# TT 79: Correlated Electrons - Poster Session

Time: Wednesday 15:00–19:00 Location: P2

TT 79.1 Wed 15:00 P2

**Electron Spin Resonance in $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ below 1 K** — Ilshat Fazlishanov[1,4], •Zakir Seidov[1,5], Jörg Sichelschmidt[2], Hans-Albrecht Krug von Nidda[1], Cornelius Krellner[3], Christoph Geibel[2], Frank Steglich[2], and Manuel Brando[2] — [1]Experimental Physics V, EKM, University of Augsburg, 86159 Augsburg — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [3]Institute of Physics, Goethe University Frankfurt, 60438 Frankfurt am Main — [4]E.K.Zavoisky Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [5]Institute of Physics, Azerbaijan National Academy of Sciences, AZ-1143 Baku, Azerbaijan

We report Electron Spin Resonance (ESR) experiments on the heavy-fermion metal $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ in the temperature range $0.75K \leq T \leq 4K$. The ESR measurements were performed at X-band frequencies using a home-built 3He cryostat. We found that below 1.3K the ESR spectra of $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ split into two lines. Such a behavior can be explained by the strong anisotropy of the ferromagnetic ground state in agreement with magnetization measurements [1].

[1] S. Lausberg, A. Hannaske, A. Steppke, L. Steinke, T. Gruner, L. Pedrero, C. Krellner, C. Klingner, M. Brando, C. Geibel, F. Steglich, Phys. Rev. Lett. **110**, 256402 (2013)

TT 79.2 Wed 15:00 P2

**Heavy fermion behaviour and structural change in high pressure $CeSb_2$** — Zhuo Feng[1], •Yang Zou[1], Terence Giles[2], Philipp Niklowitz[2], Heribert Wilhelm[3], Giulio I. Lampronti[4], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Dep. of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK — [3]Beamline I15, Diamond Light Source, Didcot OX11 0DE, UK — [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 transition 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 9 K and 12 K [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 $p_c$. Whereas in the low pressure structure, $CeSb_2$ is local moment magnet, in the high pressure structure it exhibits tranport 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 79.3 Wed 15:00 P2

**de Haas-van Alphen oscillations in (La,Ce)$TiGe_3$** — R. Seerig[1,5], •M. Uhlarz[1], W. Kittler[2], V. Fritsch[2], O. Stockert[3], T. Förster[1], P. Canfield[4], J. Wosnitza[1,5], and H. v. Löhneysen[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [4]Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA — [5]Institut für Festkörperphysik, TU Dresden, 01062 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 hexagonal perovskite structure [1, 2]. We report on de Haas-van Alphen (dHvA) oscillations in single crystals grown from Ge flux, measured in magnetic fields up to 13 T in a cantilever-type torque magnetometer. We found four dHvA frequencies ranging from 60 T to 4300 T, with effective masses between $0.31\,m_0$ and $1.31\,m_0$, featuring a comparatively weak angular dependence. Further, we give an interpretation of our results on the basis of DFT calculations of the electronic bandstructure of $LaTiGe_3$.

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

TT 79.4 Wed 15:00 P2

**Evolution of ferromagnetic correlations in $FeGa_{3-x}Ge_x$ probed by $^{69,71}$Ga nuclear quadrupolar resonance** — •M. Majumder, M. Wagner-Reetz, P. Khuntia, Yu. Grin, and M. Baenitz — Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany

Binary Fe based semimetals like FeSi, $FeSb_2$ and $FeGa_3$ earned great attention because of their unconventional ground state (possible Kondo insulators) and good thermoelectric performance. Metallic behavior and Fe based magnetism can be introduced by various substitutions. In contrast to $FeSb_2$ (where Te substitution results in a disorder dominated Griffiths phase) [1], the system $FeGa_3$ seems to be an ideal candidate to study the evolution of ferromagnetic quantum criticality (FMQC) by magnetic resonance. Recently it was shown that Fe(Ga, $Ge)_3$ develops FMQC behavior without strong disorder effects [2,3]. The nuclear quadrupolar resonance (NQR) spectra provide direct information about the degree of local disorder (line width) and the critical fluctuations at the verge of FM ordering (spin lattice relaxation at zero field). In $FeGa_3$ four NQR lines have been found, of which two lines are from the two Ga sites in the crystal structure and other two are due to the two Ga isotopes [4]. $^{69,71}$Ga NQR investigation have been performed in $FeGa_{3-x}Ge_x$ polycrystalline sample with $x$=0.1 (absent magnetic order), 0.2 ($T_C \simeq 6$ K) and $x_c \approx 0.15$ (critical concentration for FMQC).

[1] Phys. Rev. Lett. **109**, 256401 (2012)
[2] Phys. Rev.B **86**, 144421, (2012)
[3] arXiv: 1304.1897 (2013)
[4] arXiv: 1311.1501 (2013)

TT 79.5 Wed 15:00 P2

**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], 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 79.6 Wed 15:00 P2

**Phase diagram of the effective Ising spin-1/2 chain system $CoNb_2O_6$ in transverse magnetic field and comparison with the 1D Ising model** — •Victoria Cho[1], Simon Scharffe[1], Oliver Breunig[1], Martin Valldor[1], Markus Garst[2], Eran Sela[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Insitut für Theoretische Physik, Universität zu Köln

$CoNb_2O_6$ is a model system to investigate the quantum phase transition of Ising spins in a transverse magnetic field. The interesting physics exclusively takes place within the magnetic $CoO_6$ layers, separated by non-magnetic $NbO_6$ layers. The edge-sharing oxygen octahedrons link the $Co^{2+}$spins and form 1D ferromagnetic chains along the $c$ axis. Due to crystal field effects an easy-axis anisotropy is present, which leads to an effective spin-1/2 system described by the Ising model. Small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$ cause long-range antiferromagnetic order, which is incommensurate below $T_{N1}$=2.95 K and becomes commensurate at $T_{N2}$=1.97 K. A magnetic field parallel to the $b$ axis is normal to the easy axis and allows to study the

quantum phase transition in transverse field. Above 5 T the system is driven through its quantum critical point to a quantum paramagnet. Only few studies of the transverse field case are available. We present measurements of specific heat and magnetization in a temperature range from about 0.3 up to 10 K and discuss the phase diagram. We compare our measurements with the theoretical predictions of the 1D Ising model in a transverse field.

This work was supported by the DFG through SFB 608.

TT 79.7 Wed 15:00 P2

**Magnetic excitations in quantum-critical Ce($Pd_{0.86}Ni_{0.14}$)Al** — •O. Stockert[1], K. Schmalzl[2], V. Fritsch[3], and H. v. Löhneysen[3] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France — [3]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

The heavy-fermion compound CePdAl offers the opportunity to study quantum criticality in the presence of geometrical frustration. The antiferromagnetic order in CePdAl decreases strongly when substituting nickel for palladium and a quantum critical point is approached in $CePd_{1-x}Ni_xAl$ for $x = 0.14$. We performed extensive inelastic neutron scattering to study the low-energy magnetic excitations in $Ce(Pd_{0.86}Ni_{0.14})Al$, i.e., the alloy where magnetic order is just suppressed. We find spin fluctuations being broad in $q$-space indicating only short-range dynamic spin correlations. We discuss their $q$-space and temperature dependence and will compare the results to the spin excitations in the magnetically ordered parent compound CePdAl.

TT 79.8 Wed 15:00 P2

**Hidden energy scale in CePdAl** — Chien-Lung Huang[1], Kai Grube[1], •Christian Taubenheim[1], Veronika Fritsch[1], Sarah Woitschach[2], Zita Huesges[2], Oliver Stockert[2], and Hilbert v. Löhneysen[1] — [1]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

CePdAl is a partially geometrically-frustrated heavy-fermion antiferromagnet with a Néel temperature $T_N = 2.7\,K$ crystallizing in the hexagonal ZrNiAl structure. We measured the thermal expansion $\alpha_{a,c}$ and the magnetostriction $\lambda_{a,c}$ along both crystallographic axes in the temperature range of $0.02\,K \leq T \leq 10\,K$ and magnetic fields of up to 14 T. From $\alpha_{a,c}$ and $\lambda_{a,c}$ we derive the $T$-$B$ phase diagram below 1 K. Across the magnetic phase boundaries into the paramagnetic state $\alpha_{a,c}/T$ shows a peak moving to $T \to 0$ at $B^* = 3.5\,T$, which is concomitant with maxima in $\lambda(B)$, entropy $S(B)$, and magnetic susceptibility $\chi(B)$. This suggests a possible hidden energy scale in CePdAl, which might be tuned by applying pressure. To this end, we investigated the pressure dependence of the magnetization and performed magnetoresistivity measurements between $1.8\,K \leq T \leq 10\,K$ and $B \leq 5\,T$. As a first result the pressure dependence is found to be very weak, since $\alpha_a$ and $\alpha_c$ have opposite signs. This explains the different values for $T_N$ found in literature.

TT 79.9 Wed 15:00 P2

**Effect of Ni-doping on the geometrically frustrated heavy-fermion system CePdAl** — •Stefan Lucas[1], Zita Huesges[1], Sarah Woitschach[1], Oliver Stockert[1], Veronika Fritsch[2], and Hilbert von Löhneysen[2] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The heavy-fermion compound CePdAl is an interesting system for investigations of quantum criticality in combination with geometric magnetic frustration, which arises from the hexagonal crystal structure of the system. In zero magnetic field, the Néel temperature of 2.7 K can be reduced by doping nickel on the palladium sites. At a doping level of about 14 %, the Néel temperature becomes zero and a quantum critical point is reached. To follow the magnetic order upon nickel doping and investigate the effect of magnetic frustration closer to the quantum critical point, we performed extensive heat capacity measurements on a 5 % Ni-doped single crystal. $CePd_{0.95}Ni_{0.05}Al$ orders below $T_N \approx 1.85\,K$ via a second-order phase transition in contrast to the weakly first-order transition in pure CePdAl. Our measurements reveal for $CePd_{0.95}Ni_{0.05}Al$ a critical magnetic field $B_C \approx 3\,T$ ($B \parallel c$, $T \to 0$) to fully suppress the antiferromagnetic phase. We will discuss the resulting magnetic $B-T$ phase diagram and compare it with the parent compound CePdAl.

