPt_5$ as well as the dependence of the Raman features on temperature and thickness of the intermetallic film.

[1] J. Kemmer, C. Praetorius *etal.*, Phys. Rev. B **90**, 195401 (2014).

TT 71.9 Wed 15:00 Poster B

Electronic and magnetic structure of $RENi_2Mn_x$-compounds (RE = rare earth, x = 0, 0.25, 0.5, 0.75, 1, 1.25) with respect to $ErNi_2Mn_x$ — •Kamil Balinski[1], Artur Chrobak[3], T.V. Kuznetzsova[2], N.V. Mushnikov[2], V.V. Marchenkov[2], and Karsten Küpper[1] — [1]Department of Physics, Osnabrück University, Germany — [2]Institute of Metal Physics, 620990 Ekaterinburg, Russia — [3]Department of Physics, University of Silesia in Katowice, Poland

Rare earth (RE) and transition metal (T) compounds are research field since the 1960s. Because of huge magnetocalorical effect and giant magnetostriction the RE-T-compounds are excellent for applications like magnetic cooling or hydrogen storage devices. Besides of that RE-Ni_2-type of alloys are, due to the relatively simple crystal structure and the fact that Ni_2 does not indicate any magnetic moment, excellent candidates for studies of magnetic behavior of RE's and their binding partners. The electronic structure of $ErNi_2Mn_x$ (x = 0, 0.25, 0.5, 0.75, 1, 1.25) is characterized by XPS and ResPES, the magnetic structure is investigated by SQUID and PPMS techniques, and resistivity measurements are made. Variation in Mn concentration revealed the position of Mn 3d-states at 1.7 eV. The XPS intensity at 1.7 eV can be correlated with the behavior of the Curie temperature and the resistivity. While similar $RENi_2Mn_x$-systems, where RE had been replaced by Gd and Tb, highest resistivity, Curie temperature and the highest Mn 3d-valence band state intensity were observed at x = 0.5. $ErNi_2Mn_x$-system behave different and show the mentioned maxima at x = 1.25.

TT 71.10 Wed 15:00 Poster B

Multi-impurity Anderson models: geometry and entanglement — •Benjamin Mille, Tizian Müller, and Ralf Bulla — Institut für Theoretische Physik, Universität zu Köln

Block-tridiagonalisation methods allow to map multi-impurity Anderson models in arbitrary geometry and dimension onto models of M coupled chains (M = number of impurities). The resulting chain model can then be used as a starting point for renormalization group and iterative methods. Here we discuss how to combine the logarithmic discretization - an essential feature of Wilson's Numerical Renormalization Group - with the general tridiagonalisation scheme. This corresponds to the mapping of the original model onto a Wilson ladder, the generalization of the Wilson chain obtained for the single-impurity case. Furthermore we investigate - via exact diagonalization of small clusters - how the entanglement between two spatially separated Anderson impurities falls off with their distance.

TT 71.11 Wed 15:00 Poster B

Nonequilibrium dynamics of the pseudo gap single impurity Anderson model — •Julian Musshoff[1], Christian Kleine[2], and Frithjof B. Anders[2] — [1]Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, Germany — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

In the single impurity Anderson model with a pseudo-gap density of states, modeled by a power law $\rho(\epsilon) \propto |\epsilon|^r$, a local moment phase and a strong coupling phase are separated by a quantum critical point (QCP). We investigate the real-time dependence of the double occupancy of the impurity due to quenches in one phase and over the QCP using the time-dependent numerical renormalization group (TD-NRG). We show that the double occupancy equilibrates to a steady state for long times. We present a time-dependent perturbation theory which becomes exact at short times. The short-time evolution of our TD-NRG data excellently agrees with this perturbation theory providing an analytical expression of the relevant time scales for the short-time dynamics. We are able to trace back the differences between the results obtained by a time-dependent Gutzwiller variational approach and by the TD-NRG to the wave-function ansatz in the Gutzwiller approach.

TT 71.12 Wed 15:00 Poster B

Cobalt adatoms on Graphene: role of the realistic interaction matrix in a QMC simulation — •Igor Krivenko[1], Maria Valentyuk[1], Ersoy Sasioglu[2], Priyanka Seth[3], Michel Ferrero[3], Olivier Parcollet[4], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich — [3]Centre de Physique Théorique, École Polytechnique, France — [4]Institut de Physique Théorique, CEA-Saclay, France

We have theoretically studied the local spectra and magnetic properties of the cobalt impurities on the graphene at the low temperatures. In our studies we have employed the DFT++ method in the projector augmented wave (PAW) basis set using the VASP code, and a new hybridization expansion CT-QMC solver from the TRIQS project (Toolbox for Research on Interacting Quantum Systems). We have been interested in the observation of the spin and orbital Kondo effect in the different adatom geometries (hollow-position/top-position). Another question of the interest has been to study the effect of different approximations for the local interaction matrix on the impurity spectrum. In order to reproduce the multiplet structure of the cobalt d-shell, one has to consider interactions beyond a simple density-density approximation. With our new hybridization expansion solver we have been able to treat a U-matrix, parametrized by 3 Slater integrals (129 non-vanishing matrix elements) and a realistic U-matrix, obtained by

means of the Constrained RPA method (157 elements).

TT 71.13 Wed 15:00 Poster B

Multi-spin multi-channel Kondo box problem — •Mirek Hänsel, Andrej Schwabe, and Michael Potthoff — Institut für Theoretische Physik, Universität Hamburg

In a quantum box, where one or several quantum spins are coupled by a weak antiferromagnetic local exchange J to a system of non-interacting conduction electrons, the standard Kondo effect is cut by the finite system size. The residual finite-size Kondo effect can be described by perturbation theory in J. We show that the effective low-energy physics is given by a central-spin model where typically each impurity spin couples to the spin of a completely delocalized conduction-electron eigenstate at the Fermi edge. Different screening channels are given for the case of orthogonal eigenstates. We discuss the general case of several spins and several channels by analyzing various geometries, e.g., one-dimensional chains and two-dimensional lattices with different boundary conditions, and different geometrical setups of the impurity spins. The couplings in the effective central-spin model and the resulting magnetic structure are calculated as functions of the conduction-electron density and the geometry.

TT 71.14 Wed 15:00 Poster B

Towards a Matrix Product State based description of steady-state non-equilibrium physics in 1D correlated quantum systems using Lindblad driving — •Frauke Schwarz[1], Ireneusz Weymann[2], Jan von Delft[1], and Andreas Weichselbaum[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany — [2]Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

The Kondo effect in quantum impurity models in equilibrium is well-understood by means of the Numerical Renormalization Group (NRG). To extend the description of Kondo physics to situations of steady state non-equilibrium, we want to combine the ideas of NRG with the Lindblad approach to open quantum systems. For this purpose, we introduce additional reservoirs described by Lindblad terms in the Liouville equation which restore the continuum properties of the discretized leads that are coupled to the impurity. This enables us to define the temperature and the chemical potential for each lead independently. To reduce the dimensionality of the problem we employ the stochastic quantum trajectory approach to solve the underlying Lindblad equation.

Several ideas on how to define adequate Lindblad operators will be presented together with their implications for the calculation of the quantum trajectories based on Matrix Product States.

TT 71.15 Wed 15:00 Poster B

Temperature dependent properties in the infinite-dimensional Hubbard model with a magnetic field — •Markus Dutschke[1], Liviu Chioncel[1,2], and Junya Otsuki[3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Department of Physics, Tohoku University, Sendai 980-8578, Japan

We investigate the temperature and field dependence of the spectral function, the effective mass enhancement and the magnetisation of the infinite-dimensional Hubbard model in a magnetic field. We compare results for different interaction strengths at half-filling, near half-filling and quarter-filling. These are achieved by using dynamical mean-field theory (DMFT) with a continuous-time quantum monte carlo (CT-QMC) impurity solver and are compared with some NRG results.

TT 71.16 Wed 15:00 Poster B

Influence of strong disorder on incoherent transport near the Mott transition: Statistical DMFT approach — •Milos Radonjic[1,2], Darko Tanaskovic[2], and Vladimir Dobrosavljevic[3] — [1]Center for Electronic Correlations and Magnetism, Theoretical Physics III, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA

We present the study of disordered half-filled Hubbard model within the Statistical dynamical mean field theory, which is a unique theoretical method reliable and controllable in a wide temperature, disorder and interaction range. We have successfully applied this method, for the first time, on the finite size cubic lattice, at finite temperature.

The results show that the finite size effects are negligible already on the lattice with 6*6*6 sites (except at the lowest temperatures, deep in the Fermi liquid regime). Also we confirmed that disorder is strongly screened on the metallic side of the Mott MIT and that inelastic scattering is dominant outside of the Fermi liquid region. We defined a local resistivity and proposed a resistor network method for calculating lattice dc resistivity. Two types of sites can be identified: strongly correlated - with the local occupation close to 1, and weakly correlated - away from local half-filling. Strongly correlated sites are responsible for strong, non-monotonic temperature dependence of the resistivity.

TT 71.17 Wed 15:00 Poster B

Electronic correlations and spin-orbit coupling in d^4 osmates — •Vladislav Pokorný[1] and Jan Kuneš[2] — [1]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

We employ the combination of the density functional theory and the dynamical mean-field theory to investigate the electronic correlations in heavy transition metal compounds with partially filled t_{2g} levels such as d^4 osmates which were prepared recently. Using the hybridization-expansion, continuous-time quantum Monte Carlo impurity solver we study the combined influence of electron correlations and spin-orbit coupling effects on the the electronic and magnetic structure of these systems.

