TT 19: Poster Session: Correlated Electrons 1

Time: Monday 15:00–19:00 Location: P2-EG

TT 19.1 Mon 15:00 P2-EG

Bulk and surface properties of $SmRh_2Si_2$ single crystals — •Jacintha Banda[1], Kristin Kliemt[2], Alla Chikina[3], Alexander Generalov[4], Kurt Kummer[5], Monika Güttler[3], Victor N. Antonov[6], Yuri Kucherenko[6], Steffen Danzenbächer[3], Christoph Geibel[1], Clemens Laubschat[3], Denis V. Vyalikh[3,7,8,9], Cornelius Krellner[2], and Manuel Brando[1] — [1]MPI CPfS, Dresden, Germany — [2]Goethe-University Frankfurt, Frankfurt, Germany — [3]Dresden University of Technology, Dresden, Germany — [4]MAX IV Laboratory, Lund, Sweden — [5]ESRF, Grenoble, France — [6]National Academy of Sciences of Ukraine, Kiev, Ukraine — [7]Saint Petersburg State University, Saint Petersburg, Russia — [8]Donostia International Physics Center, San Sebastian, Spain — [9]IKERBASQUE, Bilbao, Spain

We present the properties of $SmRh_2Si_2$. Using a modified Bridgman method with indium flux we obtained platelet-shaped $SmRh_2Si_2$ single crystals. The magnetic ground state was characterized by magnetization, specific heat and electrical transport measurements. $SmRh_2Si_2$ orders antiferromagnetically below $T_N = 62\,K$ with pronounced anomalies in C(T) and ρ(T). Due to the layered structure, the crystals could be cleaved easily parallel to the Sm-layers leading to well-defined atomically flat surfaces allowing to perform ARPES to investigate the valence of the Sm ions in the bulk and at the surface [1]. We found that, in spite of the antiferromagnetic order, Sm reveals divalent admixtures to the almost trivalent ground state both in the bulk and at the surface. [1] A. Chikina et al., to be published

TT 19.2 Mon 15:00 P2-EG

An Ultrasonic Study of the Heavy-Fermion Metal $YbNi_4P_2$ — •Yeekin Tsui, Lars Postulka, Bernd Wolf, Ulrich Tutsch, Kristin Klimt, Cornelius Krellner, and Michael Lang — Goethe-Universität, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M), Germany

$YbNi_4P_2$ is a stoichiometric heavy-fermion Kondo-lattice system with a Kondo temperature TK $\sim$ 8 K. The material exhibits unique features among the heavy-fermion compounds including its quasi-1D crystalline and electronic structure. Furthermore, $YbNi_4P_2$ undergoes a second-order ferromagnetic (FM) phase transition at 0.17 K, which can be suppressed by doping with a small amount of As leading to a FM quantum-critical point (QCP). The 4f-spins remain strongly fluctuating down to the lowest measured temperatures which influence the thermodynamic and transport properties of $YbNi_4P_2$. Therefore, $YbNi_4P_2$ is the first clean system situated in the close vicinity of an FM QCP [1]. Ultrasonic measurements have proven to be a powerful probe for characterizing the intriguing properties of heavy-fermion metals. Here we present ultrasonic measurements on a single crystal of $YbNi_4P_2$ over a wide temperature range. Our data show clear features in the ultrasound velocity and the attenuation corresponding to crystal-electric-field effects around 30 K. Further ultrasonic measurements are being conducted at temperatures around the FM phase transition.

[1] C. Krellner et al., New Journal of Physics 13 (2011) 103014

TT 19.3 Mon 15:00 P2-EG

Low Energy Dynamics in Charge Ordered $R_{0.5}Sr_{0.5}MnO_3$ (R = Nd and Pr) Manganite Thin Films — •Rakesh Rana[1], Johannes Schmidt[1,2], Jorg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The half-doped $Pr_{0.5}Sr_{0.5}MnO_3$ manganite represents a unique stripe type CO-orbital order that induces transport and magnetic anisotropy whereas the CO in $Nd_{0.5}Sr_{0.5}MnO_3$ is charge-exchange (CE)-type which is isotropic in nature.

We have systematically explored epitaxial manganite thin films grown on (100), (110), and (111) oriented $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ substrates by pulsed laser deposition technique. Our Terahertz time-domain spectroscopic data reveal charge density wave (CDW) resonance centered around 5-6 meV for (110) oriented films and Drude-like conductivity for (100) and (111) oriented films. The CDW resonance in the optical conductivity spectra can be tuned from 4 meV to 6 meV for (110) oriented films and depends on the amount of ferromagnetic phase fraction in the CO matrix and corroborates well with the magnetization measurements. The nonlinear conductivity related to the sliding of the pinned CDW character makes the studied systems promising candidates for ultrafast coherent control of charge transport by resonant THz pumping.