TT 79.10 Wed 15:00 P2

**QPI in singlet, triplet and non-centrosymmetric unconventional superconductors** — •Alireza Akbari[1] and Peter Thalmeier[2] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]MPI for the Chemical Physics of Solids, Dresden, Germany

The technique of quasiparticle interference (QPI) has recently been successfully applied to heavy fermion compounds to determine the unconventional superconducting gap symmetry. It was proposed [1] and proven [2,3] that QPI can distinguish between the d-wave singlet candidates of superconducting $CeCoIn_5$. The QPI theory has now also been developed for non-centrosymmetric (NCS) superconductors [4] with mixed singlet-triplet gap function. Qualitatively new effects in the QPI pattern originate from Rashba spin-orbit coupling: Distinct differences between charge- and spin QPI and anisotropies appear due to additional Rashba coherence factors. We use Born approximation and full t-matrix theory to calculate the QPI spectrum and apply it to a 2D model for the NCS heavy fermion unconventional superconductor $CePt_3Si$. We discuss the new QPI features for a gap model with accidental node lines due to its composite singlet-triplet nature. Furthermore we predict the quasiparticle interference spectrum for the multiband chiral p-wave superconductor $Sr_2RuO_4$ [5] and the possible chiral d-wave superconductor SrPtAs.

[1] A. Akbari et al, PRB 84 , 134505 (2011)
[2] M. P. Allan et al, Nat. Phys. 9, 468 (2013)
[3] B. B. Zhou et al, Nat. Phys. 9, 474 (2013)
[4] A. Akbari and P. Thalmeier, EPL, 102, 57008 (2013)
[5] A. Akbari and P. Thalmeier, PRB 88, 134519 (2013)

TT 79.11 Wed 15:00 P2

**Theory of Magnetic Excitations in Van Vleck-type Mott insulator on Square Lattice** — •Alireza Akbari and Giniyat Khaliullin — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

We study magnetism in Van Vleck-type $d^4$ Mott insulators with square lattice symmetry. A theory includes the exchange interactions, tetragonal crystal field splitting, and spin orbit coupling. We found two different magnetic phases, with in-plane and out-of-plane magnetization for the higher and lower values of the crystal field splitting, respectively. We calculated the excitation spectra for paramagnetic and two magnetically ordered phases. The results are discussed in the context of $d^4$ Mott insulator $Ca_2RuO_4$.

TT 79.12 Wed 15:00 P2

**Magnetostriction and thermal expansion of the triple-layered $Sr_4Ru_3O_{10}$ System** — •W. Schottenhamel[1], R. Fittipaldi[2], A. Vecchione[2], A.U.B. Wolter[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany — [2]Univ. Salerno, Dipartimento Fis ER Caianiello, I-84084 Fisciano, Italy

$Sr_4Ru_3O_{10}$ is a member of the $(Sr,Ca)_{n+1}Ru_nO_{3n+1}$ Ruddlesden Popper series and displays spontaneous ferromagnetism at $T_c \sim 102\,K$ along the c axis coexisting with orbital-dependent intralayer metamagnetism around $T^* \sim 50\,K$ [1]. Since a strong spin-phonon coupling has been proposed in this material, we performed detailed thermodynamic investigations by means of dilatometry as well as by SQUID magnetometry under pressure. Measurements of magnetostriction, thermal expansion and magnetization were performed on single crystalline samples in the temperature range $T = 2$–$200\,K$ at magnetic fields up to 15 T. The crystal expansion exhibits a highly anisotropic behavior. Signatures of the ferromagnetic phase-transition were found for both directions. Further distinct anomalies are visible in the lower temperature region, which could be correlated to the metamagnetic transition at $T^*$. By combining the changes of the thermal expansion and the heat-capacity at the ferromagnetic transition, a strong volumetric pressure dependence of $dTc/dp \sim$ -8 K/ GPa has been revealed. Additional measurements of magnetization under hydrostatic pressure have been done in order to verify this big negative value.

[1] V. Granata et. al., J. Phys.: Cond. Mat. 25 (2013) 056004

TT 79.13 Wed 15:00 P2

**Realistic Calculation of Optical Spectra of Layered Ruthenates** — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

Within the LDA + dynamical mean field theory, the optical conductivity of layered ruthenates is investigated for various temperatures, in the framework of linear response theory and Kubo's formalism. The anisotropic properties of charge dynamics and temperature dependence

of in-plane and out-of-plane conductivity are studied. The effect of spin-orbit coupling in the spectrum is considered.

TT 79.14 Wed 15:00 P2

**Ab initio study of electronic correlation in $SrRuO_3$** — •Liang Si, Zhicheng Zhong, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

4d ferromagnetic oxide $SrRuO_3$ (SRO) has a great potential for future oxide electronic device applications, so the deep understanding and masterful control are important to its development and application. The ferromagnetic-to-nonmagnetic and metal-to-insulator transitions in SRO thin film, which depend on film thickness, are fancy properties, whereas there is no conclusion whether such two transitions are intrinsic properties because both DFT and DFT+U methods fail in simulation of such experimentally observed ferromagnetic-to-nonmagnetic and metal-to-insulator transitions. We employed DFT+DMFT method to study the electronic structures of SRO in bulk and thin film systems in order to explain the experimentally observed transitions at thin film. According to our calculations we suggest the following two conclusions regarding the experimentally observed transitions: firstly, both transitions in SRO thin films are intrinsic properties due to strongly electronic correlation rather than surface relaxation and defects effect, secondly, dynamic mean filed theory is necessary in studying of transition metal oxides especially for interface or thin film systems.

TT 79.15 Wed 15:00 P2

**Critical scaling analysis of the itinerant ferromagnet $Sr_{1-x}Ca_xRuO_3$** — •Dirk Fuchs, Markus Wissinger, Jörg Schmalian, Chien-Lung Huang, Rudolf Schneider, and Hilbert von Löhneysen — Karlsruhe Institute of Technology, Karlsruhe, Germany

The critical behavior of $Sr_{1-x}Ca_xRuO_3$ was investigated by a scaling analysis based on the Arrott-Noakes equation of state. The critical exponents $\beta$, $\gamma$, and $\delta$ of the magnetic critical behavior were extracted for samples with $0 \leq x \leq 0.6$. The ferromagnetic system exhibits a smooth suppression of the Curie temperature $T_C$ to zero at a critical concentration $x_c \approx 0.7$. For $x = 0$, mean-field like exponents are observed. With increasing $x$ the critical exponents $\beta$, $\gamma$, and $\delta$ change nearly linearly from $\beta \approx 0.5$, $\gamma \approx 1$ and $\delta \approx 3$ for $x = 0$ to $\beta \approx 1$, $\gamma \approx 0.9$ and $\delta \approx 1.6$ for $x \approx 0.6$. Despite the systematic evolution of the critical exponents as a function of $x$ the exponents can not be described by a universality class of known classical standard models.

TT 79.16 Wed 15:00 P2

**Doping Induced Spin State Transition in $LaCoO_3$: Dynamical Mean-Field study** — •Pavel Augustinsky[1], Vlastimil Krapek[1,2], and Jan Kunes[1] — [1]Institute of Physics, ASCR, Prague, Czech Republic — [2]CEITEC, Brno Univesity of Technology, Czech Republic

Hole and electron doped $LaCoO_3$ is studied using dynamical mean-field theory. The one-particle spectra are analyzed and compared to the available experimental data, in particular the x-ray absorption spectra. Analyzing the temporal spin-spin correlation functions we find the atomic intermediate spin state is not important for the observed Curie-Weiss susceptibility. Contrary to the commonly held view about the roles played by the $t_{2g}$ and $e_g$ electrons we find narrow quasiparticle bands of $t_{2g}$ character crossing the Fermi level accompanied by strongly damped $e_g$ excitations.

TT 79.17 Wed 15:00 P2

**Excitonic instability in Two-Band Hubbard Model** — •Pavel Augustinsky and Jan Kunes — Institute of Physics, ASCR, Prague, Czech Republic

We report a newly observed instability in the two-band Hubbard model close to the spin-state transition [1]. Using unbiased search for the particle-hole instabilities in DMFT, we found that the earlier observed high-spin low-spin checker-board order is competing with the excitonic phase characterized by condensed spinful excitons. We present both numerical results and an analytic description in the strong-coupling limit.

[1] arXiv:1310.0669

TT 79.18 Wed 15:00 P2

**Signatures of electronic correlations in half-metals** — •Markus Dutschke[1], Liviu Chioncel[1,2], and Junya Otsuki[1,3] — [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

The distinctive feature of the electronic correlations in half-metals is the existence of Non-quasiparticle states, within the half-metallic gap, predicted previously in model as well as realistic LDA+DMFT calculations. We revisit this problem considering a simplified Hubbard model solved in DMFT using the CT-QMC impurity solver. In the same time we present an implementation of the hybridization expansion quantum impurity solver, based on the segment representation.