TT 71.18 Wed 15:00 Poster B

NMR on the quantum critical ferromagnet $YbNi_4P_2$: Evidence for a large basal plane local anisotropy — •Rajib Sarkar[1], Marco Günter[1], Cornelius Krellner[3], Michael Baenitz[2], Christoph Geibel[2], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]MPI-CPFS, D-01187 Dresden, Germany — [3]Goethe University Frankfurt, D-60438 Frankfurt am Main, Germany

In the last 10 years there was growing evidence both from theoretical work and experimental observations that a ferromagnetic (FM) quantum critical point (QCP) cannot exist in a pure system, because the transition becomes first order before reaching the QCP. Therefore the recent report of clear evidence for a FM-QCP in the heavy fermion compound $YbNi_4P_2$ attracted considerable attention. While the Bravais lattice of this compound is tetragonal, resulting in isotropic in-plane macroscopic magnetic properties, the local symmetry on the Yb site (and on the P-site) is lower, orthorhombic. Therefore some in-plane anisotropy of local magnetic properties is expected, which could however not yet been studied because of the absence of related effects on macroscopic properties. We performed ^{31}P NMR investigations on a grain aligned polycrystalline sample of $YbNi_4P_2$. We observed three structures in the NMR spectra, which present quite different T-dependence of the respective Knight shifts. An analysis of these results provides a clear evidence for strong local in-plane anisotropy of the Yb-moment due to the orthorhombic crystal electric field. Implication for the magnetic ordered state shall be discussed.

TT 71.19 Wed 15:00 Poster B

Single crystal growth of the heavy fermion compounds $YbRh_2Si_2$ and $YbNi_4P_2$ — •Constantin Butzke, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

Heavy fermion systems are model systems to unravel the exciting physics around quantum-phase transitions. Studying these emergent phenomena necessitates the preparation of large and high-quality single crystals. We report on the optimization of the single crystal growth for two Yb-based quantum critical materials, $YbRh_2Si_2$ and $YbNi_4P_2$. The prototype heavy-fermion system $YbRh_2Si_2$ is situated extremely close to an unconventional antiferromagnetic (AF) quantum critical point (QCP). The AF ordering (T_N = 70 mK) can be further lowered by chemically induced negative pressure using Ir-substitution. The QCP is reached for an Ir-substitution of x ≈ 0.1 in $Yb(Rh_{1-x}Ir_x)_2Si_2$ [1]. Here, we report on the optimization of the crystal growth of the substitution series as well as of the unsubstituted compound. We also report on our attempts to determine the melting point of $YbRh_2Si_2$ and present a phase analysis of the molten compound. In the heavy fermion metal, $YbNi_4P_2$, a ferromagnetic (FM) transition

at $T_C = 0.17$ K was observed recently and a FM QCP is reached at $x \approx 0.1$ in $YbNi_4(P_{1-x}As_x)_2$. We report on the crystal growth of $YbNi_4P_2$ by Czochralski method out of a Ni-P flux from a levitated melt. The obtained crystals were characterized by Laue X-ray scattering, X-ray powder diffraction, EDX microprobe analysis and resistivity measurements.

[1] S. Friedemann *et al.*, Nature Phys. **5**, 465 (2009).

TT 71.20 Wed 15:00 Poster B

Magnetic resonance in transverse-field Ising magnet LiHoF4 through quantum and thermal phase transitions — •Ivan Kovacevic, Peter Babkevich, Mingee Chung, Giovanni Boero, and Henrik Ronnow — Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland

Coplanar resonators and vector network analyzer (VNA) were used to measure the susceptiblity in wide frequency range up to 6 GHz. The investigated temperatures from 0.2 K to 4.2 K and field range from 0 to 9 T cover the thermal transition into a ferromagnetically ordered phase below 1.53 K in zero-field as well as the quantum phase transition into a quantum-disordered paramagnetic phase above critical field 4.95 T at zero temperature. Entangled electro-nuclear states in LiHoF4 were probed by excitation field matching the hyperfine transitions at resonant frequencies. Absorption line was obtained by sweeping the transverse field at different frequencies. The model calculations within the mean-field approximation enable to track the evolution of the hyperfine levels as a function of field and temperature through quantum and thermal transitions, and show indeed excellent agreement with the experimental results. The presented methodology may find immediate applications to other important rare-earth containing materials such as spin ice, particularly close to the quantum phase transitions.

TT 71.21 Wed 15:00 Poster B

Thermodynamics of the Ising chain compound $CoNb_2O_6$ in transverse magnetic field — •Daniel Brüning[1], Simon Scharffe[1], Victoria Cho[1], Martin Valldor[1,2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

$CoNb_2O_6$ is a model system to investigate a quantum phase transition in magnetic fields. The structure consists of layers of CoO_6 octhahedrons separated by non-magnetic NbO_6 layers. The edge-sharing oxygen octahedrons link the Co^{2+}spins through Co-O-Co superexchange and form 1D ferromagnetic zigzag chains along the orthorhombic c axis. Crystal field effects lead to an easy-axis anisotropy of the Co^{2+} moments in the ac plane and to an effective spin-1/2 chain system described by the Ising model. A purely 1D Ising chain develops long-range order at zero temperature only and a transverse field induces a quantum phase transition into a quantum disordered state. Due to small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$, $CoNb_2O_6$ shows 3D long-range antiferromagnetic order below T_N=2.95 K. Because a magnetic field parallel to the b axis is normal to the easy-axis of the spin chain it is possible to study the complex interplay of 3D ordering and 1D quantum phase transitions. We present specific heat and magnetization measurements from about 0.3 to 10 K and discuss the phase diagram. The theoretical model of the Ising chain in transverse magnetic field is completely solvable and we compare our measurements to the corresponding calculations.

TT 71.22 Wed 15:00 Poster B

Ferromagnetic quantum critical point in $CeTi_{1-x}V_xGe_3$ — •Wolfram Kittler[1], Christian Taubenheim[1], Veronika Fritsch[1,2], Paul C. Canfield[3], and Hilbert v. Löhneysen[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, Germany — [2]Universität Augsburg, Institut für Physik, Experimentalphysik VI, Germany — [3]Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

$CeTiGe_3$ is a moderate heavy-fermion system, crystallizing in a hexagonal perovskite structure. It orders ferromagnetically at $T_C = 14.3$ K. Experiments on polycrystals have shown that the substitution of Ti with V suppresses the magnetic order, suggesting the existence of a ferromagnetic quantum critical point [1]. We have successfully grown single crystals of $CeTi_{1-x}V_xGe_3$. The strong uniaxial anisotropy with the easy axis along the c-axis is reduced with increasing x and turns into an easy ab-plane anisotropy for $x = 1$. The magnetic ordering temperature is indeed shifted to $T_C \to 0$ at a V concentration $x_c \approx 0.4$. We present data of magnetization, electrical resistivity and specific heat down to $T = 100$ mK of $CeTi_{1-x}V_xGe_3$. These data support the existence of a ferromagnetic quantum critical point.

[1] W. Kittler *et al.*, Phys. Rev. B **88**, 165123 (2013).

TT 71.23 Wed 15:00 Poster B

High-pressure transport properties of CrB_2 — •Alexander Regnat[1], Julian Becker[1], Jan Spallek[1], Andreas Bauer[1], Alfonso Chacon[1], Robert Ritz[1], Christian Blum[2], Sabine Wurmehl[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Leibniz Institute for Solid State and Materials Research IFW, D-01171 Dresden, Germany

High quality single crystals of the itinerant antiferromagnet CrB_2, $T_N = 88$ K, were grown by means of optical float zoning. Bulk, transport and de Haas-van Alphen measurements were carried out [1,2]. Here, we present a comprehensive study of the high-pressure transport properties. Samples were investigated under hydrostatic, uniaxial and quasi-hydrostatic conditions. As a result we are able to attribute contradictory reports for the pressure dependence of T_N to uniaxial strain [3, 4]. Perhaps most interestingly, we find a pronounced low temperature resistivity anomaly around 3 GPa in the quasi-hydrostatic case.

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[2] Brasse et al., PRB 88, 155138 (2013).
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[4] Grechnev et al., J. Low Temp. Phys. 35, 531 (2009).

TT 71.24 Wed 15:00 Poster B

Impact of Local Magnetic Moments on the Anderson Metal-Insulator Transition — •Daniel Jung[1], Keith Slevin[2], and Stefan Kettemann[1] — [1]School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany — [2]Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

We study the effects of classical magnetic impurities on the Anderson metal-insulator transition numerically. In particular we find that while a finite concentration of Ising impurities lowers the critical value of the site-diagonal disorder amplitude W_c, in the presence of Heisenberg impurities, W_c is first enhanced with increasing exchange coupling strength J due to time-reversal symmetry breaking. The resulting scaling with J is analyzed and compared to analytical predictions by Wegner [1]. The results are obtained numerically, based on a finite-size scaling procedure for the typical density of states, which is the geometric average of the local density of states. The latter can efficiently be calculated using the kernel polynomial method (KPM). We extend previous approaches by combining the KPM with a finite-size scaling analysis. We also discuss the relevance of our findings for systems like phosphor-doped silicon, which are known to exhibit a quantum phase transition from metal to insulator driven by the interplay of both interaction and disorder, accompanied by the presence of a finite concentration of magnetic moments.

[1] F. Wegner, Nucl. Phys. B 280, 210 (1987).

TT 71.25 Wed 15:00 Poster B

Suppression of critical fluctuations of electronic Ising-nematicity by coupling to the crystal lattice — •Christopher Max[1], Achim Rosch[1], Indranil Paul[2], and Markus Garst[1] — [1]Institute for theoretical Physics, Universitiy of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot-Paris 7 & CNRS, UMR 7162, 75205 Paris, France

Nematic instabilities of the electronic Fermi surface are relevant for various strongly-correlated systems like the ruthenates or the Fe-based superconductors. At the same time, they serve as a theoretical paradigm for quantum phase transitions in metals whose properties at lowest temperature still remain unclear and are the topic of current research. In the present work, we point out that the Ising-nematic order parameter strongly hybridizes with the strain field of the crystal, and, as a consequence, the nematic transition is naturally accompanied with a tetragonal-orthorhombic distortion. Due to the long-range shear forces of the crystal, the quantum critical properties will be eventually governed by quantum critical elasticity [1]. Upon approaching the quantum critical point, a crossover occurs from critical non-Fermi liquid behavior to conventional metallicity while the phonon sectors becomes soft resulting in an anomalous phonon specific heat $C_{\rm ph} \sim T^{2.5}$ at lowest temperature. We discuss the various crossovers for thermodynamics as well as for the electronic spectral function.