TT 19.4 Mon 15:00 P2-EG

DFT simulations of rare-earth hexaborides using hybrid functionals — •Florian Sohn[1] and Peter Blöchl[1,2] — [1]Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für theoretische Physik, Technische Universität Clausthal, Leibnizstr. 10, 38678 Clausthal-Zellerfeld

Rare-earth hexaborides (REB_6) are strongly correlated materials, where the strong Coulomb interaction between electrons in the rare-earth's f-electron shell influence the electronic properties of the whole material decisively.

Rare-earth hexaborides exhibit a variety of low-temperature phenomena, including antiferromagnetic ordering for most partially filled f-shells, ferromagnetic ordering in EuB_6, superconductivity in LuB_6, topological insulating behavior in SmB_6 and a complex phase diagram with Kondo behavior in CeB_6. We present results of density functional theory calculations using the local hybrid functional PBE0. The hybrid functional accounts for some of the more important correlations and thus provides a viable starting point for many-particle calculations using more sophisticated many-particle methods. The calculations are done with the PAW method using our CP-PAW code, which describes the f-electrons explicitly. The electronic structure is rationalized on the basis of the projected density of the systems and their changes throughout the series.

We gratefully acknowledge financial support by the DPG project PR298/19-1.

TT 19.5 Mon 15:00 P2-EG

Coupling of Co atoms on Cu(111) through monatomic chains — •Neda Noei, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

Using a low temperature scanning tunneling microscope we investigated how the Kondo resonance of a single Co atom on Cu(111) changes when it is attached to monatomic Cu chains. Cu chains with lengths up to 100 nm were repeatedly fabricated. They are one type of dislocations which arise after dipping the tip into Cu(111). In order to evaluate a long range interaction between magnetic atoms, Co atoms were attached to the copper chains at different distances from each other. We observed a nonuniform variation of the Kondo resonance in amplitude and width.

TT 19.6 Mon 15:00 P2-EG

Realistic description of multi-orbital Kondo Anderson impurities on metal surfaces — •Francisco Meirinhos, Ammar Nejati, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

The detailed understanding of the STM spectra of magnetic atoms adsorbed on a metal surface is hampered by the complexity of the atomic level scheme consisting of multiple local orbitals, occupied by several electrons. We develop a quantitative theory for the description of such complex Anderson impurities which proceeds in three steps. (1) We transform the atomic multi-orbital, multi-electron states to the local eigenstate basis, involving Hund's rules and the Clebsch-Gordan coefficients, in order to determine the multiplet of low-lying spin-orbit Kramers doublets of the magnetic atom. Taking into account local charge fluctuations by at most one unit, this defines an effective multi-orbital, infinte$-U$ Anderson impurity model. (2) The parameters of this model are determined by fitting the (magnetically polarized) spectra of the mean-field solution to the results of spin-polarized density functional theory (DFT). This is accurate for the high-energy spectral features. (3) Finally, we calculate the low-energy Kondo-Fano spectra for the obtained parameters using the multi-orbital non-crossing approximation (NCA). The results will be compared with experimental STM dI/dV spectra.

TT 19.7 Mon 15:00 P2-EG

Ward identities versus two-particle self-consistency — •Friedrich Krien[1], Erik G.C.P. van Loon[2], Hartmut Hafermann[3], Alexander I. Lichtenstein[1], and Mikhail I. Katsnelson[2] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Radboud University, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands — [3]Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., 92100 Boulogne Billancourt, France

Some diagrammatic extensions of (E)DMFT (EDMFT+GW, Trilex, Dual Boson and others) introduce retarded interactions into the Anderson-Impurity model to fix a two-particle self-consistency condition. We take a close look at the fate of conservation laws under this pretext and demonstrate that Φ-derivability à la Baym-Kadanoff is not a sufficient criterion for spin conservation. We propose direct numerical validation to verify Ward identities.

TT 19.8 Mon 15:00 P2-EG

Electron spin resonance as a function of frequency, field, temperature, and angle using broadband and resonant planar microwave devices applied to $YbRh_2Si_2$ and ruby — •Linda Bondorf[1], Manfred Beutel[1], Wolfgang Voesch[1], Markus Thiemann[1], Kristin Kliemt[2], Cornelius Krellner[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Goethe-Universität, Frankfurt am Main, Germany

The quantum-critical heavy-fermion material $YbRh_2Si_2$ shows strong magnetic anisotropy and exhibits antiferromagnetic order at temperatures below 70 mK and magnetic fields below 60 mT. Electron spin resonance (ESR) measurements on $YbRh_2Si_2$ at such low temperatures and fields are highly desired but out of reach for conventional ESR spectrometers. These limitations can be overcome with resonant and broadband planar microwave devices as ESR probes [1, 2].

Here we present an ESR setup that enables frequency-, magnetic field-, temperature-, and angle-dependent measurements using coplanar structures. We demonstrate this technique through broadband ESR measurements (up to 20 GHz) on ruby with in-situ sample rotation inside a ^{4}He cryostat. Angle-dependent measurements with enhanced sensitivity on $YbRh_2Si_2$ are performed down to 4.4 GHz and 1.6 K using a superconducting coplanar resonator, and extensions of this approach to mK temperatures will be discussed.