TT 79.19 Wed 15:00 P2

**Bulk and interface half-metallicity in heterostructures based on $Co_2MnAl$** — •Andreas Held[1], Kathrin Garb[1], Igor Di Marco[2], Stanislav Chadov[3], and Liviu Chioncel[1,4] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We study electronic correlation effects in bulk $Co_2MnAl$ and ($Co_2MnAl$/CoMnVAl) heterostructures within a combined density functional and Dynamical Mean Field Theory. We analyze the changes in the topology of the bulk Fermi surface as well as in the electronic properties by approaching the interface via a function of temperature and the strength of the local Coulomb interaction U.

TT 79.20 Wed 15:00 P2

**Importance of electronic correlations for the phase stability of $V_2O_3$** — •Ivan Leonov and Dieter Vollhardt — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

We report results for $V_2O_3$ obtained by a novel implementation of the LDA+DMFT approach for the computation of the total energy of materials with strongly interacting electrons. It includes a fully self-consistent calculation of the charge density, whereby correlation-induced changes in the effective Kohn-Sham Hamiltonian are taken into account. This scheme is employed to study the electronic structure and phase stability of $V_2O_3$ near a pressure-induced Mott-Hubbard metal-insulator transition. 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. In agreement with experiment, we observe that the metal-insulator transition is accompanied by a remarkable change of the $c/a$ ratio. Full charge self-consistency is shown to be important to understand the phase stability of $V_2O_3$ near the Mott-Hubbard metal-insulator phase transition.

TT 79.21 Wed 15:00 P2

**The correlated semiconductor $CrSb_2$** — •Anna Galler, Jan Tomczak, and Karsten Held — Institut für Festkörperphysik, Technische Universität Wien

Intermetallic-based correlated semiconductors display an intriguing temperature dependence in their physical properties: while at high temperatures a Curie-Weiss-like susceptibility develops, a regime of notably large thermopower is found at low temperatures. Between the two regimes optical spectra exhibit large transfers of spectral weight.

Here, we present a theoretical many-body study for a member of this class of materials: $CrSb_2$. We compute interaction matrix elements from first principles using the constrained random-phase-approximation (cRPA) and study many-body spectra and response functions within LDA+DMFT (local density approximation combined with dynamical mean field theory).

TT 79.22 Wed 15:00 P2

**Real-Time Dynamics in Bose-Fermi Impurity Models** — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We consider the real-time dynamics in a nano-device coupled to a

fermionic lead and subject to additional charge noise or coupling to a phononic bath. We have extended the recently adopted numerical renormalisation group (NRG) to Bose-Fermi models in equilibrium to non-equilibrium quenches by employing the time-dependent NRG. It is known that such Bose-Fermi models show very rich physics in equilibrium manifested in a variety of different fixed points governing the phase transitions between different ground states. We present relaxation rates of different physical properties such as the local occupancy or spin polarisation across the quantum phase transition between the localised/delocalised phases in the Bose-Fermi Kondo model as well as in the more general Bose-Fermi Anderson model.

TT 79.23 Wed 15:00 P2

**Magnetic phase-diagram of the spin-diluted Kondo-lattice model** — •Matthias Peschke, Maximilian Aulbach, and Michael Potthoff — Universität Hamburg I. Institut für Theoretische Physik, Hamburg , Germany

We analyze the magnetic phase diagram of the spin-diluted Kondo-lattice model for strong antiferromagnetic Kondo couplings $J$ and fillings ranging from quarter filling down to the magnetic-polaron limit with a single conduction electron. This range of electron densities permits to employ the Lanczos method for systems consisting of a moderate number of lattice sites and local spins. At quarter filling, and for a "diluted" system where every second site of the conduction-electron system couples to a local quantum spin $s = 1/2$, the formation of almost local Kondo singlets results in a non-magnetic ground state. For low densities we expect a state with magnetic long-range order of the local spins mediated by extremely heavy polarons. In the single conduction-electron limit, an almost fully polarized ferromagnet is enforced by a generalized Lieb-Mattis theorem. While the size of the Kondo clouds is predominantly controlled by $J$, the polaron size is additionally determined by the degree of spin dilution. We study the crossover from polaron-mediated magnetism to a non-magnetic state with local spins screened individually for different degrees of dilution and for different $J$ in the strong-coupling regime.

TT 79.24 Wed 15:00 P2

**Multi-Fermi Points in the Kondo-vs.-RKKY Quantum Box** — •Mirek Hänsel, Andrej Schwabe, and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Germany

The competition between the Kondo effect and the indirect (RKKY) magnetic exchange is studied for nanoscale systems where, besides the Kondo temperature and the RKKY coupling, the finite-size gap represents a third relevant energy scale.

As has been shown recently [1] for the typical "on resonance" case with a single electron at the non-degenerate Fermi level, a Kondo-type screening of an impurity spin is possible, depending on the system's geometry. This leads to an unconventional Kondo-vs.-RKKY competition with a re-entrant behavior that manifests itself in an unusual J dependence of spin correlations and a total ground-state spin deviating from the predictions of standard RKKY theory.

Here, we extend our studies by applying the density-matrix renormalization group as well as weak-coupling perturbation theory to multi-impurity Kondo models on confined one- and two-dimensional lattices where the conduction-electron system has a degenerate Fermi level. In this case and for weak J, the system is perturbatively mapped onto an effective central-spin model where typically each impurity spin couples to a different itinerant spin in the central region. We discuss the geometry dependence of the effective couplings and the resulting magnetic structure.

[1] A. Schwabe, D. Gütersloh and M. Potthoff, Phys. Rev. Lett. 109, 257202 (2012).

TT 79.25 Wed 15:00 P2

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

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

TT 79.26 Wed 15:00 P2

**Exact diagonalization techniques for strongly correlated systems** — •Sareh Motahari and David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Gaining an understanding of strongly correlated electron materials and nanoscale devices is one of the main challenges of condensed matter physics. One of the most important models in this context is the Anderson impurity model which is central to the understanding of the Kondo effect [1] and is at the heart of the Dynamical Mean-Field Theory [2]. Here we explore different techniques based on exact diagonalization of finite Anderson models for the description of strong correlations in nanoscale systems and molecules with transition metal centers. In particular, we explore the use of the novel Distributional Exact Diagonalization [3] method for the description of the Kondo effect in realistic systems.

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TT 79.27 Wed 15:00 P2

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

Wilson's Numerical Renormalization Group (NRG) allows to describe many quantum impurity problems in equilibrium. But it remains a challenge to extend the use of NRG to situations of steady-state non-equilibrium, such as current through a quantum dot at finite bias. In our approach we consider additional baths coupled to the fermionic leads of the given impurity problem. The effect of these additional baths on the leads can be described by using Lindblad operators [1,2] in the Liouville equation for the density matrix of the dot and the leads. To efficiently solve the Liouville equation we use the stochastic quantum trajectory method [2].

Here we present first results how the Lindblad operators could be chosen to hold the leads in thermal equilibrium at a specific chemical potential and temperature and how the quantum trajectory method can be implemented in terms of time-dependent NRG based on complete basis sets.

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TT 79.28 Wed 15:00 P2

**The Numerical Renormalization Group as impurity solver within the Dynamical Mean-Field - Theory for multi-band lattice models** — •Katharina Stadler, Andreas Weichselbaum, and Jan von Delft — Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center of NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Dynamical Mean-Field Theory (DMFT) provides a non-perturbative many-body approach to describe the local dynamics of strongly correlated materials by mapping a lattice model self-consistently onto an effective quantum impurity model, which is then solved by a non-perturbative method, such as Quantum Monte Carlo simulations (QMC) or the Numerical Renormalization Group (NRG) approach.

Here, we use NRG as DMFT impurity solver to treat multi-band models. Typically, the application of NRG in this context is strongly limited since the numerical cost increases exponentially with the number of bands. To deal with this limitation, we investigate two strategies: First, for multi-band models with intrinsic symmetries, we implement these explicitly in our numerical code using non-abelian channel symmetries [1] where applicable. Second, for models without symmetries we investigate the feasibility of using interleaved Wilson chains, as recently proposed [2]. We also test the reliability of the latter method

by applying it to models with symmetries and comparing the results to those obtained by the explicit treatment of the non-abelian channel symmetry.
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TT 79.29 Wed 15:00 P2

**Charge order and frustration in two-dimensional Falicov-Kimball models** — •YOUNES JAVANMARD, ANDREY ANTIPOV, PEDRO RIBEIRO, and STEFAN KIRCHNER — Max Planck Institute for Physics of Complex Systems, Nöthnitzer Str 38, 01187 Dresden, Germany

The Falicov-Kimball model is frequently employed in a number of contexts ranging from the melting of charge order to the metal-insulator transition. Its popularity is in part due to its solvability in the limit of infinite coordination number, i.e. within the Dynamical Mean Field Theory (DMFT).

At sufficiently large interaction strength the Falicov-Kimball model can be mapped to an Ising model on the same lattice. On the square lattice at half-filling, the DMFT fails to capture the interacting nature of the charge-ordering transition and predicts a continuous transition of mean-field character for all coupling strengths. In contrast, a recent study suggest the transition of the two-dimensional square lattice to be of first order at small interaction strength [1].

We set up a Monte Carlo algorithm for the two-and three-dimensional Falicov-Kimball model and study the nature of the transition in the half-filled Falicov-Kimball model on the square lattice and extend the study to lattice types allowing for geometrical frustration, like the triangular lattice [2].
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[2] M. Zonda, P. Farkasovsky, H. Cecarikova, Sol. State Comm. 149 (2009).