[1] M. Zacharias, I. Paul and M. Garst, arXiv:1411.6925

TT 71.26 Wed 15:00 Poster B

Magnetic field and impurity studies in Kitaev and Kitaev Heisenberg models — •Sitikantha Das[1], Zhu Zengwei[2], Ross McDonald[2], Suchitra Sebastian[1], and Vikram Tripathi[3] — [1]Cavendish Labs, Cambridge — [2]National High Magnetic Field Laboratory, Los Alamos — [3]Tata Institute of Fundamental Research, Mumbai

In an effort to find an experimental realisation of Kitaev physics in solid state systems, the layered alkali iridates A_2IrO_3 (A = Li, Na), seem to be promising material candidates. Although the spin-1/2 Kitaev model has a quantum spin-liquid ground state with short ranged spin correlations and low-energy emergent excitations that are dispersing Majorana fermions, it has now been established that Na_2IrO_3 orders into a zig-zag state below 15 K. We have performed pulsed magnetic field torque experiments on Na_2IrO_3 at various field orientations and we observe strong angular dependence. Using negative Kitaev-Heisenberg as a model, we attempt to study the magnetisation and torque using exact diagonalization with a view to understand the experimental data.

We also study the effect of coupling an external magnetic impurity to a Kitaev model numerically. Antiferromagnetic coupling of the impurity spin results in the creation of finite flux excitations, which is now known from analytical calculations. This is verified numerically and we also study the effect of tuning the coupling strength from antiferromagnetic to ferromagnetic interaction.

TT 71.27 Wed 15:00 Poster B

The phase diagram of the XXZ model on the anisotropic triangular lattice — •Shijie Hu[1], Jize Zhao[2,3], Xuefeng Zhang[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Applied Physics and Computational Mathematics, Beijing 100088, China — [3]Beijing Computational Science Research Center, Beijing 100084, China

We use the density-matrix renormalization group (DMRG) in two dimensions to systematically study the full phase diagram of a general antiferromagnetic XXZ model on the anisotropic triangular lattice (called J_z-J_x-J'_z-J'_x model). In the strong-coupling limit of large J_z/J_x, we find a broad incommensurate supersolid phase in between the 1/2 filled Néel phase and 1D-decoupled-chain phase as a function of anisotropy. The incommensurate vector of this coplanar phase is related to the quantized density of domain walls along the vertical axis. In the other limit of large J_x/J_z, we find an incommensurate superfluid phase (cone phase). The transition region from supersolid phase to superfluid phase for intermediate coupling strength J_z/J_x, shows a rich physical behavior and provides a hint about the existence of a gapped 'spin-liquid' phase proposed by P. W. Anderson several decades ago.

TT 71.28 Wed 15:00 Poster B

Quantum Monte Carlo calculations for frustrated spin systems — Andreas Honecker[2], •Rene John Kerkdyk[1], Thomas Pruschke[1], and Stefan Wessel[3] — [1]Georg-August-Univesität Göttingen — [2]Université de Cergy-Pontoise, Laboratoire de Physique Théorique et Modélisation — [3]RWTH Aachen

Using Quantum Monte Carlo methods to examine the behavior of frustrated spin systems at low temperatures is usually problematic due to the sign problem. Our research focuses on a cluster approach to a model-specific elimination or reduction of the sign problem. We have implemented this approach in a worm algorithm for a one-dimensional spin-1/2 Heisenberg ladder and show that it permits access to the thermodynamic behaviour over the entire temperature range.

TT 71.29 Wed 15:00 Poster B

Optical absorption of the spin-1/2 Heisenberg antiferromagnet on a triangular lattice — •Boris Celan and Wolfram Brenig — Institute for Theoretical Physics, Technische Universität Braunschweig

We investigate the optical absorption of the spin-1/2 antiferromagnetic Heisenberg model on the two-dimensional anisotropic triangular lattice.

Vertex functions for the absorption of light are derived within a model of phonon-assisted multimagnon excitations and their momentum dependence is analyzed. For the magnetic excitations we use linear spin-wave theory. For the optical conductivity we derive a Bethe-Salpeter equation including quasi-particle renormalization and irreducible vertex functions to order 1/S. Numerical solutions of this integral equation are discussed on finite lattices up to 33x33 sites with and without final-state interactions.

We find the optical absorption to be qualitatively insensitive to the inclusion of final-state interactions. Results will also be presented for optical vs acoustic phonons. For low frequencies we derive asymptotic analytic expressions for the absorption which will be compared to our numerical results.

TT 71.30 Wed 15:00 Poster B

Insight in orbital resolution of lattice susceptibilities of strongly correlated electron systems — •Lewin Boehnke[1], Alexander Lichtenstein[2], Mikhail Katsnelson[3], and Frank Lechermann[2] — [1]University of Fribourg, Switzerland — [2]University of Hamburg, Germany — [3]University Nijmegen, The Netherlands

Recent advances in the numerical ascertainment of lattice susceptibilities of strongly correlated electron systems [1] in a rigorous manner on a similar footing as the dynamical mean field theory (DMFT) allow to step out of the comfort zone of a single orbital approximation to realistic materials.

Outside this zone, new challenges and opportunities lie in the physical interpretation of these versatile quantities.

We show the wave-vector dependent variation of orbital resolution of the magnetic susceptibility of Sr_2RuO_4, culminating in unexpected lack thereof at its incommensurate peak as well as the intrinsically non-local order parameter of the hidden-order phase in $LiVS_2$[2].

[1] Boehnke, Hafermann, Ferrero, Lechermann, Parcollet, PRB **84** (2011)

[2] Boehnke, Lichtenstein, Katsnelson, Lechermann, arXiv: 1407.4795 (2014)

TT 71.31 Wed 15:00 Poster B

High-temperature heat transport in spin-1/2 quantum magnets — •Christian Hess[1,2], Oleg Mityashkin[1], Ashwin Mohan[1], Chinnathambi Sekar[1], Gernot Krabbes[1], Sabine Wurmehl[1], Bernd Büchner[1,2], Romuald Saint-Martin[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany — [3]Laboratoire de Physico-Chimie de L'Etat Solide, Université Paris-Sud, 91405 Orsay, France

Some years ago, a new, magnetic mode of heat transport has been discovered in low-dimensional spin-1/2 quantum magnets, i.e. spin planes, spin-ladders, and chains as realized in cuprate materials with large magnetic exchange $J/k_B \sim 2000$ K, and is intensely studied since then. The magnetic heat conductivity of such quantum magnet materials can be exceptionally large (even at room temperature), dwarfs the phonon heat conduction and thereby leads to an overall magnitude of the heat conductivity which can be comparable to that of metals. Here we present recent results which extend the accessible temperature range towards high temperature, approaching, for the first time, $k_BT \approx J/2$. The data provide fresh experimental input that allows to rationalize the high-temperature scattering processes for elementary excitations of the quantum magnets.

TT 71.32 Wed 15:00 Poster B

Crystal growth of frustrated materials with kagome-lattices — •Christian Klein, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität, Frankfurt, Germany

Kagome-lattices are promising materials to investigate frustrated quantum spin systems with a possible quantum spin liquid (QSL) ground state [1]. High-quality single crystals are essential to distinguish between disordered magnetic ground-states and a true QSL.

We report on synthesis and characterization of the materials Herbertsmithite ($Cu_3Zn(OH)_6Cl_2$) and Barlowite($Cu_4(OH)_6BrF$), which represent model systems for two-dimensional Kagome-layered structures [2]. The kagome-layers are build up by copper ions and separated from each other through a transition-metal cation, so that a quasi-two-dimensional system is created [3]. Single crystals were grown under hydrothermal conditions.

We present the details of the crystal growth and preliminary substitution experiments to study their influence on the magnetic properties.

[1] P. A. Lee, Science 321, 1306 (2008).
[2] M. Shores et al., J. Am. Chem. Soc. 127, 13462 (2005).

[3] S. Chu et al., Appl. Phys. Lett. 98, 092508 (2011).

TT 71.33 Wed 15:00 Poster B

Spin dynamics in the kagome compound $YBaCo_3AlO_7$ — •M. Iakovleva[1,2], E. Vavilova[1,2], H.-J. Grafe[1], M. Valldor[3], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Zavoisky Physical-Technical Institute, 420029 Kazan, Russia — [3]MPI CPfS, 01069 Dresden, Germany

$YBaCo_3AlO_7$ is a transition metal oxide compound with a magnetic kagome substructure where unconventional ground states such as a spin liquid can be expected. We have investigated the ground state and low energy spin dynamics of this material by ^{27}Al nuclear magnetic resonance spectroscopy.

The characteristic features of the spectral shape and of the relaxation rate temperature dependences show that short-range quasi static correlations occur in the system but not a long-range antiferromagnetic order. We compare our NMR results with AC and DC susceptibility measurements and discuss a possible realization of a spin glass state due to intrinsic structural disorder in this material.

TT 71.34 Wed 15:00 Poster B

NMR of the Shastry-Sutherland lattice $SrCu_2(BO_3)_2$ in pulsed magnetic fields — R. Stern[1], J. Kohlrautz[2], J. Haase[2], •H. Kuehne[3], E.L. Green[3], and J. Wosnitza[3] — [1]National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia — [2]Universität Leipzig, Faculty of Physics and Earth Sciences, 04103 Leipzig, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

$SrCu_2(BO_3)_2$ is a quasi-two-dimensional spin system consisting of Cu^{2+} ions which form orthogonal spin-singlet dimers, also known as the Shastry-Sutherland lattice. This system has been studied extensively using a variety of techniques to probe the spin-triplet excitations, including recent magnetization measurements over 100 T. Spectroscopic techniques, such as nuclear magnetic resonance (NMR), can provide further insight into the spin-coupling mechanisms and excitations. We present ^{11}B NMR spectra measured in pulsed magnetic fields up to 54 T, and compare those with prior results obtained in static magnetic fields at 41 T. Herewith, we prove the feasibility and efficacy of this technique, yielding the capability for extended studies at highest magnetic fields up to the 100 T regime that determine the spin structure in the 1/3 magnetization plateau and beyond.