[1] M. Scheffler *et al.*, Phys. Status Solidi B **250**, 439 (2013).
[2] Y. Wiemann *et al.*, Appl. Phys. Lett. **106**, 193505 (2015).

TT 19.9 Mon 15:00 P2-EG

Characterization of As substituted $YbNi_4P_2$ single crystals — •Philipp Ross, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe-University Frankfurt, D-60438 Frankfurt, Germany

The tetragonal compound $YbNi_4P_2$ has a low Curie temperature, T_C = 0.17 K, which can be further suppressed by substituting P by As. The rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at x≈0.1 [1,2].

Single crystals of $YbNi_4(P_{1-x}As_x)_2$, with various As concentrations were grown by the Czochralski method [3]. Strong effort was undertaken to determine the precise orientation of the as-grown crystals and prepare single-crystalline pieces. These crystals were characterized by electrical transport, heat capacity and magnetization measurements. Here we present the measured data these measurements down to T = 2 K. Furthermore, we characterized the room temperature crystal structure by powder X-ray diffraction and determined the change in the lattice constants for increasing As content using Rietveld refinement.

[1] C. Krellner et al., New J. Phys. 13, 103014 (2011)
[2] A. Steppke et al., Science 339, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth 449, 129-133 (2016)

TT 19.10 Mon 15:00 P2-EG

Magnetic anisotropy in $YbNi_4P_2$ — •Sven Friedemann[1], Sara Karbassi[1], Saman Ghannadzadeh[2], Manuel Brando[3], Kristin Kliemt[4], and Cornelius Krellner[4] — [1]HH Wills Laboratory, University of Bristol, UK — [2]High Field Magnet Laboratory, University of Radboud, Nijmegen, NL — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a rare example of a heavy-fermion compound with ferromagnetic (FM) order. It allows to study the emergence of a FM quantum critical point (QCP) which marks a long-standing challenge in metallic compounds as FM QCPs are avoided in most systems through a change of the transition to 1st order or through an intervening antiferromagnetic phase. $YbNi_4P_2$ by contrast was demonstrated to have a readily accessible QCP when suppressing the FM order with substitution of phosphorous by arsenic [1]. An alternative route to access the FM QCP could be via a transverse field tuning for strongly anisotropic FM order. We use angular dependent magnetoresistance measurements to extract the anisotropy of the Landé g factor. This will be the basis to understand under which conditions a FM QCP may be accessed via transverse field tuning.

[1] Steppke, A., et al., Science, **339**, 933 (2013).

TT 19.11 Mon 15:00 P2-EG

Evolution of the entropy in the magnetic phases of partially frustrated CePdAl — •Kai Grube[1], Stefan Lucas[2], Chien-Lung Huang[1,2,3], Akito Sakai[4], Sarah Woitschach[2], Elizabeth L. Green[5], Sebastian Kuntz[1], J. Wosnitza[5], Veronika Fritsch[4], Philipp Gegenwart[4], Oliver Stockert[2], and Hilbert von Löhneysen[1,3] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [4]Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, Germany — [5]Hochfeld-Magnetlabor Dresden (EMFL-HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany

In the heavy-fermion metal CePdAl long-range antiferromagnetic order coexists with geometric frustration of one third of the Ce moments. At low temperatures the Kondo effect tends to screen the frustrated moments. We use magnetic fields B to suppress the Kondo screening and studied the magnetic phase diagram and the evolution of the entropy with B employing thermodynamic probes. We estimate the frustration by introducing a definition of the frustration parameter based on the enhanced entropy, a fundamental feature of frustrated systems. In the field range where the Kondo screening is suppressed the liberated moments tend to destabilize the magnetic order and strongly enhance the frustration.

TT 19.12 Mon 15:00 P2-EG

Magnetic correlations in Ce(Pt,Pd)Al_3 — •Stefan Weber[1], Petr Cermak[2], Christian Franz[1], Wolfgang Simeth[1], Kirill Nemkovskiy[2], Astrid Schneidewind[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, Garching, DE — [2]Jülich Centre for Neutron Science, MLZ, Garching, DE

The nature of quantum phase transitions in selected Ce compounds is still heavily discussed [1]. The properties of these systems are characterized by the interplay of several competing energy scales. In the Ce$T$$Al_3$ (T=transition metal) series, T=Pt and Pd compounds are located at the border of antiferromagnetic ordering but not known to order yet [2]. Extensive measurements of the bulk properties (magnetization, susceptibility and specific heat) suggest the possible collapse of energy scales across the quantum phase transition in these systems [3]).