TT 79.30 Wed 15:00 P2

**Optimizing Matrix Product State Codes Using SciPAL: Parallelisation and GPU Portability** — •THOMAS KÖHLER[1], JOHANNES HAGEMANN[2], SALVATORE R. MANMANA[1], and STEPHAN C. KRAMER[3] — [1]Institut f. Theoretische Physik, Universität Göttingen — [2]Institut f. Röntgenphysik, Universität Göttingen — [3]Max-Planck-Institut f. biophysikalische Chemie, Göttingen

We apply the SciPAL library [1] to matrix product states (MPS), as used in the context of density-matrix renormalization group (DMRG) methods, which are important tools for treating low-dimensional strongly correlated quantum systems as realized in certain materials like quantum magnets (e.g. Azurite) and typically described by Hubbard-like or Heisenberg models. SciPAL (scientific parallel algorithms library) is a C++-based, hardware-independent open-source library, compatible with the widely used finite element library deal.II. By its link to CUDA, it provides the flexibility to extend existing codes to work on graphics processors. SciPAL's core asset is a user-friendly API to BLAS and NVidia's CUBLAS which allows to use an operator-based formulation of typical linear algebra operations. We discuss the extension of SciPAL to a domain-specific formulation of the numerical methods for computing the properties of MPS and their performance on graphics cards. A. K. Mitchell et al. [1] SciPAL: Expression Templates and Composition Closure Objects for High Performance Computational Physics with CUDA and OpenMP, S. C. Kramer and J. Hagemann, submitted to ACM TOPC.

TT 79.31 Wed 15:00 P2

**Accelerations of Diagrammatic Determinantal Quantum Monte Carlo Calculations using GPUs** — •MARKUS SCHMITT[1], IAIN BETHUNE[2], and THOMAS PRUSCHKE[3] — [1]Georg-August-Universität, Göttingen, Germany — [2]EPCC (University of Edinburgh), Edinburgh, UK — [3]Georg-August-Universität, Göttingen, Germany

Diagrammatic Determinantal Quantum Monte Carlo (DDQMC) algorithms are used to solve quantum impurity models such as the Anderson model. The calculation of acceptance rates and observables during the Monte Carlo walk involves linear algebra operations whose computational expense increases with decreasing temperature. Thus, the lower boundary of the treatable temperature range is limited by the available compute capacity. In order to make use of GPUs as cheap and powerful accelerators parts of a DDQMC code were ported to CUDA. The measurement of the observables turned out to be well suited for acceleration on GPUs and a speedup of more than 100 times over the unaccelerated version was obtained for the largest problem size under consideration.

TT 79.32 Wed 15:00 P2

**Superconducting gap at a ferromagnetic quantum critical point** — •MATTHIAS EINENKEL[1], HENDRIK MEIER[2], CATHERINE PÉPIN[3], and KONSTANTIN B. EFETOV[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Department of Physics, Yale University, New Haven, CT 06520, USA — [3]IPhT, CEA-Saclay, L'Orme des Merisiers, 91191 Gif-sur-Yvette, France

We discuss the quantum critical behaviour of a two-dimensional quantum ferromagnet in the context of the spin-fermion model. In this system fermions interact with critical bosonic excitations. We investigate the system by first performing a mean-field analysis, and show that close to the quantum critical point a superconducting gap appears which has spin triplet symmetry. Further, we calculate the action of the Goldstone modes associated with this symmetry breaking and derive a non-linear sigma model. These fluctuations turn out to be not suppressed by any small parameter and therefore eventually destroy the order. This reveals the failure of the large N expansion which was reported by previous works.

TT 79.33 Wed 15:00 P2

**Disorder-driven Coulomb gas transitions** — •STEFAN WOLFF and SIMON TREBST — Institut for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Coulomb gases with power-law correlations emerge as effective low-temperature description of various frustrated magnets where the low-temperature states obey certain local constraints. An even more direct realization of a Coulomb phase is provided by close-packed dimer models on bipartite lattices. Here we report results from extensive numerical simulations of such dimer models, where we study the characteristics of the phase transition induced by static disorder of the lattice, i.e. site and/or bond percolation.

TT 79.34 Wed 15:00 P2

**LDA+Slave-Boson Mean-Field Theory: itinerant electrons, magnetism and dynamics in realistic materials with multi-orbital degrees of freedom** — •CHRISTOPH PIEFKE, MALTE BEHRMANN, and FRANK LECHERMANN — Uni Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) in combination with the LDA framework is used to investigate strongly interacting systems [2]. In a tailored correlated subspace the multi-orbital Hubbard Hamiltonian is mapped onto an itinerant quasiparticle part and localized bosonic degrees of freedom. This decouples complex interactions (e.g. spin-flip, pair-hopping, spin-orbit coupling), quartic in the original electron operators, at the cost of a set of constraints. At saddle-point, a self-consistent mean-field solution is obtained. With rigorous derivation of the slave-boson formalism by matrix calculus over complex numbers and group theory, we show how to reduce the number of parameters in our functional. The connection to similar approaches within the Gutzwiller formalism [2] will be discussed. Finally, we also investigate the dynamical behaviour of quasiparticles and multiplets after sudden changes of interaction parameters via the time-dependent extension of the RISB method [3].
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[2] N. Lanatà, H. Strand, X. Dai, B. Hellsing, Phys. Rev. B 85, 035133 (2012)
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TT 79.35 Wed 15:00 P2

**ESR studies of $CoCr_2O_4$** — •ALEXEY PONOMARYOV[1], MYKHAYLO OZEROV[1], JOACHIM WOZNITZA[1], VLADIMIR TSURKAN[2,3], ALOIS LOIDL[2], and SERGEI ZVYAGIN[1] — [1]High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Institute of Applied Physics, Academy of Science of Moldova, Chisinau, Republic of Moldova

$CoCr_2O_4$ is a ferrimagnet ($T_C \sim 97K$) with cubic spinel structure and two magnetic ions ($Co^{2+}$ and $Cr^{3+}$) in the elementary cell. Significant spin-lattice coupling and magnetic frustration are important features of $CoCr_2O_4$, defining its very unusual phase diagram [1]. Here, we report on high-field electron spin resonance (ESR) studies of single-crystalline samples of $CoCr_2O_4$ performed in the frequency range from 90 to 1000 GHz in magnetic fields up to 16 T. Two modes were observed. Pecu-

liarities of the ESR excitation spectra are discussed.

This work was partly supported by the DFG.

[1] Tsurkan et al., Phys. Rev. Lett. 110, 115502 (2013)

TT 79.36 Wed 15:00 P2

**Magnetic ground state and low-energy spin dynamics in single crystals of the frustrated magnet $CoAl_2O_4$** — •S. Zimmermann[1,2], A. Alfonsov[1], M. Iakovleva[3], E. Vavilova[3], H.-J. Grafe[1], H. Luetkens[4], O. Zaharko[4], H.-H. Klauss[2], A. Maljuk[1], S. Wurmehl[1], T. Dey[1], V. Kataev[1], and B. Büchner[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Zavoisky Phys.-Tech. Inst., RAS, Kazan, Russia — [4]PSI Villigen, Switzerland

Frustrated magnetic systems are of special interest because they can exhibit exotic magnetic ground states like spin ice or spin liquid. The compound $CoAl_2O_4$ belongs to the A-site spinels, where the Co ions form a diamond lattice and the frustration originates from competing nearest- and next-nearest neighbor interactions. Thus the frustration tends to suppress long-range magnetic ordering and favors short-range spin correlations. This effect can be supported by disorder, e.g., site inversion. Due to the recent breakthrough in the growth of high-quality single crystals [1], it has become possible to study the magnetic ground state of $CoAl_2O_4$ in detail. Recent neutron scattering results give strong indications that a spin liquid like magnetic ground state is realized in such $CoAl_2O_4$ single crystals [2]. To further clarify this question, we have studied these crystals with high field high frequency ESR, NMR and $\mu$-SR techniques. The experimental results have enabled to obtain important insights into the properties of the ground state, spin dynamics and magnetic interactions in this compound which will be discussed in this presentation.

[1] A. Maljuk et al., J. Cryst. Growth **311**, 3997 (2009)
[2] O.Zaharko et al., Phys. Rev. B **84**, 094403 (2011)

TT 79.37 Wed 15:00 P2

**Thermal expansion and magnetostriction measurements at sub Kelvin temperatures - experiments on the frustrated quantum magnet $Cs_2CuCl_4$** — •satya krishna Thallapaka, Bernd Wolf, and Michael Lang — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR49, D-60438 Frankfurt (M), Germany.

We describe the device suitable for high-resolution thermal expansion and magnetostriction measurements using a capacitive dilatometer [1] which measures length changes with a sensitivity of $\Delta l \geq 10^{-2}$ Å, corresponding to a relative resolution of $\Delta l/l \sim 10^{-10}$. The system operates down to 40 mK and in magnetic fields up to 18 T. We report measurements on the spin S = 1/2 triangular-lattice Heisenberg antiferromagnet $Cs_2CuCl_4$ aiming at exploring its field-induced quantum critical point.

[1] R. Pott and R. Schefzyk, J. Phys. E **16**, 444 (1983)

TT 79.38 Wed 15:00 P2

**Localized states on triangular traps and low-temperature properties of the antiferromagnetic Heisenberg and repulsive Hubbard models** — •Mykola Maksymenko[1,3], Johannes Richter[2], and Oleg Derzhko[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38 01187 Dresden — [2]Institut für theoretische Physik, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Institute for Condensed Matter Physics of NAS of Ukraine

We consider the antiferromagnetic Heisenberg and the repulsive Hubbard model on two N-site one-dimensional lattices, which support dispersionless one-particle states corresponding to localized states on triangular trapping cells. We calculate the degeneracy of the ground states in the subspaces with low number of magnons or electrons as well as the contribution of these states (independent localized states) to thermodynamic quantities. Moreover, we discuss another class of low-lying eigenstates (so-called interacting localized states) and calculate their contribution to the partition function. We also discuss the effect of extra interactions, which lift the degeneracy present due to the chirality of the localized states on triangles.