TT 71.35 Wed 15:00 Poster B

Scaling of the magnetic response in $YbCo_2Si_2$ — •A. Hannaske[1], K. Schmalzl[2], N. Mufti[1], C. Geibel[1], and O. Stockert[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]JCNS at ILL, Grenoble, France

$YbCo_2Si_2$ is a moderate heavy-fermion compound and orders antiferromagnetically below $T_N = 1.7$ K. In zero magnetic field two ordered phases occur. The low-temperature commensurate magnetic structure with an ordering wave vector $k = (0.25\ 0.25\ 1)$ can be continuously suppressed in a magnetic field $B||[1\bar{1}0]$ exhibiting a critical field $B_c(T_N = 0) = 2$ T where the transition to the paramagnetic phase takes place. Extensive inelastic neutron scattering experiments have been performed on singe-crystalline $YbCo_2Si_2$ at B_c as a function of temperature. The magnetic response of the ordering wave vector shows a critical slowing down when lowering the temperature down to zero indicating the proximity to quantum criticality. Furthermore, the response has been analyzed with respect to possible scaling behavior. Assuming a spin-density-wave scenario with three-dimensional quantum-critical spin fluctuations leads to a better collapse of all measured data points than a scenario with local critical fluctuations. This finding is in line with results of the specific heat, which doesn't show any sign of divergence at lowest T at the critical field B_c.

TT 71.36 Wed 15:00 Poster B

Pressure induced magnetic ordering in $SrCo_2P_2$ — •Helge Rosner, Sarah Ackerbauer, Christoph Bergmann, Moritz Besser, Michael Nicklas, and Christoph Geibel — MPI CPfS, Dresden, Germany

Since the discovery of superconductivity in doped iron pniktides, in particular the AFe_2As_2 systems of the $ThCr_2Si_2$ structure type, the intricate interplay of crystal structure, magnetism and superconductivity in these compounds has attracted broad attention. It is widely believed that the superconductivity of this compound family is closely related tho spin fluctuations. $SrCo_2P_2$ is a structural homologue of the AFe_2As_2 compound series, exhibiting a paramagnetic ground state, but in close vicinity to a quantum critical point. In our joined experimental and theoretical study we demonstrate that under hydrostatic pressure the system undergoes an isostructural transition to the so-called tetragonal collapsed state with a strongly reduced c/a ratio by about 15%. Surprisingly, this transition is accompanied by magnetic ordering, indicated by a magnetic-field-dependent kink in the resistivity. Our results are supported by density functional electronic structure calculations.

TT 71.37 Wed 15:00 Poster B

Tuning of the magnetic interactions in the frustrated spin chain compound linarite via hydrostatic pressure — •Jonathan Noky[1], Wolf Schottenhamel[1], Stefan-Ludwig Drechsler[1], Stefan Süllow[2], Anja U. B. Wolter[1], and Bernd Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]IPKM, TU Braunschweig, Braunschweig, Germany

Linarite ($PbCuSO_4(OH)_2$) is an anisotropic, quasi-one-dimensional frustrated spin-chain compound with competing ferromagnetic nearest-neighbor and antiferromagnetic next-nearest neighbor exchange interactions. Due to small but non-negligible interchain interactions linarite shows magnetic long-range order below T = 2.8K, where a helical ground state and a rich magnetic phase diagram have been observed for magnetic fields H parallel to the chain direction [1]. The magnetic interactions and thereby the frustration ratio strongly depends on the bond angles and bond lengths between involved copper and oxygen atoms. In order to systematically change them, the application of chemical or hydrostatic pressure is a powerful tool. We present a magnetization study of linarite under high hydrostatic pressures for different magnetic fields both perpendicular and parallel to the chain direction.

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

TT 71.38 Wed 15:00 Poster B

Amorphous ferromagnetism and re-entrant magnetic glassiness in $Sm_2Mo_2O_7$ — •Giacomo Prando[1], Pietro Carretta[2], Anja Wolter-Giraud[1], Romuald Saint-Martin[3], Alexandre Revcolevschi[3], and Bernd Büchner[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Dipartimento di Fisica e Unitá CNISM di Pavia, Universitá di Pavia, I-27100 Pavia, Italia — [3]Laboratoire de Physico-Chimie de l'Etat Solide, ICMMO, UMR8182, Université Paris-Sud, F-91405 Orsay, France — [4]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

We report on the investigation of a high-quality single crystal of $Sm_2Mo_2O_7$ by means of dc magnetometry, muon spin spectroscopy and high-harmonics ac susceptibility [1]. The magnetic phase of the Mo^{4+} sublattice develops below $T_C = 78$ K and is typically discussed in the literature as a conventional itinerant ferromagnetic state. However, our results clearly detect a complicated superposition of conventional and highly disordered magnetic behaviors below 78 K sharing several common features with amorphous ferromagnetic alloys and with other insulating spin-glass pyrochlore molybdates. As typical for amorphous ferromagnets, a freezing of the transverse XY spin components of Mo^{4+} below $T \sim 25$ K is evidenced, an effect otherwise known as re-entrant spin-glass phase. Our results shed new light on the magnetic properties of $Sm_2Mo_2O_7$ and on the overall electronic phase diagram commonly accepted for pyrochlore molybdates.

[1] G. Prando et al., *Phys. Rev. B* **90**, 085111 (2014)

TT 71.39 Wed 15:00 Poster B

Local magnetic properties of diluted honeycomb iridates $Na_{3-\delta}M\mathbf{Ir_2O_6}$ (M = Zn, Cu, Ni) probed by ^{23}Na-NMR and μ^+SR — •Giacomo Prando[1], Evgeniya Vavilova[1,2], Alexey Alfonsov[1], Hans-Joachim Grafe[1], Vladislav Kataev[1], Bernd Büchner[1,3], Kristen Baroudi[4], Cindi Yim[4], John Roudebush[4], Huiwen Ji[4], and Robert Cava[4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute of RAS, Kazan, Russia — [3]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

We present an experimental investigation of the magnetic properties of a series of sodium ternary iridates $Na_{3-\delta}MIr_2O_6$ (M = Zn, Cu, Ni) by means of local spin-probe techniques. In these materials, Ir ions are arranged in hexagonal honeycomb layers while the transition metal ions M substitute the Na ions in the hexagons center, with some detected

degree of M/Ir site mixing [1]. Together with our earlier magnetization measurements [1], our results give evidence that the doping of the Ir honeycomb lattice has a remarkable impact on the overall magnetic properties. In contrast to a well-defined long-range antiferromagnetic (AF) order in Na_2IrO_3, our data clearly reveal two different regimes at low temperatures, namely a static AF ordering and a spin glass behavior with short range spin correlations. The interplay and coexistence of these regimes depends on the specific element M.

[1] K. Baroudi et al., *Journ. Sol. State Chem.* **210**, 195 (2014)

TT 71.40 Wed 15:00 Poster B

Accessing the magnetic properties of iridium oxides by means of electron spin resonance — •Stephan Fuchs[1], Giacomo Prando[1], Alexey Alfonsov[1], Vladislav Kataev[1], Bernd Büchner[1,2], Brendan Phelan[3], and Robert Cava[3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

We report on our first results of electron spin resonance (ESR) measurements performed on exemplary iridium-based oxides. These are aimed at understanding the microscopic magnetic properties of these materials which are ultimately arising from a complex interplay of spin-orbital interactions and strong electronic correlations. $La_{11-x}Sr_xIr_4O_{24}$ allows us to detect single-iridium ion spectroscopic features thanks to the large distance among iridium-oxygen cages. At the same time, the increased inter-ions interactions in Na_2IrO_3 lead to a clear broadening of the ESR signal. We discuss our preliminary results in a wide range of temperatures and magnetic fields (up to 16 T).

TT 71.41 Wed 15:00 Poster B

Hydrostatic pressure experiments on frustrated hexagonal Iridates — •Rudra Sekhar Manna, Friedrich Freund, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A = Na, Li) have novel electronic and magnetic properties due to the strong spin-orbit coupling and electronic correlations. They are proposed candidate materials for the realization of the frustrated bonding-dependent anisotropic Kitaev interaction [1, 2]. While the structure of Na_2IrO_3 and α-Li_2IrO_3 consists of a two-dimensional (2D) honeycomb lattice, a 3D, so-called hyper-honeycomb structure is realized in β-Li_2IrO_3 [3, 4]. All different materials display long-range magnetic order, in contrast to a Kitaev quantum spin-liquid, although the analysis of the magnetic properties indicates dominating Kitaev exchange interactions [3]. The Kitaev interaction sensitively depends on the Ir-O-Ir bonding angle which may be varied by external pressure. This motivates a detailed study of the hydrostatic pressure dependence of the magnetic properties of hexagonal iridates. In particular we investigate the bulk magnetization in a commercial SQUID magnetometer up to 2 GPa using Daphne oil as pressure medium and a small piece of lead as pressure sensor.

[1] Y. Singh *et al.*, PRL **108**, 127203 (2012).
[2] S. Manni *et al.*, PRB **89**, 245113 (2014).
[3] A. Biffin *et al.*, PRB **90**, 205116 (2014).
[4] T. Takayama *et al.*, arXiv:1403.3296 (2014).

TT 71.42 Wed 15:00 Poster B

Possibility of a two-dimensional spin liquid in CePdAl induced by partial geometric frustration? — •V. Fritsch[1,2], K. Grube[2], W. Kittler[2], C. Taubenheim[2], Z. Huesges[3], S. Lucas[3], E. Green[4], O. Stockert[3], and H. v. Löhneysen[2] — [1]Universität Augsburg, Institut für Physik, Experimentalphysik VI, Germany — [2]Karlsruher Institut für Technologie, Germany — [3]Max-Planck-Institut für chemische Physik fester Stoffe, Dresden, Germany — [4]Hochfeldzentrum Dresden-Rossendorf, Germany

CePdAl crystallizes in the hexagonal ZrNiAl structure, where the magnetic ions form a distorted kagomé lattice. At $T_N = 2.7$ K the onset of antiferromagnetic (AF) order is observed. Neutron scattering experiments [1] revealed a partial frustration in the distorted kagomé planes of this structure: two-thirds of the Ce moments form ferromagnetic chains, which are antiferromagnetically coupled, the remaining third do not participate in any long-range order. Along the c-axis the magnetic moments exhibit an amplitude modulation. Accordingly, the kagomé planes are stacked on top of each other, resulting in corrugated AF planes parallel to the c-axis formed by the ordered magnetic moments, which are separated by the frustrated moments [2]. It is an intriguing and yet unresolved question if this third of frustrated moments forms a spin liquid state in CePdAl. Based on measurements of specific heat, thermal expansion, magnetization and electrical resistivity we want to discuss this possibility.