We studied single crystals of $CePtAl_3$ and $CePdAl_3$ by polarized neutron diffraction on DNS (MLZ Garching) at very low temperatures. A search for long-range magnetic order in $CePtAl_3$ appears to be inconclusive so far with putative evidence for magnetic reflections and hysteresis. In contrast, in $CePdAl_3$ we find clear evidence for magnetic order at low temperatures. The possible magnetic structures of both compounds will be discussed.

[1] P. Gegenwart, Q. Si, F. Steglich e.g. Nature Physics 4, 186 (2008).
[2] C. Franz, et al., J. Alloys Compd. 688, 978 (2016)
[3] C. Franz, PhD thesis, TU Munich (2014)

TT 19.13 Mon 15:00 P2-EG

Advancing the crystal quality and dimensions in the crystal growth process of $Yb(Rh_{1-x}Ir_x)_2Si_2$ — •Sebastian Witt[1], Michael Baenitz[2], and Cornelius Krellner[1] — [1]Goethe University Frankfurt, 60438 Frankfurt am Main, Germany — [2]MPI for Chemical Physics of Solids, 01187 Dresden, Germany

In the heavy fermion compound, $YbRh_2Si_2$, a superconducting phase transition at 2mK was found recently [1]. From these measurements it is further evident, that the occurence of nuclear antiferromagnetic order slightly above T_C plays an essential role. Single crystals (SC) with isotope pure silicon and/or ytterbium enable the investigation of the nature of the superconductivity in this material. Additionaly, the

stability of the superconduction phase can be investigate by the substitution of rhodium by iridium. Due to small amounts of the isotopes and the non-nominal and non-homogenous substitution it is necessary to further optimize the crystal growth.

Here, we report the crystal growth of $Yb(Rh_{1-x}Ir_x)_2Si_2$ with the optimized accelerated crucible rotation technique. This technique enhances the crystal quality (homogeneity, less distortions and reduced flux inclusions). The process optimization is accompanied by resistivity measurements of the SCs as well as EDX measurements to ensure the homogeneity of the substituted elements. We report simulations of the growth process inside the crucible. Crystals with the silicon-29 isotope were used for first NMR measurements and results of metallothermic reduction of Yb_2O_3 to obtain the Yb-metal were presented.

[1] E. Schuberth et al., Science, **351(6272)**, 485-488, (2016).

TT 19.14 Mon 15:00 P2-EG

Novel Quantum Criticality in the Au-Al-Yb Quasicrystal — •Andreas Wörl[1], Shuya Matsukawa[2], Akito Sakai[3], Noriaki Sato[2], and Philipp Gegenwart[1] — [1]Experimentalphysics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Department of Physics, Graduate School of Science, Nagoya University, Japan — [3]Institute for Solid State Physics, The University of Tokyo, Japan

The emergence of non-Fermi liquid behavior without tuning an external control parameter has been reported for several heavy-fermion materials lately. One prime example is the icosahedral quasicrystal $Au_{51}Al_{36}Yb_{15}$, which exhibits divergent behavior of magnetic susceptibility, $\chi^{-1} \propto T^{0.51}$, and specific heat, $C/T \propto -\ln T$, in zero magnetic field [1].

To further resolve the nature of the non-Fermi liquid state, we report thermal expansion and magnetostriction measurements at ultra-low temperatures. The Grüneisen ratio, which is the most suitable physical quantity for the characterization of pressure sensitive quantum crititcal phenomena, gives no evidence of an intrinsically generated pressure sensitive quantum critical point. We conclude the formation of a novel critical state with the peculiarity of low pressure but high magnetic field sensitivity.

[1] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura and T. Ishimasa, Nat. Mater. **11**, 1013 – 1016 (2012)

TT 19.15 Mon 15:00 P2-EG

Thermal expansion measurements on $Cs_2CuCl_{4-x}Br_x$ at sub-Kelvin temperatures — •Satya Krishna Thallapaka, Christian Thurn, Ulrich Tutsch, Bernd Wolf, and Michael Lang — Physikalisches Institut, SFB/TR49, Goethe Uni Frankfurt, DE

In recent years, Cs_2CuCl_4 and Cs_2CuBr_4 have been extensively investigated both experimentally and theoretically, as they represent model systems for quasi-2D triangular-lattice quantum antiferromagnets. They attracted much attention due to their unconventional magnetic properties resulting from the interplay of strong quantum fluctuations in reduced dimensions, geometrical frustration and effects of spin-lattice interactions close to the field-induced quantum critical point (QCP). Recently, a study of the mixed system $Cs_2CuCl_{4-x}Br_x$ has identified two novel compounds [1] with well-ordered halide sublattices due to a site-selective substitution mechansim, namely $Cs_2CuCl_3Br_1$ and $Cs_2CuCl_2Br_2$. It was predicted that the latter compound is showing an even higher degree of frustration than the border compounds. Thus, the series $Cs_2CuCl_{4-x}Br_x$ is ideal to study the effects of frustration and dimensionality around the QCP. To this end, we will present measurements of the thermal expansion coefficient on Cs_2CuCl_4 down to $T = 40$ mK around the field-induced QCP. The thermal expansion coefficient has been proven to be particularly suited to probe the anomalous thermodynamics of QCPs [2]. In addition, we will compare these results to measurements of the thermal expansion on the mixed system $Cs_2CuCl_2Br_2$ and to specific heat measurements.