TT 79.39 Wed 15:00 P2

**1/d expansion for coupled dimer magnets** — •Darshan G. Joshi[1], Kris Coester[2], Kai P. Schmidt[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Theoretische Physik, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Using bond operators we develop a systematic expansion in 1/d, where d is spatial dimension, for coupled-dimer Heisenberg magnets. We apply this technique to a model of dimers on a hypercubic lattice, a generalization of the square-lattice bilayer Heisenberg model to arbitrary d. The method covers both the quantum paramagnetic and antiferromagnetic phases including the quantum critical point. Physical observables such as the phase boundary, mode dispersions and ground-state energy are shown to have a systematic expansion in powers of 1/d and are calculated to next-to-leading order. In the paramagnetic phase, an expansion in ratio of inter-dimer and intra-dimer coupling for arbitrary d is shown to be consistent with the results of the 1/d expansion.

TT 79.40 Wed 15:00 P2

**Bond randomness in Kitaev's honeycomb spin-liquid model** — •Fabian Zschocke and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The Kitaev model on the honeycomb lattice realizes a spin liquid whose emergent excitations are gapless Majorana fermions and static Z2 gauge fluxes. Upon introduction of bond randomness the model remains exactly solvable, via an equivalent tight-binding model of canonical fermions. We use this to study a number of observables as function of disorder strength, paying particular attention to properly selecting physical states within the canonical-fermion description. Specifically, we calculate the distribution of local susceptibilities, extract the NMR lineshape, and make contact with known results on the problem of disordered Dirac fermions.

TT 79.41 Wed 15:00 P2

**NMR as a local probe for 5d and 4d magnetism in honeycomb lattices $A_2TO_3$; (A=Na,Li; T=Ir,Rh)** — •Panchanana Khuntia[1], Mayukh Majumder[1], Soham Manni[2], Philipp Gegenwart[2], and Michael Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Goettingen, Germany

Recently, 5d iridates like the honeycomb lattices $(Na,Li)_2IrO_3$ and 4d analog $Li_2RhO_3$ display unconventioal magnetic properties which are driven by spin orbit coupling and frustration. There is a cross-over from Néel (zig-zag) type magnetic ordering to a spin-liquid state in the Heisenberg-Kitaev model. We report temperature (T) and field (H) dependent NMR study on $Na_2IrO_3$, $Li_2IrO_3$, and $Li_2RhO_3$. $^{23}$Na NMR in $Na_2IrO_3$ enable us to disentangle three Na sites and deduce the magnetic order parameter.The T and H dependent NMR spectra and spin lattice relaxation rate (SLR) reveal that $Na_2IrO_3$ and $Li_2IrO_3$ are magnetically ordered with $T_N$ = 15 K, additionally, $Li_2IrO_3$ exhibits features reminiscent of a spin-liquid.In $Li_2RhO_3$, magnetization and specific heat data exhibit no sign of long range ordering down to 0.3 K but a spin glass transition is observed at $T_g$=8 K. $^7$Li NMR line width and SLR in $Li_2RhO_3$, display signatures of spin correlation and emergence of slowing down of spin fluctuations on approaching the freezing temperature. The specific heat and SLR show power law behavior below $T_g$ reflecting the persistence of low lying excitations pointing towards a spin liquid state.

TT 79.42 Wed 15:00 P2

**Energy dynamics in the Heisenberg-Kitaev chain** — •Robin Steinigeweg and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Spin liquids are realized by the Kitaev model and by the Heisenberg model in one dimension, with a finite-temperature dynamics only partially resolved despite the integrability of both models. We make an essential step forward by studying the dynamics in the Heisenberg-Kitaev chain as a model of two competing spin liquids. Using analytical and numerical approaches within linear response, we show the emergence of purely ballistic energy transport at all integrable points, which manifests as pronounced Drude weights and low-frequency suppression of regular contributions. Varying several model parameters including exchange-coupling strength, ratio, and anisotropy as well as magnetic field, we find extended quantum chaotic regions with vanishing Drude weights and well-defined DC contributions. In the vicinity of the Kitaev model, we find clear signatures of the topological gap in the response function.

TT 79.43 Wed 15:00 P2

**Magnetic properties of antiferromagnetic Heisenberg chains with spin-S boundary defects in magnetic fields** — •Björn

Willenberg[1,3], Jan Grelik[2,3], Wolfram Brenig[1,3], and Holger Frahm[2,3] — [1]Institute for Theoretical Physics, Technische Universität Braunschweig — [2]Institute for Theoretical Physics, Leibniz Universität Hannover — [3]Niedersächsische Technische Hochschule, NTH

We investigate anisotropic S=1/2 Heisenberg chains with spin-S boundary defects with an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo methods based on Stochastic Series Expansion. For particular choices of parameters and at zero temperature the models we investigate are exactly solvable by means of Bethe Ansatz techniques. Results will be presented for magnetic properties as functions of uniform and edge magnetic fields, exchange-coupling constants, anisotropy, temperature, and system size. Properties include the susceptiblity and magnetization. Of special interest are bulk and boundary properties which are expressed in orders of 1/L and the magnetization with respect to the corresponding magnetic fields. We will compare our findings from both methods in the zero temperature limit.

TT 79.44 Wed 15:00 P2

**Optical absorption of a 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 in a spin-1/2 antiferromagnetic Heisenberg model on the anisotropic triangular lattice coupled to lattice degrees of freedom. We describe the scattering of light from the system via a simple model of magneto-elastic coupling to nearest neighbor bond dipoles, assuming a monoatomic unit cell. The magnetic excitations are described using linear spin wave theory including interaction to $O(1/S^2)$. The absorption cross section is evaluated in terms of two-magnon-one-phonon Greens functions. Results will be presented for the conductivity versus frequency and temperature, with and without final state interactions. The impact of anisotropy will be analyzed. The role of different phonon density of states will be considered.

TT 79.45 Wed 15:00 P2

**Magnetic phase diagram of the metallic triangular-lattice antiferromagnet $PdCrO_2$** — Jong Mok Ok[1], •M. Dietterle[2], J. Wosnitza[2], and Jun Sung Kim[1] — [1]Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — [2]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany

Due to geometrical frustration, two-dimensional triangular-lattice antiferromagnets (TAFM) exhibit a variety of magnetic phases and transitions in an applied magnetic field [1]. The phase diagram becomes fantastically rich if magnetic anisotropy and competing first- and second-neighbor interactions come into play, as it is the case in many magnetic materials [2]. $PdCrO_2$ is a rare example of a metallic TAFM consisting of stacked layers of Pd and Cr triangular lattices in a delafossite structure. The localized $S = 3/2$ spins of the $Cr^{3+}$ ions in the $CrO_2$ layer are expected to be AFM ordered in the 120-degree helical spin structure at $T_N = 37.5$ K. Previous de Haas-van Alphen experiments reveal a Fermi-surface reconstruction due to the AFM ordering, confirming the strong coupling between the itinerant electrons and the localized spins [3]. With torque magnetometry on single crystals in high pulsed magnetic fields up to 70 Tesla we investigate the phase diagram of $PdCrO_2$ and the influence of meta-magnetic transitions on the nature of coupled itinerant electrons.

[1] L. Seabra *et al.*, Phys. Rev. B **84**, 214418 (2011)
[2] L. Seabra *et al.*, Phys. Rev. B **83**, 134412 (2011)
[3] Jong Mok Ok *et al.*, Phys. Rev. Lett. **111**, 176405 (2013)

TT 79.46 Wed 15:00 P2

**Fermi condensation near Van Hove singularities in the triangular lattice** — •Daniel Hirschmeier[1], Dmitry Yudin[2], Hartmut Hafermann[3], Olle Eriksson[2], Alexander I. Lichtenstein[1], and Mikhail I. Katsnelson[4] — [1]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden — [3]Institut de Physique Théorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525, AJ Nijmegen, The Netherlands

The proximity of the Fermi surface to Van Hove singularities drastically enhances interaction effects and leads to essentially new physics. In this work we address the formation of flat bands ("Fermi condensation") within the Hubbard model on the triangular lattice and provide a detailed analysis from an analytical and numerical perspective. To describe the effect we consider both weak-coupling and strong-coupling approaches, namely the renormalization group and dual fermion methods. It is shown that the band flattening is driven by correlations and is well pronounced even at sufficiently high temperatures, of the order of 0.1-0.2 of the hopping parameter. The effect can therefore be probed in experiments with ultra cold fermions in optical lattices.

TT 79.47 Wed 15:00 P2

**Magnetic Ordering and Superconductivity in Triangular Lattices in the Hubbard Model** — Maria Daghofer and •André Fischer — IFW Dresden, Dresden, Germany

The 2D triangular lattice provides a simple model with intrinsic geometric frustration and is therefore well suited to study effects induced by electronic interactions. The aim of this work is to find possible ground state scenarios at the van-Hove filling within the Hubbard model, taking various magnetically ordered states and superconducting states into account. Using cluster perturbation theory allows us to tread the system on a level beyond mean field theory. We find a superconducting phase with unconventional symmetry to be the supported ground state in a wide parameter regime. A comparison of selected magnetically ordered states does not show a support of a previously proposed chiral phase.