[1] A. Dönni *et al.*, J. Phys.: Condens. Matter **8**, 11213 (1996).
[2] V. Fritsch *et al.*, Phys. Rev. B **89**, 054416 (2014).

TT 71.43 Wed 15:00 Poster B

Dielectric measurements of magnetic monopoles on the spin-ice compounds $(Ho/Dy)_2Ti_2O_7$ — •Manuel Pietsch, Christoph P. Grams, Jean-Francois Welter, Victoria Cho, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

In so-called spin-ice compounds a frustrated ground-state with finite zero-point entropy is stabilized via competing interactions and emergent magnetic monopoles excitations [1]. It was postulated that a magnetic monopole holds an electric dipole moment [2], which allows to investigate their dynamics via the dielectric function $\varepsilon(\nu)$.

In $Dy_2Ti_2O_7$ a critical speeding-up for frequencies up to 100 kHz was reported down to temperatures of 200 mK with a specific focus on the critical endpoint present for a [111] magnetic field [3]. In $Ho_2Ti_2O_7$ both faster relaxation dynamics compared to the sister-compound and an additional relaxation process are suspected [4].

Here we report on broadband dielectric spectroscopy measurements of $\varepsilon(\nu)$ in $Ho_2Ti_2O_7$.

Funded through the Institutional Strategy of the University of Cologne within the QM2 Excellence Initative and research grant HE-3219/2-1.

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[2] D. I. Khomskii, Nature Comm. 3 (2012) 1
[3] C.P. Grams et al., Nature Comm. 5 (2014) 4853
[4] G. Ehlers et al., J. Phys.: Cond. Mat. 16 (2004) S635

TT 71.44 Wed 15:00 Poster B

Heat Transport in dilute Spin-Ice Materials $(R_{1-x}Y_x)_2Ti_2O_7$ with R = Ho,Dy — •Jean-Francois Welter[1], Simon Scharffe[1], Gerhard Kolland[1], Martin Valldor[1,2], Victoria Cho[1], Peter Laschitzky[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Max-Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany

In the spin-ice materials $R_2Ti_2O_7$ the magnetic R^{3+} ions form a network of corner-sharing tetrahedra. Recently, these materials attracted a lot of interest due to their groundstate degeneracy and the description of the low-energy excitations as magnetic monopoles[1]. In order to investigate the influence of the monpole propagation on the thermal conductivity κ, we dilute the spin-ice compounds with non-magnetic Yttrium. We synthesized single crystals of the series $(R_{1-x}Y_x)_2Ti_2O_7$ with $0 \leq x \leq 0.75$ using the floating-zone method. Comparing the thermal conductivity for different doping levels x, the total κ can be separated into a sum of phononic (κ_{ph}) and magnetic (κ_{mag}) contributions. In both $R_2Ti_2O_7$ compounds, κ_{mag} is sizable and can be attributed to magnetic monopole excitations[2]. We find that κ_{mag} is more pronounced in $Dy_2Ti_2O_7$ and that the field dependences of κ_{ph} are of opposite signs in the Dy- and Ho-based materials[3].

This work was supported by DFG via the project LO 818/2-1.

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[2] Kolland *et al.*, Phys. Rev. B, **86**, 060402(R) (2012).
[3] Scharffe *et al.*, J. Magn. Magn. Mater. (in press, arXiv:1406.4037).

TT 71.45 Wed 15:00 Poster B

Influence of Ti deficiency on the magnetic properties in $Yb_2Ti_2O_7$ — •Marcel Naumann[1], Elizabeth L. Green[1], Sergei Zherlitsyn[1], Salim Erfanifam[1], Shadi Yasin[1], Joachim Wosnitza[1], Andrej Maljuk[2], Christian G. F. Blum[2], Rhea Kappenberger[2], Jan Trinckauf[2], Bernd Büchner[2], Sabine Wurmehl[2], Rajib Sarkar[3], Sirko Kamusella[3], Philipp Materne[3], Hans-Henning Klauss[3], Hubertus Luetkens[4], and Chris Baines[4] — [1]Hochfeld-Magnetlabor Dresden, HZDR, 01328 Dresden, Germany — [2]IFW, 01171 Dresden, Germany — [3]TU Dresden, 01069 Dresden, Germany — [4]PSI, 5232 Villigen, Switzerland

Frustrated spin systems with pyrochlore lattice exhibit a wide range of physical phenomena such as magnetic monopoles and residual entropies. In particular, $Yb_2Ti_2O_7$ has attracted attention in recent years, also due to the sample dependence of its ground state. While some works suggest a ferromagnetic ground state others see no long-

range magnetic ordering or spin freezing whatsoever.

We investigated two different samples grown under similar growth conditions using heat-capacity, ultra-sound, and μSR measurements. While one sample showed a crossover around 240 mK,the other exhibited no evidence of long-range magnetic order down to 15 mK. The results of subsequent x-ray and EDX measurements indicate a strong influence of Ti deficiency on the low-temperature magnetic properties. This offers a new tuning parameter for the ongoing search for a quantum spin liquid.

TT 71.46 Wed 15:00 Poster B

Phase separation in $Y_{0.63}Ca_{0.37}TiO_3$ — •Bernhard Zimmer[1], Raphael German[1], Thomas Koethe[1], Alexander Komarek[1,2], Markus Braden[1], and Paul van Loosdrecht[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the domain structure and Raman response of $Y_{0.63}Ca_{0.37}TiO_3$ single crystals which show a clear metal-to-insulator transition at ca. 170 K, with a wide hysteresis in the resistivity ranging down to ca. 50 K. We observe by use of a conventional optical microscope the appearance of two distinct regions at temperatures below ca. 200 K, with a characteristic length scale of order of 10 μm. By means of Raman spectroscopy we can identify the regions to correspond to the metallic and insulating domains, and follow the evolution of the domains as function of temperature down to 5 K.

TT 71.47 Wed 15:00 Poster B

Ultrasonic investigation of GaV_4S_8 — •P. T. Cong[1], S. Mombetsu[1,2], V. Tsurkan[3], A. Loidl[3], S. Zherlitsyn[1], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Department of Physics, Hokkaido University, Japan — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

In recent years, transition metal-chalcogenides with the cubic $GaMo_4S_8$-type structure have attracted much interest because of their fascinating properties such as superconductivity under pressure, metal-insulator transition, 4*d* ferromagnetism and various structural and magnetic instabilities at low temperatures. These phenomena reflect the strong coupling of structural, electronic and magnetic degrees of freedom in this system. Here, we present results of ultrasound investigations performed on a high-quality single crystal of the tetrahedral magnetic-cluster material GaV_4S_8. The temperature dependence of the sound velocity and attenuation shows a huge anomaly at $T_s = 44$ K followed by a pronounce feature at $T_c = 12.5$ K related to a structural transition and ferromagnetic ordering, respectively, as known from previous magnetic-susceptibility and specific-heat results [1]. A field-induced transition at temperatures below T_c reveals a complex magnetic structure of GaV_4S_8, suggesting a competition of several interactions. Based on these measurements, we mapped out the $B-T$ phase diagram of GaV_4S_8 and discuss the role of the lattice degrees of freedom in this material.

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TT 71.48 Wed 15:00 Poster B

Skyrmion density correlations in critical chiral paramagnets — •Laura Köhler, Achim Rosch, and Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

The interactions between critical paramagnons in chiral magnets like MnSi or Cu_3OSeO_3 suppress the critical temperature and, in addition, drive the transition weakly first-order. Within the resulting fluctuation-disordered regime strong correlations prevail that substantially renormalize the correlation length in quantitative agreement with Brazovski theory [1,2,3]. Within this regime, we theoretically address the correlations of the skyrmion density that can be identified with the local vector chirality of the magnetization. These correlations are expected to be particularly pronounced for finite magnetic fields close to the skyrmion crystal phase. We compute the corresponding correlation function within the Brazovski approximation with the aim to identify additional microwave resonances.

[1] M. Janoschek *et al.* Phys. Rev. B **87**, 134407 (2013).
[2] A. Bauer *et al.*, Phys. Rev. Lett. **110**, 177207 (2013).
[3] J. Kindervater *et al.* Phys. Rev. B **89**, 180408(R) (2014).

TT 71.49 Wed 15:00 Poster B

Scattering of high-energy magnons from a magnetic skyrmion — •Sarah Schroeter and Markus Garst — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

The skyrmion is a topologically stable soliton solution in chiral magnets and corresponds to a large-amplitude excitation of the field-polarized ground state. We consider the fluctuation spectrum around such a soliton with particular focus on the scattering of high-energy magnons. The topological winding number of the skyrmion results in a finite Aharanov-Bohm flux density in the scattering potential that leads to skew and rainbow scattering of magnons [1]. We consider the differential cross section and the magnon pressure on the skyrmion within a semiclassical approximation and derive their high-energy asymptotics.

[1] C. Schütte and M. Garst, Phys. Rev. B 90, 094423 (2014).

TT 71.50 Wed 15:00 Poster B

Magnon excitations of magnetic helices and skyrmion crystals — •Johannes Waizner and Markus Garst — Institute for Theoretical Physics, Universität zu Köln, Köln, Germany

In chiral magnets long-range ordered magnetic crystals form with a lattice spacing proportional to the inverse of spin-orbit coupling. The magnetic helix corresponds to a one-dimensional crystal while the skyrmion lattice effectively realizes a two-dimensional magnetic crystal. We study the magnon excitations of these crystals that experience a characteristic Bragg scattering off their periodicity resulting in magnon band structure. For the helix, in particular, this leads to gaps in the spectrum that prohibit magnon propagation along the pitch direction. We also compare with recent results of inelastic neutron scattering [1].