[1] Cong *et al.*, PRB **83**, 064425 (11)
[2] Zhu *et al.*, PRL 91, 066404 (03)

TT 19.16 Mon 15:00 P2-EG

Spin dynamics of $FeGa_{3-x}Ge_x$ studied by Electron Spin Resonance — Bonho Koo[1], Kristian Bader[2], Michael Baenitz[1], Peter Gille[2], and •Jörg Sichelschmidt[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden — [2]LMU, Kristallographie, München

$FeGa_3$ is a nonmagnetic, narrow-gap semiconductor which acquires itinerant ferromagnetism upon electron doping by a partial replacement of Ga with Ge. The way how this magnetism evolves is of particular interest for better understanding the *d*-electron heavy-fermion behaviour of $FeGa_{3-x}Ge_x$ (at $x < 0.15$) or the properties close to a ferromagnetic (FM) quantum critical point at the critical Ge-concentration of $x = 0.15$. For detailed studies in this direction the availability of single crystals with a high purity is a precondition.

We studied the electron spin resonance (ESR) of ultra-pure single crystals of $FeGa_{3-x}Ge_x$ for $x = 0$ and x around 0.15. For $x = 0$ we observed a well-defined ESR signal, indicating the presence of pre-formed magnetic moments in the semiconducting phase. Upon increasing x the occurrence of itinerant magnetism clearly affects the ESR properties below $T \approx 30$ K whereas at higher T an ESR signal as seen in $FeGa_3$ prevails independent on the Ge-content. We interpret the low-T ESR in terms of a resonance of conduction electron spins and consider the relaxation as being determined by exchange fields. This is supported by a comparison with the temperature dependencies of magnetisation and electrical resistivity. The present results show that the ESR of $FeGa_{3-x}Ge_x$ is an appropriate and direct tool to investigate FM correlations in the vicinity of a FM quantum critical point.

TT 19.17 Mon 15:00 P2-EG

Quantum Monte Carlo simulations of metallic quantum critical points — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot, 76100, Israel

While quantum critical phenomena in insulators are relatively well understood, their metallic counterparts pose a substantial theoretical challenge since the order parameter fluctuations can interact with gapless fermionic excitations on the Fermi surface. This interplay, however, allows for a multitude of competing orders in the vicinity of a metallic quantum critical point including e.g. the formation of superconductivity when driving the metallic system through a phase transition.

Fortunately, it has recently been demonstrated that for certain classes of metallic quantum critical points this physics can be studied by determinant quantum Monte Carlo simulations, without suffering from the notorious fermion "sign problem". I will show numerically exact studies of the antiferromagnetic quantum critical point in two spatial dimensions and discuss techniques to improve on the scalability of the determinant quantum Monte Carlo approach.

TT 19.18 Mon 15:00 P2-EG

Phase diagram of the quantum dissipative rotor model with two competing baths — •Dominik Maile[1], Sabine Andergassen[1], Wolfgang Belzig[2], and Gianluca Rastelli[2] — [1]Eberhard Karls Universität Tübingen, D-72074 Tübingen, Germany — [2]Universität Konstanz, D-78457 Konstanz, Germany

We study a quantum dissipative rotor model in which each local phase-difference and each local momentum are uniformly coupled to two different baths. Such systems can represent e.g. a chain of resistively shunted Josephson junctions [1], capacitively coupled to a diffusive metal [2]. The first dissipative coupling quenches the quantum phase fluctuations favoring the long-range phase order (i.e. superconducting ground state) whereas the second one quenches momentum fluctuations destroying phase coherence (insulating ground state).

Using the Self-Consistent Harmonic Approximation [1], we calculate the zero-temperature phase diagram as determined by the two dissipative coupling constants and the bare zero point fluctuations. As an effect of the quantum frustration for the two canonical conjugate observables [3], we obtain an interesting phase diagram with a non-monotonic behavior: for instance, the ground state can pass from superconducting to insulating phase and back to superconducting phase by increasing the dissipation.

[1] S. Chakravarty et al., Phys. Rev. Lett. **56**, 2303 (1986).
[2] A.M.Lobos, T. Giamarchi, Phys. Rev. B **84**, 024523 (2011).
[3] G. Rastelli, New J. Phys. **18**, 053033 (2016).