TT 79.48 Wed 15:00 P2

**Strongly correlated system on frustrated lattices: Beyond the flat-band scenario** — •J. Richter[1], O. Derzhko[2], O. Krupnitska[2], and T. Krokhmalskii[2] — [1]University Magdeburg, Germany — [2]Institute for Condensed Matter Physics, Ukraine

We consider the spin-1/2 antiferromagnetic Heisenberg model at high magnetic fields as well as the Hubbard model at low electron density on some frustrated lattices with almost dispersionless lowest one-particle band. Eliminating high-energy degrees of freedom we construct low-energy effective Hamiltonians which are much simpler than the initial ones. Based on the effective-model description we examine the low-temperature properties of the considered frustrated quantum Heisenberg antiferromagnets in the high-field regime. We also apply our approach to describe azurite. Interesting features of these highly frustrated spin models consist in a steep increase of the entropy at very small temperatures T and a characteristic extra low-T peak in the specific heat. The most prominent effect for spin models is the existence of a magnetic-field driven Berezinskii-Kosterlitz-Thouless phase transition occurring in the two-dimensional model [1]. For the Hubbard model we discuss the existence of ground-state ferromagnetism. While for the considered model for a completely flat band the ground state is paramagnetic, we find a transition to ground-state ferromagnetism driven by the on-site repulsion in case that the band becomes dispersive. We present the ground-state phase diagram for the Hubbard model on the frustrated diamond chain at 1/6 electron filling.

[1] O.Derzhko et al., Phys. Rev. B 88, 094426 (2013)

TT 79.49 Wed 15:00 P2

**Magnetocrystalline anisotropy in low dimensional systems** — •Kira Riedl, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We study the magnetic and electronic properties of low dimensional systems with focus on consequences of spin-orbit coupling. On the basis of density functional theory (DFT) calculations we analyze several materials regarding if effects of the magnetocrystalline anisotropy or the Dzyaloshinskii-Moriya interaction can be observed. We investigate recent reports of a significant magnetic anisotropy in the copper compound $CuBr_2$ and the pyrochlore $R_2V_2O_7$ with DFT+U+SOC calculations. As a member of another class of materials with dominant effects of spin-orbit coupling we also study the magnetic properties of the hexagonal iridate $Na_2IrO_3$. It is of high physical interest since there is no general agreement yet whether it is a realization of the Heisenberg-Kitaev model or it can rather be described with quasi-molecular orbitals.

TT 79.50 Wed 15:00 P2

**Magnetic anisotropy of azurite probed by high-field electron resonance** — •Mykhaylo Ozerov, Jochen Wosnitza, and Sergei Zvyagin — Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Electron spin resonance (ESR) studies of single crystals of the natural mineral azurite $Cu_3(CO_3)_2(OH)_2$, a spin-chain compound with a distorted diamond structure, in magnetic fields up to 16 T are reported. Two ESR modes were observed below $T_N = 1.8$ K. The ESR angular dependence measured at 248 GHz revealed an extremum at a direction of $42^o \pm 3^o$, tilted from the a axis towards to the c axis. Field dependence of the resonance frequencies was measured with magnetic fields applied parallel, as well as perpendicular, to this direction. Two gaps in the ESR excitation spectrum were found at 84 and 145 GHz (0.35 and 0.6 meV), which is consistent with results of inelastic neutron scattering measurements [Rule *et al.*, PRB 84, 184419 (2011)]. Peculiarities of the obtained frequency-field diagram evidence essential role of the Dzyaloshinskii-Moriya interaction in the microscopic picture of the magnetic interactions in this compound.

This work was partly supported by the DFG.

TT 79.51 Wed 15:00 P2

**Crystal growth and analysis of $BaCuSi_2O_6$** — •Pascal Puphal, Natalija van Well, Franz Ritter, Cornelius Krellner, and Wolf Assmus — Physikalisches Institut, Goethe-Universität Frankfurt, Deutschland

$BaCuSi_2O_6$ is of interest since it has a two dimensional BEC-Phase at low temperature from 23,2 to 49,3 T. Crystal growth of this crystal is difficult, but was achieved using oxygen partial pressure or flux-method($LiBO_2$). However, the system tends to glaze especially using $LiBO_2$ as flux. We found $NaBO_2$ to work as flux as well and $KBO_2$ to be the best. Also we could prove with an electron microscope that the flux is not incorporated in the structure. We have investigated that an alloy of platinum and gold as crucible material improves the growth since it interacts less with the material.
$BaCuSi_2O_6$ has a structural phase transition from tetragonal to orthorhombic, which we explore with low temperature powder diffraction, magnetic, and specific heat measurements. Furthermore, we investigated strontium substitution on the barium side, which we proved to be possible up to 30%. It leads to a reduction of the unit cell, which suppresses the structural phase transition already at 5% strontium. Calcium substitution behaves differently: it only leads to defects in the crystal, which also suppress the phase transition but with increasing calcium, it even destroys the dimer-coupling of cupper.

TT 79.52 Wed 15:00 P2

**Specific heat studies of the $Cs_2CuCl_{4-x}Br_x$-system** — •Markus Kuhnt, Natalija van Well, Franz Ritter, Pham Thanh Cong, Bernd Wolf, Michael Lang, Cornelius Krellner, and Wolf Assmus — Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt (M), Germany

In this contribution, we report on a systematic study of the magnetic properties on single crystals of the $Cs_2CuCl_{4-x}Br_x$-system ($0 \leq x \leq 4$), which include the well studied end components $Cs_2CuCl_4$ and $Cs_2CuBr_4$. Both are $S = \frac{1}{2}$ quasi-two-dimensional-quantum antiferromagnets, but whereas $Cs_2CuCl_4$ exhibits field-induced Bose-Einstein-condensation, in $Cs_2CuBr_4$ triplet crystallization is found. In 2011 Cong et al. studied the magnetic susceptibility of the $Cs_2CuCl_{4-x}Br_x$-system ($0 \leq x \leq 4$) above 2 K and found that the transition from $Cs_2CuCl_4$ to $Cs_2CuBr_4$ evolves discontinuously[1].

This discontinuous evolution motivates to study the magnetic properties of this system more thoroughly. Thus, we measured the specific heat at various $x$ in the temperature range $1.8 \leq T \leq 20$ K. We will discuss the magnetic part of the specific heat as well as the ratio between the maximum temperatures of magnetic specific heat and magnetic susceptibility as a function of $x$. These data will also be compared to theoretical calculations for Heisenberg antiferromagnetic chains and 2D Heisenberg triangular antiferromagnets.
[1] P.T. Cong et al., Phys. Rev. B **83**, 064425

TT 79.53 Wed 15:00 P2

**Magnetic Properties of $Cu_2OSeO_3$ under weak doping** — Markus Strobl[1], •Marco Halder[1], Tim Adams[1], Sebastian Mühlbauer[2], Michael Wagner[1], Andreas Bauer[1], Helmut Berger[3], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), Lichtenbergstr. 1, 85748 Garching, Germany — [3]Ecole Polytechnique Federale Lausanne, CH-1015 Lausanne, Switzerland

The magnetoelectric $Cu_2OSeO_3$ is the first established insulator within the class of cubic chiral helimagnets crystallizing with space group $P2_13$. Perhaps most fascinating, these compounds give rise to a regular lattice of topologically non-trivial spin whirls, the so-called Skyrmion lattice. The magnetoelectric coupling in $Cu_2OSeO_3$ thereby promises novel phenomena compared to itinerant magnets such as MnSi, $Fe_{1-x}Co_xSi$, or FeGe. While in the latter systems the influence of doping on the magnetic properties was already investigated in detail, no corresponding data are available for $Cu_2OSeO_3$. Here, we report a comprehensive study by means of magnetization and small-angle neutron scattering focusing on the determination of the magnetic phase diagram of vapor-transport-grown samples of $Cu_2OSeO_3$ substitutionally doped with various transition metals.

TT 79.54 Wed 15:00 P2

**Phase-space Berry phases in chiral magnets: Skyrmion charge, Dzyaloshinskii-Moriya interaction and Hall effect** — •Robert Bamler[1], Frank Freimuth[2], Yuriy Mokrousov[2], and Achim Rosch[1] — [1]Universität zu Köln, Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present a theory for electronic properties of systems with spin-orbit coupling and smooth magnetic textures, such as chiral magnets. We show that Berry phases in mixed position/momentum space play an important role for both equilibrium and non-equilibrium properties.

In magnetic materials without inversion symmetry (chiral magnets) the spin-orbit coupling can lead to smooth whirls (skyrmions) in the magnetization. They give rise to a strong Hall signal due to the Berry phase an electron picks up when it moves in position space. At the same time, spin-orbit interactions in chiral magnets lead to Berry-phase effects in momentum space, such as the anomalous Hall effect.

In our work we show that the combination of spin-orbit coupling and a magnetic texture leads to new effects due to Berry phases picked up on closed loops in mixed position/momentum space. Using a gradient expansion of the Green's function we identify mixed phase-space Berry phases as the cause of Dzyaloshinskii-Moriya interactions and the charge of skyrmions in metals. By applying the gradient expansion to the Kubo formula we recover the known contributions to the Hall conductivity due to Berry phases in position and momentum space and discuss new contributions due to mixed phase-space Berry phases.

TT 79.55 Wed 15:00 P2

**Large lattice distortions associated with the magnetic transition in $La_{0.7}Sr_{0.3}MnO_3$** — •Frank Weber[1], Dimitri Argyriou[2,3], Oleksandr Prokhnenko[4], and Dmitry Reznik[5] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany — [2]European Spallation Source ESS AB, PO Box 176, SE-221 00 Lund, Sweden — [3]Department of Synchrotron Radiation Research, Lund University, Box 118, Lund, Sweden — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [5]Department of Physics, University of Colorado - Boulder, Boulder, CO 80309

Colossal magnetoresistance (CMR) is associated with the phase transition from a metallic ferromagnetic to insulating paramagnetic phase, which can be controlled by an applied magnetic field. The insulating phase occurs due to trapping of the charge carriers by polaronic lattice distortions, which raise the resistivity. Theories based on local physics predict that the magnitude of the resistivity jump at $T_C$ is determined by how much, on average, the amplitude of these distortions increases at the phase transition. Using neutron scattering, we measured the average distortion amplitude in $La_{0.7}Sr_{0.3}MnO_3$. Surprisingly, its increase from below to above $T_C$ is just as large as in other manganites, which have a much larger resistivity jump. This result suggests that the strength of CMR is determined not by the size of distortions, but by their cooperative nature, specific to each compound. Existing theories need to be extended to include correlations between different unit cells to explain and predict the strength of CMR.