[1] M. Kugler, G. Brandl, R. Georgii, K. Seemann, M. Janoschek, J. Waizner, M. Garst, A. Rosch, C. Pfleiderer, and P. Böni (unpublished)

TT 71.51 Wed 15:00 Poster B

Critical behavior of collective GHz excitations of Skyrmions and spin helices — •Ioannis Stasinopoulos[1], Stefan Weichselbaumer[1], Thomas Schwarze[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2], and Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department, FG Magnetische Materialien, TU München, Garching, Germany — [3]EPFL, Institut de physique de la matiere complexe, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]IMX, EPFL, Lausanne, Switzerland

Skyrmions are topologically stable spin textures with the spins pointing in all directions wrapping up a sphere. They emerge in chiral-magnets, e.g. MnSi, and arrange in a hexagonal lattice with typical lattice constants of several tens of nm. Our group uses an all-electrical microwave spectroscopy setup based on a vector analyzer and lithographically fabricated coplanar waveguides to excite and simultaneously probe the spin states. We study and compare the temperature dependence of the dynamics both in the ordered magnetic phases and the regime just above T_c. This study addresses the dynamics of a suspected "Skyrmion liquid" above T_c and aims ultimately at deepening the microscopic understanding of crystallization processes in magnetism. Financial support by the DFG via TRR80 and NIM is acknowledged.

TT 71.52 Wed 15:00 Poster B

Collective GHz excitations of Skyrmions and spin helices in Cu_2OSeO_3 — •Stefan Weichselbaumer[1], Ioannis Stasinopoulos[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2], and Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department, FG Magnetische Materialien, TU München, Garching, Germany — [3]EPFL, Institut de physique de la matiere complexe, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]IMX, EPFL, Lausanne, Switzerland

Skyrmions are topologically stable spin textures with the spins pointing in all directions wrapping up a sphere. We investigate collective excitations of Skyrmions and spin helices in the GHz-regime in the insulating multiferroic Cu_2OSeO_3. Using an all-electrical microwave spectroscopy setup based on a vector analyzer and lithographically fabricated coplanar waveguides (CPW) we excite and simultaneously probe the dynamics. By modifying the sample shape, CPW design, and excitation configuration, we address the dynamic modes differently. We compare our results with a mean-field theory taking into account dipolar interaction between the spins. The control over the dynamics opens the way towards helimagnet-based high-frequency de-

vices. Financial support by the DFG via TRR80 is acknowledged.

TT 71.53 Wed 15:00 Poster B

Corbino resistance measurements of the cubic helimagnet MnSi — •Marco Halder, Christoph Schnarr, Andreas Bauer, and Christian Pfleiderer — Technische Universität München, Physik-Department E21, D-85748 Garching, Germany

In recent years the transport properties of the itinerant helimagnet MnSi were heavily investigated. In particular, the topological Hall contribution arising from a regular arrangement of spin whirls, the so-called Skyrmion lattice, attracted great scientific interest. In addition, it was shown that already ultra-low current densities are sufficient to move the magnetic texture leading to emergent electrodynamics. Here, we report measurements on a disk-shaped sample with a coaxial contact arrangement, i.e., in a Corbino geometry, addressing geometrical contributions to the magnetoresistance of MnSi. We report the Corbino resistance of high-quality single crystals of MnSi over a wide range of temperatures from 2 K to 300 K under magnetic fields up to 9 T.

TT 71.54 Wed 15:00 Poster B

Chiral fluctuations in Cu_2OSeO_3 and FeGe in their field modulated states: ^{63,65}Cu and ^{57}Fe NMR study — •Mayukh Majumder, Hiroshi Yasuoka, Panchanan Khuntia, Markus Schmidt, and Michael Baenitz — Max Plank Institute for Chemical Physics of Solids, Dresden, Germany

Insulating Cu_2OSeO_3 (ferrimagnetic transition temperature at 58 K) and metallic FeGe (ferromagnetic transition temperature at 280 K) show different field modulated states such as helical, conical along with topological Skyrmion phase [1,2,3]. We employed ^{63,65}Cu and ^{57}Fe NMR as a on site probe of field modulated states. The evolution of spectral shape from helical to conical to ferrimagnetic (for Cu_2OSeO_3) or ferromagnetic state (for FeGe) have been investigated. Further the spin-lattice relaxation rate ($1/T_1$) and spin-spin relaxation rate ($1/T_2$) provide the nature of chiral spin excitations across different field modulated phase boundaries.

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[2] Phys. Rev. Lett. 107, 127203(2011).
[3] Nature 8 153(2013).

TT 71.55 Wed 15:00 Poster B

Pressure induced insulator-to-metal transition in $FePS_3$ — •Matthew John Coak[1], Charles Robert Sebastian Haines[1,2], and Siddarth Shankar Saxena[1] — [1]Cavendish Laboratory, University of Cambridge — [2]CamCool Research Ltd UK

$FePS_3$ is structurally and magnetically two-dimensional, with a magnetic ground state in which spins are ordered as ferromagnetic chains coupled antiferromagnetically. At ambient pressure, it is an insulator with a direct gap of approximately 0.5 eV and a room temperature resistivity of approximately 104 Ωcm. We present the results of exploratory resistivity, magnetisation and dielectric measurements under pressure for this material. The insulating phase is suppressed at a pressure in the range 40-70 kbar giving way to a new metallic phase. As yet unexplained intermediate behaviour is seen at pressures around the transition. At high pressure, the resistivity develops linear temperature dependence similar to that observed in Cuprates. At lower temperature, there is an upturn in resistivity which may indicate a low temperature phase transition or impurity scattering.

TT 71.56 Wed 15:00 Poster B

Field-dependent de Haas-van Alphen frequencies in the non-centrosymmetric compound CrGe — •J. Klotz[1,2], K. Götze[1,2], J. Bruin[3], C. Geibel[4], H. Rosner[4], K. Weber[4], M. Schmidt[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]High Magnetic Field Laboratory, Radboud University, Netherlands — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

CrGe is a transition-metal germanide with the B20 non-centrosymmetric cubic structure. It does not exhibit any magnetic order in fields up to 60 T but the temperature dependence of the susceptibility and resistivity indicate its proximity to ferromagnetism [1]. Since CrGe has no inversion symmetry, it was expected to exhibit anti-symmetric spin-orbit interaction with split dHvA frequencies which are field dependent [2]. We present dHvA-effect data that were obtained employing rotatable capacitive torque magnetometers in a 18 T/30 mK and a 33 T/340 mK system. We found a clear field dependence of the dHvA frequencies as well as enlarged effective masses as was expected from the enhanced Sommerfeld coefficient of $\gamma = 19$ mJ/mol K^2

[1] T. Sato and M. Sakata, J. Phys. Soc. Jpn. **52** (1983), 1807
[2] V. P. Mineev and K. V. Samokhin, Phys. Rev. B **72** (2005), 212504.

TT 71.57 Wed 15:00 Poster B

Resistivity of MnB_4 — •Nico Steinki[1], Dirk Schulze Grachtrup[1], Stefan Süllow[1], Arno Knappschneider[2], and Barbara Albert[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, TU Darmstadt, Germany

In an effort to develop super hard materials, MnB_4 was recently synthesized for the first time in single crystalline form, with micro scale crystals of about 200 μm length. Subsequently, the magnetic properties have been studied experimentally, and band structure calculations have been carried out [1,2]. Based on these calculations and preliminary resistivity measurements, it was argued that the material is semiconducting, although a definite conclusion could not be reached.

In order to determine whether MnB_4 is a semiconductor or a metal we have carried single crystal resistivity measurements at temperatures 2 to 300 K. For this purpose a setup for measuring micro-scale samples was developed and characterized. The setup is based on a modified two point configuration and the resistivity of MnB_4 was measured as function of temperature. With these measurements MnB_4 was identified to be a semiconductor.

[1] A. Knappschneider et al., Angew. Chem. **126** (2014) 1710
[2] H. Gou et al., Phys. Rev. B **89** (2014) 064108

TT 71.58 Wed 15:00 Poster B

Signatures of the magnetostructural phase transition in CrN probed by temperature-dependent infrared spectroscopy — •Jihaan Ebad-Allah[1,2], Benjamin Kugelmann[1], Francisco Rivadulla[3,4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt — [3]Center for Research in Biological Chemistry and Molecular Materials, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — [4]Department of Physical Chemistry, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

During the last decades, CrN has attracted great interest due to its superior high-temperature oxidation resistance, hardness, wear and corrosion resistance, and good chemical and thermal stability. In addition, CrN has remarkable electronic, optical, and magnetic properties. At the Neel temperature (T_N= 273-286 K) CrN undergoes a paramagnetic to antiferromagnetic phase transition, concomitant with a structural distortion from cubic rock-salt to orthorhombic [1].

We carried out temperature-dependent absorption measurements on CrN powder in the frequency range 250-7500 cm^{-1}. At ambient conditions, the absorption spectrum shows a phonon mode in the far-infrared range, a strong absorption band at around 0.17 eV, and a charge gap at ≈ 0.7 eV [2]. Below T_N, the phonon mode splits and the absorption edge shows a slight blue shift.

[1] A. Filippetti et al., Phys. Rev. B **59**, 7043 (1999).
[2] D. Gall et al., J. Appl. Phys. **91**, 5882 (2002);
A. Herwadkar et al.,Phys. Rev. B **79**, 035125(2009).

TT 71.59 Wed 15:00 Poster B

Influence of doping and quasi-lowdimensionality on the thermoelectric properties of strongly correlated materials — •Raphael Richter[1], Lewin Boehnke[2], Daniel Grieger[3], and Frank Lechermann[1] — [1]1. Institut fur Theoretische Physik, Universität Hamburg, Germany — [2]Département de Physique, University of Fribourg, Switzerland — [3]International School for Advanced Studies (SISSA), Trieste, Italy

Strongly correlated materials are among the most interesting and complicated systems in condensed matter physics. Large Seebeck coefficients are found in some of these compounds, which highlight the possibility for thermoelectric applications.

In this work, we study the thermoelectric properties of such systems by means of the charge self-consistent density functional theory (DFT) plus dynamical mean-field theory (DMFT) scheme, build on a mixed basis pseudopotential framework combined with a continuous time quantum Monte-Carlo solver. By means of this methodology we consider doping effects by constructing pseudopotentials with frac-

tional nuclear charge or within a supercell approach. For the investigation of the thermoelectric response, the (anisotropic) Seebeck tensor is calculated within the Kubo formalism at different temperatures.