TT 19.19 Mon 15:00 P2-EG

Competing phases in spin ladders with ring exchange and frustration — •Alexandros Metavitsiadis[1] and Sebastian Eggert[2] — [1]Institute for Theoretical Physics Technical University Braunschweig, Braunschweig, Germany — [2]Department of Physics and OPTIMAS Research Center, University of Kaiserslautern, Kaiserslautern, Germany

The ground state properties of spin-1/2 ladders are studied, emphasizing the role of frustration and ring exchange coupling. We present a unified field theory for ladders with general coupling constants and

geometry. Rich phase diagrams can be deduced by using a renormalization group calculation for ladders with in chain next nearest neighbor interactions and plaquette ring exchange coupling. In addition to established phases such as Haldane, rung singlet, and dimerized phases, we also observe a surprising instability towards an incommensurate phase for weak interchain couplings, which is characterized by an exotic coexistence of self-consistent ferromagnetic and anti-ferromagnetic order parameters.

TT 19.20 Mon 15:00 P2-EG

Magnetic phase diagram of $LuFe_4Ge_2$ under high pressure probed by μSR — •Shanu Dengre[1], Rajib Sarkar[1], M.O. Ajeesh[2], Philipp Materne[1], Rustem Khasanov[3], Katharina Weber[2], Christoph Geibel[2], Michael Nicklas[2], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU-Dresden, 01069-Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187-Dresden, Germany — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232-Villigen, Switzerland

$LuFe_4Ge_2$ is a geometrically frustrated magnetic system with antiferromagnetic (AFM) ordering at $T_N = 36$ K. In this work, we used μSR spectroscopy to study the pressure evolution of magnetic phase diagram of $LuFe_4Ge_2$. Previous electrical transport investigations showed a continuous suppression of T_N to zero temperature at 1.7 GPa and suggested the existence of a second pressure-induced magnetic phase. Our transverse field - μSR experiments find a 100% magnetic volume below T_N in the low pressure AFM phase. Further, they prove the presence of a second long-range antiferromagnetically ordered phase at higher pressures and also indicate that the complete sample volume is magnetically ordered in this phase. The obtained ordering temperatures are in good agreement with the electrical resistivity data. The low temperature muon precision frequency does not change between zero and 2.25 GPa, which is consistent with a similar size of the ordered moment in the two different magnetic phases.

TT 19.21 Mon 15:00 P2-EG

Magnetic order and spin dynamics in a helical magnetic system $Fe_3PO_4O_3$ — •Rajib Sarkar[1], Sirko Kamusella[1], Sascha Albert Bräuninger[1], Stefan Holenstein[2], Hubertus Luetkens[2], James Neilson[3], Michael Tarne[3], Kate Ross[3], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Physics, Colorado State University, Fort Collins, Colorado 80523-1875, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

The 3d-electronic spin dynamics and the magnetic order in $Fe_3PO_4O_3$ were investigated by μSR and the ^{57}Fe Mössbauer experiments. Zero field (ZF)-μSR and the ^{57}Fe Mössbauer studies prove the static long range magnetic ordering below $T_N \approx 163$ K. Both transverse field (TF) and ZF-μSR results evidence 100% magnetic volume fraction in the ordered state. ZF-μSR time spectra can be best described by a Bessel function which is consistent with the helical type of magnetic structure as proposed by the neutron scattering experiments. ^{57}Fe Mössbauer results are also consistent with the helical magnetic structure. While spin-lattice relaxation rate (λ) exhibits a peak at the magnetic ordering related to the critical fluctuations, another peak shows up also at around 35 K signaling the presence of secondary relevant energy scale in $Fe_3PO_4O_3$.

TT 19.22 Mon 15:00 P2-EG

Magnetic order and spin dynamics in $La_2O_2Fe_2O(S/Se)_2$ probed by ^{57}Fe Mössbauer and ^{139}La NMR spectroscopy — •Sirko Kamusella[1], Rajib Sarkar[1], Felix Brückner[1], Vadim Grinenko[1], Hans-Henning Klauss[1], and Byron Freelon[2] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA

We present ^{57}Fe Mössbauer and ^{139}La NMR studies on $La_2O_2Fe_2OS_2$ in the magnetically ordered state and paramagnetic state. Similar to $La_2O_2Fe_2OSe_2$ [1] we observed a non collinear magnetic structure in $La_2O_2Fe_2OS_2$, accounting for the explicitly broken x-y-symmetry in the layered structure. The magnetism in this compound is based on frustrated J1-J1'-J2 interactions and single-ion anisotropy. However, unexpected observations occurred: The continuous reduction of the principal component V_{zz} of the EFG below $1.4T_N$ for both compounds and the continuous slowing down of the spin fluctuations as reflected in the NMR spin lattice relaxation rate ($^{139}T_1$) could be discussed in the context of spin-nematicity.

Therefore, parts of our investigations can be related to advanced theoretical concepts which are used to model the physics in these materials, such as orbital selective Mottness [2], biquadratic spin interactions and two magnon relaxation.