TT 79.56 Wed 15:00 P2

**Crystal growth and physical properties of doped honeycomb lattice systems $A_2IrO_3$ (A=Na, Li)** — •Friedrich Freund, Soham Manni, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Honeycomb-lattice iridates have recently attracted interest in the context of novel electronic and magnetic states like spin-orbit Mott or quasi-molecular orbital insulators, Kitaev-Heisenberg magnets or correlated topological insulators. Starting from $Na_2IrO_3$ and $Li_2IrO_3$, which display insulating antiferromagnetic ground states, we investigate the influence of various dopings on the magnetic interaction and electronic properties. Single and polycrystals are synthesized using

solid state reactions under appropriate conditions.

TT 79.57 Wed 15:00 P2

**Interplay of Spin-Orbit Coupling and Electron Correlations in Iridate Compounds** — •Alexander Hampel and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

This work deals with the investigation of the electronic structure of perovskite iridates, such as $Ba_2IrO_4$. Recent experiments exploring different iridate compounds found out that the cooperation of strong electron correlations and spin-orbit coupling plays an important role in the correct description of their physical behaviour. The reason for this are large spin-orbit interaction energies in the 5d transition metal oxides, which have the same order of magnitude as the local Coulomb interaction.
We apply a combination of density functional theory (DFT) with explicit many-body methods to handle the realistic electronic correlations within the relativistic environment. More explicitly, the mixed-basis pseudopotential approach is allied with rotational-invariant slave bosons in order to address the intriguing correlated spin-orbit physics.

TT 79.58 Wed 15:00 P2

**Electronic structure of $Sr_2IrO_4$ polycrystals and PLD grown thin films** — •Ozan Kirilmaz[1], Atsushi Yamasaki[2], Michael Sing[1], Akira Sekiyama[3,4], Masaaki Isobe[5], Shigemasa Suga[3,4], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Faculty of Science and Engineering, Konan University, Kobe 658-8501, Japan — [3]Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan — [4]RIKEN SPring-8 Center, Sayo, Hyogo 679-5148, Japan — [5]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

Novel physics induced by strong spin-orbit coupling has attracted strong attention from both theory and experiment in recent years. $Sr_2IrO_4$ has an insulating ground state which seems to be driven by the strong spin-orbit coupling and relatively weak Coulomb interaction. The electronic structure near the Fermi level in $Sr_2IrO_4$ is characterized by $J_{eff} = \frac{1}{2}$ states. In order to provide deeper insight into these states, we have carried out high energy-resolution photoemission spectroscopy on both polycrystalline and thin film perovskite iridates. Photoemission spectroscopy in a wide range of excitation energies enables us to identify the bulk and surface electronic structure including their origin in the valence band.

TT 79.59 Wed 15:00 P2

**Effect of Gd doping and O deficiency on the Curie temperature of EuO** — •Nuttachai Jutong[1], Thomas Mairoser[2], Ulrich Eckern[1], and Udo Schwingenschlögl[3] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany — [3]KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effect of Gd doping and O deficiency on the electronic structure, exchange interaction, and Curie temperature of EuO in the cubic and tetragonal phases is modeled by means of density functional theory. We observe a maximum in the Curie temperature around 6.25% Gd doping, originating from a combination of f-d hopping and indirect exchange. However, the effect is suppressed at high doping. An increased Curie temperature is found in the case of O deficiency and is attributed to a double exchange mechanism, which is suppressed in the tetragonal phase due to Jahn-Teller distortions.

TT 79.60 Wed 15:00 P2

**Investigations on the Fermi surface of $SrCo_2P_2$** — •K. Götze[1,2], J. Klotz[1,2], C. Geibel[3], C. Bergmann[3], H. Rosner[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden-Rossendorf — [2]Institut für Festkörperphysik, TU Dresden — [3]Max-Planck-Institut CPfS, Dresden

$SrCo_2P_2$ is a non-superconducting member of the 122 pnictides with $ThCr_2Si_2$ tetragonal structure type. Although band-structure calculations predict ferromagnetic ordering in this compound, it only exhibits Stoner-enhanced paramagnetism [1]. However, peculiarities of the electronic structure depend on details of the crystal structure (like the P $z$ coordinate) which are not known precisely enough. Therefore, an experimental determination of the Fermi surface is desirable to explain this discrepancy. Probing the de Haas-van Alphen effect by use of a capacitive torque magnetometer setup, we measured the full angular dependence of quantum oscillations and effective masses of $SrCo_2P_2$. Our experiments were carried out in a top-loading dilution refrigerator and a $^3$He system at temperatures ranging from 25 mK to 4.2 K, and in magnetic fields up to 35 T. In combiniation with density-functional band-structure calculations, our results provide detailed information about the Fermi surface of $SrCo_2P_2$.
[1] S. Jia *et al.*, Phys. Rev. B. **80**, 165107 (2009).

TT 79.61 Wed 15:00 P2

**Algebraic-diagrammatic algorithm for the high-order perturbation expansion of the Green's function in the Mott-Hubbard insulator in high dimensions** — Eva Kalinowski[1], Walter Apel[2,3], •Martin Paech[3,1], and Eric Jeckelmann[3] — [1]Academy of Computer Science and Management, Bielsko-Biała, Poland — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Leibniz Universität, Hannover, Germany

One of the open problems in the theory of Mott-Hubbard insulators is the shape of the Hubbard bands in the single-particle density of states (DOS). In particular, for the Hubbard model on a Bethe lattice in the limit of an infinite coordination number, dynamical mean-field theory (DMFT) calculations reveal some unexplained sharp structures at the low-energy edges of the Hubbard bands in both the Mott insulating phase and the metallic phase in the critical region. Previous analytical expansions (up to second order for the Hubbard model and up to third order by solving the DMFT self-consistency equation) cannot fully explain the observed structures.

We show that the calculation of the DOS can also be formulated in a form, which is amenable to an algebraic-diagrammatic approach. We prove this procedure for the case of the Falicov-Kimball model and determine manually the DOS and the gap up to the fourth order for the Hubbard model. Additionally, we outline the generalization of an algorithm [1], which is well established for the ground-state energy and related critical properties up to the 15th order, for the computation of higher orders of the Green's function and the gap.
[1] PRB 85, 045105

TT 79.62 Wed 15:00 P2

**Generalization of the Time-Dependent Numerical Renormalization Group Method to Finite Temperatures and General Pulses** — •Hoa Nghiem and Theodoulos A. Costi — Peter Grünberg Institut and Institute for Advanced Simulation, Research Centre Jülich, 52425 Jülich, Germany

We generalize the time-dependent numerical renormalization group method (td-NRG)[1] to study the time evolution of an observable of an interacting quantum impurity system after a sudden quench at an arbitrary temperature without truncating the length of the Wilson chain [2]. This generalization requires the use of the full density matrix [3], and determining all the terms of the projected density matrix appearing in the time evolution. To evaluate these terms, we introduce efficient recursion relations. The numerical results are shown to be exact in the short time limit, while, in the long time limit, they strongly depend on the discretization parameter of NRG. We also consider the time evolution due to general continuous pulses, acting in a finite time interval. The calculation is done by discretizing the pulse into a sequence of small quenches, and generalizing the td-NRG to an arbitrary number of quenches.
[1] F. B. Anders and A. Schiller, Phys. Rev. Lett. 95, 196801 (2005).
[2] H. Nghiem and T. A. Costi, Preprint (2013).
[3] A. Weichselbaum and J. von Delft, Phys. Rev. Lett. 99, 076402 (2007).

TT 79.63 Wed 15:00 P2

**Self-energy and analytic continuation for multi-orbital quantum impurity models** — •Andreas Hausoel, Nicolaus Parragh, and Giorgio Sangiovanni — University of Würzburg, Germany

Continuous-time quantum Monte Carlo (CTQMC) allows us to treat quantum-impurity problems with several orbitals and general interactions. We present strategies to reduce the computational effort exploiting conserved quantities of the local Hamiltonian. In order to perform the analytic continuation of the self-energy from the Matsubara to the real axis the high frequency behavior is needed. We discuss how the necessary measurements can be implemented in hybridization-expansion CTQMC for multi-orbital problems and show first applications.

TT 79.64 Wed 15:00 P2

**Hierarchical Master Equation Approach to Nonequilibrium Green's Functions: From Transport through Interacting Quantum Dots to Dynamical Mean Field Theory** — •Rainer Härtle[1,2], Guy Cohen[3], David R. Reichman[3], and Andrew J. Millis[2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Columbia Universtiy, New York, USA — [3]Department of Chemistry, Columbia Universtiy, New York, USA

We extend the hierarchical quantum master equation methodology [1,2,3] to the computation of the Green's function of an impurity system that can be driven out of equilibrium. We employ an auxiliary lead method [4], which involves a smearing over a certain energy range, and a direct method, where besides the reduced density matrix correlations between the impurity and its environment have to be included [5]. We compare both methods, studying nonequilibrium quantum transport through an interacting double quantum dot [3] and discuss applications to nonequilibrium dynamical mean field theory.

[1] Y. Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).
[3] R. Härtle *et al.*, arXiv:1309.1170 (2013).
[4] G. Cohen *et al.*, arXiv:1310.4151 (2013).
[5] S. Wang *et al.*, arXiv:1301.6850 (2013).