TT 71.60 Wed 15:00 Poster B

Matrix-product-state method with local basis optimization for bosonic systems out of equilibrium — •Christoph Brockt[1], Eric Jeckelmann[1], Florian Dorfner[2], Lev Vidmar[2], and Fabian Heidrich-Meisner[2] — [1]Leibniz Universität Hannover, Germany — [2]Ludwig-Maximilians-Universität München, Germany

We present a method for simulating the time evolution of quasi-one-dimensional correlated systems with bosonic degrees of freedom using matrix product states. Our goal is the accurate description of systems with large bosonic fluctuations for long periods of time. For this purpose we combine the time-evolving block decimation (TEBD) algorithm [1] with a local basis optimization approach which yields so-called optimal boson states [2]. We discuss the performance of this approach in comparison to TEBD with a bare boson basis, exact diagonalizations, and diagonalizations in a limited functional space. First, we test our method for the non-equilibrium dynamics of a Holstein polaron [3] and show that it allows us to study the regime of strong electron-phonon coupling. Second, the method is applied to the scattering and self-trapping of an electronic gaussian wave packet traveling through a quantum wire with electron-phonon coupling. Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] G. Vidal, PRL **93**, 040502 (2004)
[2] C. Zhang, E. Jeckelmann, and S.R. White, PRL **80**, 2661 (1998)
[3] F. Dorfner et al., arXiv:1411.5074 (2014)

TT 71.61 Wed 15:00 Poster B

Nonlinear charge transport in interacting ring structures: transient and steady state dynamics — •Benedikt Schönauer and Peter Schmitteckert — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

We investigate the effect of density-density interactions in various ring structures coupled to non-interacting leads on the transient and the steady state currents. To this end we use a time dependent density matrix renormalization group method to calculate the time resolved current in response to a quench in the charge balance. Our results suggest that an asymmetry of the ring structures gives rise to interesting new features of the long time limit of the local current in the rings. In addition finite size effects seem to be significantly increased for these systems as compared to strictly one-dimensional structures.

TT 71.62 Wed 15:00 Poster B

Time-dependent Gutzwiller wave function for the finite-dimensional Hubbard model in nonequilibrium — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universitität Augsburg

We apply the time-dependent Gutzwiller wave function (GWF) to the fermionic Hubbard model in nonequilibrium in two and three dimensions. For this purpose we combine two variational formalisms for the GWF, one that starts from the limit of infinite dimensions [1] and one that applies in arbitrary dimensions [2]. Similar to the one- and infinite-dimensional case, the resulting equations of motion are conservative and yield oscillatory behavior for an interaction quench, which we compare with the prethermalization dynamics on short timescales.
[1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010).
[2] M. Kollar and C. Gramsch, see Talk in TT.

TT 71.63 Wed 15:00 Poster B

Bound state fragmentation of a spin line in 2 dimensions — •Jonathan Lux and Achim Rosch — Institute for theoretical Physics, Cologne

We investigate the dynamics of a line of down-spins embedded in the ferromagnetic spin-up ground state of a two-dimensional XXZ model close to the Ising limit. We treat the system as an open 1 dimensional system, and use a Schrieffer Wolff transformation in combination with a semiclassical approximation to tackle this quantum quench problem. During the time evolution, the line is fragmented into free and bound states of down-spins. We determine the statistics of the bound states, which, in principle, can be measured in cold atom systems using a quantum microscope.

TT 71.64 Wed 15:00 Poster B

Enforcing conservation laws in nonequilibrium cluster perturbation theory — •Christian Gramsch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

Recently it has been proposed to solve the nonequilibrium Dyson equation by numerically decomposing the self-energy into its Lehmann representation [1]. This allows to replace the interaction term in the Hamiltonian by noninteracting bath degrees of freedom. In our present work we analytically construct the Lehmann representation of the self-energy for arbitrary interacting systems. For any finite system, e.g. a cluster system, the number of resulting noninteracting bath sites is finite. While this can already be used to solve nonequilibrium cluster perturbation theory (NE-CPT) [2] for arbitrary long times, we improve upon NE-CPT by enforcing local continuity equations for density and energy to be respected. Total energy and particle number are then conserved during the time evolution.

[1] K. Balzer and M. Eckstein, Phys. Rev. B 89, 035148 (2014)
[2] M. Balzer and M. Potthoff, Phys. Rev. B 83, 195132 (2011)

TT 71.65 Wed 15:00 Poster B

Quench dynamics studied by means of non-equilibrium self-energy-functional theory — •Felix Hofmann[1], Martin Eckstein[2], and Michael Potthoff[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Universität Hamburg - CFEL

The non-equilibrium self-energy-functional theory (SFT) [1] provides a general framework for the systematic construction of non-perturbative approximations to study strongly correlated systems out of equilibrium. On the space of non-equilibrium self-energies, given on the Keldysh-Matsubara contour, the grand potential can be written as a functional which is stationary at the physical non-equilibrium self-energy. The corresponding variational principle is exploited by restricting the variations to variations of self-energies that are generated by an exactly solvable reference system.

Here we present first results obtained for Hubbard models where the real-time dynamics is induced by a quantum quench of the interaction parameter and using different reference systems. We discuss the details of the numerical implementation, present internal consistency checks, discuss the total energy conservation, and compare with literature data from the non-equilibrium dynamical mean-field theory.

[1] F. Hofmann, M. Eckstein, E. Arrigoni, and M. Potthoff, PRB 88, 165124 (2013)

TT 71.66 Wed 15:00 Poster B

Nonequilibrium Green functions approach to transport properties in strongly coupled finite quantum systems — •Niclas Schlünzen, Sebastian Hermanns, and Michael Bonitz — ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel, Germany

Transport properties of strongly correlated quantum systems are of central interest in condensed matter, ultra-cold atoms and in dense plasmas[1]. There, the proper treatment of strong correlations is important. This can be achieved by using the nonequilibrium Green functions framework with a suitable chosen many-body approximation. In this contribution, we study transport properties of finite spatially inhomogeneous Hubbard systems with the T-matrix approximation[2]. The diffusion is analyzed for different spatial geometries in one to three dimensions as a function of the particle number and interaction strength.

[1] Balzer et al., Phys.Rev. B **79** 245306 (2009).
[2] Bonitz et al., Contrib.Plasma Phys. (2014), DOI: 10.1002/ctpp.201400065

TT 71.67 Wed 15:00 Poster B

Correlated lattice systems far from equilibrium—a nonequilibrium Green functions approach — •Sebastian Hermanns, Niclas Schlünzen, and Michael Bonitz — ITAP, Christian–Albrechts–Universität Kiel, Leibnizstr. 15, 24098 Kiel, Germany

The study of dynamical processes in lattice systems reveals a great variety of electronic phenomena which occur on an ultrafast time scale[1]. They include the build-up of inter-particle correlation as well as dynamically screening of the interaction. To describe these processes theoretically, the framework of non-equilibrium Green functions is very well suited. It provides a controlled way to generate various classes of many-body approximations focussed on different aspects of the experiment. In this contribution, we analyze the specific features covered

by the second order Born, GW and T-matrix approximation in combination with the Generalized Kadanoff-Baym ansatz [2] for Hubbard systems in arbitrary dimensions in nonequilibrium.

[1] Kajala et al., Phys.Rev.Lett. **106** 206401 (2011).
[2] Hermanns et al., Phys.Rev. B **90** 125111 (2014).

TT 71.68 Wed 15:00 Poster B

Nonlocal quantum kinetic theory — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

A quantum kinetic equation of nonlocal and non-instantaneous character is derived which unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in dense Fermi systems. The numerical solution is not more expensive than solving the Boltzmann equation since large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors. The balance equations for the density, momentum and energy include quasiparticle contributions and the correlated two-particle contributions beyond the Landau theory. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy.

[1] V. Špička, P. Lipavský, K. Morawetz,
Phys. Rev. B. **55**, 5084 (1997); 5095 (1997)
[2] K. Morawetz, V. Spička, P. Lipavský, H.N. Kwong,
Phys. Rev. **C 59**,6 (1999) 3052-3059;
[3] P. Lipavský, K. Morawetz, and V. Špička,
Annales de Physique, Paris, 2001, No. 26, 1.

TT 71.69 Wed 15:00 Poster B

Electronic structure of substitutionally disordered systems: orbital based CPA within a pseudopotential approach — •Alexander Herbig, Rolf Heid, and Robert Eder — Institute for Solid State Physics, Karlsruhe Institute of Technology

Investigating the electronic structure of substitutionally disordered systems (e.g. doped compounds) is a challenge for density functional-based methods. A straightforward supercell approach is limited to special impurity concentrations due to its huge computational effort. In order to perform calculations at arbitrary impurity concentrations effective medium theories come into play. Among them the coherent potential approximation (CPA) has been successfully applied in the KKR-DFT-framework but rarely has been used within other DFT-frameworks. Blackman, Esterling and Berk (BEB) suggested an extension to the CPA which allows to handle off-diagonal disorder on the level of hopping-terms[1]. Based on ealier work[2], we developed a fully charge self-consistent BEB-CPA for a nonorthogonal LCAO-basis. This basis is obtained via projection from a mixed-basis pseudopotential calculation. We discuss the method itself as well as its numerical verification in comparison to model calculations for a tight binding binary alloy Hamiltonian solved by exact diagonalization. Furthermore we present first applications of the method to real materials.

[1] J.A. Blackman et al., Phys. Rev. B 4, 2412 (1971)
[2] K. Koerpenik et al., Phys. Rev. B 55, 5729 (1997)

TT 71.70 Wed 15:00 Poster B

Metal-Insulator Transition and Lattice Instability of Paramagnetic V_2O_3 — •I. Leonov[1], V. I. Anisimov[2,3], and D. Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]Ural Federal University, Yekaterinburg, Russia

We determine the electronic structure and phase stability of paramagnetic V_2O_3 at the Mott-Hubbard metal-insulator phase transition, by employing a combination of *ab initio* methods for calculating band structures with dynamical mean-field theory [1]. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and calculate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. The structural transformation associated with the metal-insulator transition is found to occur upon a slight expansion of the lattice volume by ~ 1.5 %, in agreement with experiment. Our results show that the structural change precedes the metal-insulator transition, implying a complex interplay between electronic and lattice degrees of freedom at the transition. Electronic correlations and full charge self-consistency are found to be crucial for a correct description of the properties of V_2O_3.

[1] I. Leonov, V. I. Anisimov, and D. Vollhardt, arXiv:1410.5399 (2014).