[1] M. Günther *et al.*, Phys. Rev. B. **90** 184408 (2014)
[2] L. Craco *et al.*, J. Phys. Condens Matter. **26**, 145602 (2014)

TT 19.23 Mon 15:00 P2-EG

Persistent spin dynamics in $NaCaCo_2F_7$ as evidenced by μSR — •Sascha Albert Bräuninger[1], Rajib Sarkar[1], Jason W. Krizan[2], Shanu Dengre[1], Philip Materne[1], Chris Baines[3], Hubertus Luetkens[3], Robert J. Cava[2], and Hans-Henning Klauss[1] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

The fluoride pyrochlore $NaCaCo_2F_7$ is a newly discovered frustrated pyrochlore with a frustration index of $f = \frac{|\theta_{CW}|}{T_f} \approx 56$. While recent NMR experiments on $NaCaCo_2F_7$ suggested a spin frozen state below 3 K, neutron scattering experiments on the other hand proposed XY like antiferromagnetic spin clusters at low energies. We present μSR studies on $NaCaCo_2F_7$. Present results indicate the slowing down of the magnetic spin fluctuation upon cooling towards the NMR and neutron scattering spin frozen state transition temperature of $T_{sf} \approx 3.0$ K. The μSR relaxation rate increases slightly below this frozen state, and remains constant down to 20 mK. In the μSR window there is no indication of static magnetism in $NaCaCo_2F_7$. In longitudinal field (100-4000 G) the relaxation rate do not vary indicating that the spin fluctuations are dynamic, and this is persistent even at $T \approx 20$ mK. While persistent spin dynamics (PSD) appears to be a generic feature of frustrated magnetic systems, it is not clear so far for the present case whether this is associated with quantum fluctuations, spin-liquid physics, or some other effect.

TT 19.24 Mon 15:00 P2-EG

Magnetostriction and Thermal Expansion of α-$RuCl_3$ — •Mohammad Hossein Haghighi[1], Laura T. C. Bohórquez[1], Anja U. B. Wolter[1], Paula J. Kelley[3,4], Stephen E. Nagler[4], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA — [4]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

α-$RuCl_3$ crystallizes in a layered honeycomb structure and has been proposed as a candidate to realize a fractionalized Kitaev model with strongly frustrated, bond-dependent, anisotropic interactions between Ru^{3+} magnetic moments. We report on angular dependent dilatometric measurements of α-$RuCl_3$, probing the thermal expansion of its lattice as well as its coupling to the magnetic spins via magnetostriction experiments in a wide range of temperatures and magnetic fields. By combining the changes of the thermal expansion and the heat capacity at the magnetic transition via the Ehrenfest relation, strong and anisotropic uniaxial pressure dependencies of α-$RuCl_3$ have been revealed.

TT 19.25 Mon 15:00 P2-EG

High-field ESR studies of the strong-leg spin-1/2 ladder antiferromagnet DIMPY — •A.N. Ponomaryov[1], J. Wosnitza[1,2], K. Povarov[3], D. Schmidiger[3], A. Zheludev[1], and S.A. Zvyagin[1] — [1]Hochfeld-magnet Labor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Dresden, Germany — [3]Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zürich, Switzerland

We report on high-field ESR studies of the Cu^{2+}-based strong-leg spin-1/2 ladder antiferromagnet $(C_7H_{10}N)_2CuBr_4$ (also known as DIMPY). ESR spectra were measured at frequencies from 58 to 450 GHz at 1.5 K. In addition to the gapped mode observed previously [M. Ozerov et al., Phys. Rev. B **92**, 241113(R) (2015)] a fine structure of the gapless mode was revealed. The data were analyzed employing ESR exchange narrowing theory, allowing us to estimate the interladder exchange interaction, $J' = 77$ mK. Further peculiarities of the ESR spectra of

DIMPY will be discussed.

This work was partly supported by the DFG.

TT 19.26 Mon 15:00 P2-EG

Low temperature thermodynamic properties of the quantum spin liquid candidate $YbMgGaO_4$ — •Sebastian Bachus, Yoshifumi Tokiwa, Andreas Wörl, Yuesheng Li, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

A quantum spin liquid (QSL) is a new state of matter which shows no ordering of its magnetic moments even at lowest temperatures. It has attracted a lot of attention in the last years due to its exotic behaviour as well its relevance for high temperature superconductors [1].
Recently, the very promising QSL candidate $YbMgGaO_4$ has been found, where the Yb^{3+}-ions form a triangular lattice. Heat capacity and Muon spin relaxation measurements down to 0.05 K provide evidence for the formation of a U(1) QSL ground state [2-4].
Since the antiferromagnetic coupling constant J is in the order of 1 K, further investigations of the low temperature properties are crucial for a better understanding of this compound.
Here, we report various low temperature measurements of specific heat, thermal expansion and magnetostriction down to 40 mK.