TT 79.65 Wed 15:00 P2

**Electronic structure of substitutionally disordered systems within a pseudopotential approach** — •Alexander Herbig and Rolf Heid — Institut for solid state physics, Karlsruhe Institute of Technology

The study of the electronic structure of substitutionally disordered systems (e.g. doped compounds) via density functional-based methods is a challenge. A common approach based on supercells is limited to special impurity concentrations. Green's function based methods seem to be more promising to deal with arbitrary impurity concentrations where interesting physics can emerge. One of these methods, the coherent potential approximation (CPA), has already been successfully applied in the KKR-DFT-framework. In this work we discuss the development and first results of a CPA-like treatment of disorder based on a mixed-basis-pseudopotential DFT-code. After projection of the Kohn-Sham-orbitals onto a nonorthogonal localized basis we apply an extension of CPA based on the formalism of Blackman, Esterling and Berk (BEB) [1]. This method on the one hand allows to handle off-diagonal disorder and on the other hand can be implemented in a very natural way within an LCAO-framework [2]. Finally charge self-consistency will be achieved by feeding the BEB-CPA-results back into the DFT-calculation.

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

TT 79.66 Wed 15:00 P2

**Green functions approach to Hubbard nano-clusters with the GKBA and T-matrix approximation** — •Niclas Schlünzen, Sebastian Hermanns, and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

The Hubbard model describes narrow-band solid state systems in terms of sites, on which the electrons can interact, and hopping amplitudes between these sites. It exhibits the quantum characteristics of solids and recently can also be experimentally realized in finite systems, e.g., ultracold atoms in optical lattices. To describe the out-of-equilibrium dynamics of those systems, the theoretical framework of non-equilibrium Green functions is well suited [1]. It provides a controlled way to apply different many-body approximations. The equations of motion for the Green function can be solved very efficiently by using the generalized Kadanoff–Baym ansatz (GKBA), which has shown accurate results for weak coupling [2]. To describe strongly interacting systems, the T-matrix many-body approximation is a convenient choice [3]. In this contribution, we show first benchmark results for the non-equilibrium dynamics of Hubbard nano-clusters with T-matrix+GKBA comparing them with exact solutions as well as results from different many-body approximations.

[1] K. Balzer, and M. Bonitz, *Nonequilibrium Green's Functions Approach to Inhomogeneous Systems*, Springer (2013)
[2] K. Balzer et al., J. Phys. Conf. Ser. **427**, 012006 (2013)
[3] M. Puig von Friesen et al., Phys. Rev. Lett. **103**, 17 (2009)

TT 79.67 Wed 15:00 P2

**Thermalization dynamics of finite Hubbard nano-clusters with non-equilibrium Green functions** — •Sebastian Hermanns and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

The Hubbard model is widely used for the description of narrow-band solid state systems in terms of sites, on which the electrons interact, and hopping amplitudes between these sites. Recently, the Hubbard model has attracted new experimental interest with the ability to perform measurements on only a few ultracold atoms in an optical trap [1]. To describe these processes theoretically, the framework of non-equilibrium Green functions is very well suited, since it provides a controlled way of approximations, is non–perturbative in the exciting field and has shown good results for 1D and 2D Hubbard nano-clusters [2]. In this contribution, we focus on the thermalization dynamics in finite Hubbard systems analyzing the free evolution from strong non-equilibrium initial conditions. We examine the occurence of different relaxation stages and their dependence on the interaction strength, particle number as well as the dimensionality and filling factor.

[1] D. Jaksch et al., Ann. Phys. (N.Y.) **315**, 1452 (2005)
[2] M. Bonitz et al., Contrib. Plasma Phys. **53**, 778-787 (2013)

TT 79.68 Wed 15:00 P2

**Reduced density matrix functional theory via a wave function based approach** — •Robert Schade[1], Peter Blöchl[1], and Thomas Pruschke[2] — [1]Clausthal University of Technology, Clausthal, Germany — [2]University of Goettingen, Goettingen, Germany

We propose a new method for the calculation of the electronic and atomic structure of correlated electron systems based on reduced density matrix functional theory (rDMFT). The density matrix functional is evaluated on the fly using Levy's constrained search formalism. The present implementation rests on a local approximation of the interaction reminiscent to that of dynamical mean field theory (DMFT). This wave function based approach can be integrated into the existing DFT framework by making use of natural orbitals.

TT 79.69 Wed 15:00 P2

**Time-resolved Auger electron spectroscopy** — •Roman Rausch and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg

Motivated by the recent time-resolved measurements of Auger spectra, we develop a theory of time-resolved Auger electron spectroscopy (AES) for strongly correlated many-body systems. The temporal correlation of the two conduction-band holes in the final state is described within the framework of the Hubbard model, extended by core states to account for the dynamics of core-hole screening. Using a numerically exact Chebyshev polynomial expansion technique (kernel polynomial method) in the low hole-density limit, the time-dependent cross section is computed for different setups. We also discuss the time-dependence of correlation-induced satellites, the validity of a two-step description and the effects resulting from a non-perturbative treatment of the Auger process.

TT 79.70 Wed 15:00 P2

**Singular-mode functional renormalization group vs. Fermi surface patching: A comparison of two FRG schemes applied to the 2D Hubbard model** — •Julian Lichtenstein[1] and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA - Fundamentals of Future Information Technology

We analyze the capabilities of the singular-mode functional renormalization group (SM-FRG) which was introduced in [1]. The most important dependencies of the two particle vertex on Matsubara frequencies are included in our implementation. Moreover, the role of the self energy feedback has been investigated. We apply this method to the 2D Hubbard model and compare the results to those from previous studies that have used FRG via Fermi surface patching.

[1] W.-S. Wang *et al.*, Phys. Ref. B **85** (2012) 035414

TT 79.71 Wed 15:00 P2

**Competing order in correlated electron systems made simple** — Jing Wang[1,2], •Andreas Eberlein[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We derive an efficient and unbiased method for computing order parameters in correlated electron systems with competing instabilities. Charge, magnetic and pairing fluctuations above the energy scale of spontaneous symmetry breaking are taken into account by a functional renormalization group flow, while the formation of order below that scale is treated in mean-field theory. The method captures fluctuation driven instabilities such as d-wave superconductivity. As a first application we study the competition between antiferromagnetism and superconductivity in the ground state of the two-dimensional Hubbard model.

TT 79.72 Wed 15:00 P2

**Information entropies in Fe and Ni: Numerical evidence for electronic correlation in Momentum space** — •Wilhelm Hans Appelt[1,2], Diana Benea[3], and Liviu Chioncel[1,2] — [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 — [3]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania

Various momentum-space properties are computed for Fe and Ni within the framework of a combined Density Functional and Dynamical Mean Field theory. We asses the effects of electron correlation in momentum space by making a comparison with the results obtained from the Local Density Approximation. We study the information entropy using the one-electron density in momentum space along different directions and as a function of local Coulomb parameter $U$.

TT 79.73 Wed 15:00 P2

**Hydrodynamic long-time tails after a quantum quench** — Jonathan Lux[1], •Jan Müller[1], Aditi Mitra[1,2], and Achim Rosch[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Department of Physics, New York University

After a quantum quench, a sudden change of parameters, generic many particle quantum systems are expected to equilibrate. While a few collisions of quasi particles are usually sufficient to establish approximately local equilibrium, the eventual global equilibrium is, however, much more difficult to detect: conserved quantities have to be transported for long distances to build up a characteristic pattern of fluctuations, which takes a very long time.

Here we investigate a quantum quench of the one-dimensional bosonic Mott insulator from infinite to finite interaction strength using semiclassical methods for weak, and exact diagonalization for strong quenches. We demonstrate that equilibrium is approached only slowly, as $t^{-1/2}$ with subleading corrections, consistent with predictions from hydrodynamics.

TT 79.74 Wed 15:00 P2

**Stochastic mean-field approach to non-equilibrium dynamics of correlated systems** — Christopher Hinz, •Sebastian Hermanns, and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

One major obstacle for the simulation of strongly interacting many-particle systems is the exponential growth of the state space with the number of particles—the so-called curse of dimensionality. One possibility to mitigate this problem is the application of the stochastic formulation of quantum mechanics. Within this framework, one can impose approximations on the ensemble and the equations of motion. An example for such an approximate treatment is the stochastic mean-field method (SMF) [1,2], which aims at embedding some of the correlations into the initial ensemble, while using the time-dependent Hartree-Fock method to propagate different stochastic realizations of the system independently of each other. As a benchmark system, we use the time evolution of Hubbard nano-clusters in one to three dimensions.

[1] S. Ayik, Phys. Lett. B **658**, 174 (2008)
[2] D. Lacroix et al., Phys. Rev. C **85**, 041602(R) (2012)

TT 79.75 Wed 15:00 P2

**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 consistent kinetic equation of nonlocal and non-instantaneous character is derived which unifies the achievements of transport in dense gases with the quantum transport of dense Fermi systems. The numerical solution is not more expensive than solving the Boltzmann equation. In order to achieve this, large cancellations in the off-shell motion have been used which are buried usually in non-Markovian behaviors. The remaining effects are: (i) off-shell tails of the Wigner distribution, (ii) renormalization of scattering rates and (iii) of the single-particle energy, (iv) collision delay and (v) related non-local corrections to the scattering integral. The balance equations for the density, momentum and energy now include besides known quasiparticle parts additionally two-particle contributions exceeding the Landau theory. Different aplications are worked out. The collision delay results into the correlated density and consequently the number of quasiparticles is not conserved. In superconductors this leads to a shift of the chemical potential and the compensating electrostatic potential known as Bernoulli potential.