TT 71.71 Wed 15:00 Poster B

Investigating disorder effects in fabricating photonic quantum simulators on a kagome geometry: PEPS versus exact-diagonalization analysis — •Amin Hosseinkhani[1,2], Ali T. Rezakhani[3], and Hamed Saberi[4,5] — [1]Peter Grunberg Institute (PGI-2), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [3]Department of Physics, Sharif University of Technology, Tehran 14588, Iran — [4]Department of Optics, Faculty of Science, Palacký University, 17. listopadu 12, 77146 Olomouc, Czech Republic — [5]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), University of Paderborn, D-33098 Paderborn, Germany

The energy spectra and photon transfer dynamics of a unit kagome cell is being explored by using a flexible numerical framework. A projected-entangled pair state (PEPS) ansatz to the many-photon wave function allows us to gain a detailed understanding of the effects of undesirable disorder in fabricating well-controlled and scalable photonic quantum simulators. The correlation functions associated with the propagation of two-photon excitations reveal intriguing interference patterns peculiar to the kagome geometry. Our results justify the use of the proposed PEPS technique for addressing the role of disorder in such quantum simulators and promises sophisticated numerical machinery for yet further explorations of the scalability of the resulting kagome arrays.

TT 71.72 Wed 15:00 Poster B

Calculating atomic multiplets across the periodic table — •Qian Zhang and Erik Koch — German Research School for Simulation Sciences, 52428 Jülich

The calculation of the multiplet structure of atoms with open shells requires two main ingredients: (i) realistic Coulomb matrix elements and (ii) the construction of states with well defined total angular momentum and spin. For the first we perform density functional calculations for isolated atoms or ions to determine the Slater-integrals of the electron-electron repulsion. For the second we use a simple ladder operator method to construct the multiplet states. We have implemented this approach in a web based application that allows the interactive calculation of multiplets for any atom/ion in the periodic table. In addition we can include the effects of spin-obit coupling. This allows us to compare the perturbative Russell-Saunders L-S and j-j coupling schemes to the more accurate intermediate coupling in which Coulomb repulsion and spin-orbit coupling are treated on the same footing.

TT 71.73 Wed 15:00 Poster B

Single-Particle Green's Function from the time-dependent Gutzwiller Approximation — •Konstantin Hobuss, Jörg Bünemann, and Florian Gebhard — Universität Marburg, Fachbereich Physik, Renthof 6, 35037 Marburg

We calculate the single-particle Green's function of the single-band Hubbard model from the time-dependent Gutzwiller Approximation within a Lagrange formalism [1]. In our approach, we add an electron with fixed wave vector $\vec{k}$ which can be interpreted as a small perturbation of the system. The Euler-Lagrange equations yield the dynamics of the corresponding variational parameters caused by the small perturbation. For the special case of a half-filled paramagnetic ground state, we find oscillations of the double occupancy with a frequency $\Omega^2 = 16\varepsilon_0^2\left(1-u^2\right)$ where $u = U/U_{\mathrm{BR}}$ is the interaction strength in terms of the Brinkman-Rice energy and ε_0 is the energy per site of the noninteracting system. From the dynamics of the variational parameters, we can compute the single-particle Green's function for all frequencies. At small excitation energies, we recover previous results for the Gutzwiller quasi-particle dispersion [2].

[1] J. Bünemann et. al., *New J. Phys.* **15** (2013), 053050.
[2] J. Bünemann et. al., *Phys. Rev. B* **67** (2003), 075103.

TT 71.74 Wed 15:00 Poster B

Configuration Path Integral Monte Carlo Simulations of the

Degenerate Homogeneous Electron Gas at Finite Temperatures — •Tim Schoof, Simon Groth, Jan Vorberger, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts Universität zu Kiel, Germany

Quantum Monte Carlo simulations of the homogeneous electron gas (HEG) in the highly degenerate regime are generally hampered by the Fermion sign problem [1]. However, accurate data for thermodynamic properties over a full range of densities at finite temperatures are of great interest for many systems, including warm dense matter, and for numerical modeling serving as input to finite-temperature DFT calculations [2]. The Configuration PIMC (CPIMC) method does not suffer from the Fermion sign problem in the non-interacting limit and allows for efficient ab-initio simulations of the HEG at high densities ($r_s \leq 1$) and low to moderate temperatures ($T/T_F \leq 1$) [3]. Comparisons of the method with approximate results from Montroll-Ward and higher order pertubation theory and Restricted PIMC calculations will be presented.

[1] E. W. Brown, B. K. Clark, J. L. DuBois, and D. M. Ceperley, Phys. Rev. Lett. 110, 146405 (2013).
[2] V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, Phys. Rev. Lett. 112, 076403 (2014).
[3] T. Schoof, S. Groth, and M. Bonitz, Contrib. Plasma Phys. (2014), DOI: 10.1002/ctpp.20140072

TT 71.75 Wed 15:00 Poster B

Periodization in Cluster Dynamical Mean-Field Theory — •Malte Harland, Igor Krivenko, and Alexander Lichtenstein — Uni Hamburg, Hamburg, Germany

The Dynamical Mean Field Theory (DMFT) maps the lattice problem onto a single site coupled to an electron bath, i.e. the Mean Field. To include spatial correlations we use CDMFT, the cluster extension that connects a cluster of many correlated sites to an electron bath with a matrix-valued hybridization function. Whereas there is only one possible DMFT scheme for the single site, there are different schemes proposed for cluster calculations. They differ in the way they incorporate the lattice symmetry into the cluster calculation done by the impurity solver. We present a comparison of the self-energy and the cumulant periodization for different cluster sizes, applying it to a 1-dimensional chain as well as to the frustrated Kagome lattice. The CDMFT scheme we use is formulated in the real space. We solve the Hubbard cluster impurity model within a Hybridization Expansion Quantum Monte Carlo solver and compare the lattice Green's function and the local density of states to results of the Density Matrix Renormalization Group method.

TT 71.76 Wed 15:00 Poster B

Electronic correlations at the two-particle level: from bulk to the nanoscale — •Angelo Valli[1,2], Thomas Schäfer[2], Patrik Thunström[2], Georg Rohringer[2], Sabine Andergassen[3], Giorgio Sangiovanni[4], Karsten Held[2], and Alessandro Toschi[2] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Of- ficina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy — [2]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [3]Institute for Theoretical Physics and CQ center for collective quantum phenomena, University of Tübingen, Tübingen, German — [4]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

We discuss the properties of local two-particle vertex functions within the framework of dynamical mean-field theory (DMFT). Their knowledge is required, e.g., to compute the local vertex corrections to dynamical response functions, and in order to include non-local spatial correlations within diagrammatic extensions of DMFT. Within the dynamical vertex approximation (DΓA) non-local spatial correlations can be generated by the (self-consistent) numerical solution of the parquet equations. This allows to treat fluctuations in all particle-hole and particle-particle scattering channels on equal footing, and to describe their interplay. As an application, we show how the information enclosed in the local vertex of DMFT can be exploited to *disentangle* the role of local and non-local correlations in Hubbard nano clusters.

TT 71.77 Wed 15:00 Poster B

Kinks and low-energy dynamics of correlated electron systems — •Markus Greger and Marcus Kollar — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

We present a physical interpretation of kinks in the effective dispersion seen in angle-resolved photoemission spectroscopy (ARPES) within the framework of dynamical mean-field theory (DMFT). We relate the energy scale of kinks to the binding energy of the local quasiparticles, i.e., Kondo singlet. This interpretation of kinks provides a direct connection to an important intrinsic property of the quasiparticles in Fermi liquids. The Kondo singlet wavefunction is further characterized using the density matrix renormalization group (DMRG).

TT 71.78 Wed 15:00 Poster B

Development and Application of Full Configuration Interaction Quantum Monte Carlo Techniques for Strongly Correlated Electron Lattice Models — •Werner Dobrautz — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Applications of Quantum Monte Carlo techniques to strongly correlated electron lattice models, like the Hubbard model, are severely hindered by the existence of the renowned sign problem.

In diffusion Monte Carlo methods this problem can be avoided by imposing a certain nodal structure on the emerging ground state solution. This necessary prior knowledge is not needed in the recently developed Full Configuration Interaction Monte Carlo algorithm, but emerges during a simulation due to its formulation of particle dynamics in a fully anti-symmetrized space of Slater determinants. But the ensure convergence to the correct ground state a cancellation of positive and negative weighted particles on Slater determinants during simulation has to happen. But the required amount of simulated particles heavily depends on the chosen single-particle basis functions in which the Slater determinants are constructed.

The unitary group approach to the non-relativistic electron problem allows us to efficiently formulate the FCIQMC method in the space of eigenfunctions of the spin operator S. This not only greatly decreases the Hilbert space size of the problem, but also allows us to restrict solutions to specific total spin quantum numbers.

TT 71.79 Wed 15:00 Poster B

Non-local spin correlations in strongly interacting electron systems — •Friedrich Krien[1], Erik G. C. P. van Loon[2], Hartmut Hafermann[3], A.N. Rubtsov[4], and A.I. Lichtenstein[1] — [1]I. Institute of theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands — [3]Institut de Physique Theorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France — [4]Department of Physics, Moscow State University, 119991 Moscow, Russia

We investigate a modified Hubbard model with non-local spin-spin coupling by means of EDMFT and the recently developed Dual Boson approach. Severe complications in the underlying impurity model are circumvented by coupling impurity spins only to spin waves along the z-axis. We develop and apply an approximation to optimally recover the impurity susceptibilities of the desired rotationally invariant system.

TT 71.80 Wed 15:00 Poster B

Spin-orbit coupling and its influence on the competing orders in the functional renormalization group method — •Mario Fink, Christian Platt, Werner Hanke, and Ronny Thomale — Institut für Theoretische Physik und Astrophysik Fakultät für Physik und Astronomie Am Hubland D - 97074 Würzburg, Germany

The effect of spin-orbit coupling plays an essential role in current research on topological insulators and topological superconductivity. To investigate the influence of spin-orbit coupling on the competing orders of quantum many-body systems, the functional renormalization group (FRG) seems to be one method of choice. We present an extended FRG method, which incorporates a spin-dependent formulation of the FRG flow equations. The unconventional superconductor Sr_2RuO_4 is considered one candidate system which exhibits an intricate interplay between spin-orbit interactions and competing many-body instabilities. In this context, our method is capable of testifying e.g. the symmetry and the origin of the superconducting gap on the α, β, and γ bands.