[1] P. A. Lee, Rep. Prog. Phys., **71** (2008)
[2] Y. Li et al., Sci. Rep., **5**, 16419 (2015)
[3] Y. Li et al., Phys. Rev. Lett., **115**, 167203 (2015)
[4] Y. Li et al., Phys. Rev. Lett., **117**, 097201 (2016)

TT 19.27 Mon 15:00 P2-EG

Characterization and optimized synthesis parameters of haydeeite α-$Cu_3Mg(OH)_6Cl_2$, an S = 1/2 kagome magnet — •Joy Desor, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

Haydeeite α-$Cu_3Mg(OH)_6Cl_2$ is one of the few examples of $S = \frac{1}{2}$ kagome magnets, that do not show the conventional Néel order at low temperatures[1]. It is the Mg equivalent of kapellasite, the isostructural compound of the prominent spin liquid candidate herbertsmithite.

We present the results of the haydeeite synthesis via the known reflux and a new hydrothermal approach. We have varied several parameters, as e.g. molar ratios, time and temperature gradient. The results were analyzed by PXRD and EDS. This will serve as a starting point for the crystal growth under hydrothermal conditions. Observation of the magnetic properties at low temperatures and specific heat reveals the features of highly frustrated kagome systems.

[1] R.H. Colman, A. Sinclair, and A.S. Wills, Chem. Mat. 22, 5774 (2010).

TT 19.28 Mon 15:00 P2-EG

New 3d-5d double perovskites containing Ir^{5+} — •Klaus K. Wolff[1], Martin Jansen[2], Alexander C. Komarek[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Double perovskites with the general formula $A_2BB'O_6$ (A = alkaline-earth or rare earth metal, B = 3d transition metal, B' = 4d or 5d transition metal) with an ordered rock-salt-like arrangement of corner-sharing alternating BO_6 and $B'O_6$ units are functional materials that have been extensively studied and are suitable for many applications, especially new magnets. For instance, Sr_2FeMoO_6 is a half-metallic ferromagnet (T_C = 415 K) showing colossal magnetoresistance, and Sr_2CrOsO_6 exhibit ferrimagnetic ordering up to very high temperatures (T_C = 725 K).

There are several representatives of double perovskites of the type A_2BIrO_6 (B = trivalent metal) containing Iridium in the formal oxidation state +5. The combination $SrLaBB'O_6$ gives the possibility to combine divalent transition metal ions with Ir^{5+}. By this approach, we were able to synthesize the new compounds $SrLaNiIrO_6$ and $SrLaCuIrO_6$. The first compound crystallizes monoclinically, whereas the second material presents higher tetragonal symmetry with significant Jahn-Teller distortion in the coordination sphere of the $3d^9$ ion Cu^{2+}. Both compounds show isolating behavior. Electronic transport and magnetic data of the powder samples will be presented.

TT 19.29 Mon 15:00 P2-EG

The α-$RuCl_3$ honeycomb system: magnetic anisotropy, high field torque magnetometry and Li- intercalation — •Michael Baenitz[1], Christof Haas[2], Kimberly Modic[1], Mayukh Majumder[1], Hiroshi Yasuoka[1], Helge Rosner[1], Alexander Tsirlin[2], Ernst Wilhelm Scheidt[2], Wolfgang Scherer[2], and Markus Schmidt[1] — [1]MPI for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institut fuer Physik, Universitaet Augsburg, 86135 Augsburg, Germany

4*d*- and 5*d*-magnets show a wide variety of magnetic ground states due to crystal electric field (CEF) splitting and strong spin-orbit coupling (SOC). The Heisenberg-Kitaev model (HKM) was successfully applied for the competing bond-dependent exchange interactions in the 5*d*-honeycomb iridates. α-$RuCl_3$ turns out to be an excellent candidate for that model because the low-spin 3+ state of Ru ($4d^5$) is equivalent to the low-spin 4+ state of Ir ($5d^5$). α-Ru trichloride exhibit a strong magnetic anisotropy evidenced from specific heat and magnetization measurements on single crystals [1]. Here we present torque magnetometry in fields up to 65 T combined with angular dependent magnetization measurements in fields up to 7 T on highly pure single crystals. Furthermore we succeeded in the intercalation of Li into the α-$RuCl_3$ lattice which leads to a suppression of the 8K magnetic order and a reduction of the Curie Weiss moment. Reducing the valency of Ru 3+ towards the 2+ state is rather interesting and opens up a new route to tune this qunatum magnet towards the spin liquid state.

[1] M. Majumder et al. PRB 91 (2015)

TT 19.30 Mon 15:00 P2-EG

Crystal growth and magnetic characterization of kagome-type materials — •Christian Klein[1], Ranjith Kumar[2], Mahmoud Abdel-Hafiez[1], Michael Baenitz[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-University, D- 60438 Frankfurt am Main, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

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

We report on synthesis and characterization of the spin-1/2 antiferromagnet material Barlowite ($Cu_4(OH)_6BrF$), which represents a model system for two-dimensional kagome-layered structures[2]. The kagome-layers are build up by copper ions and separated from each other through a transition-metal cation, so that a quasi-two-dimensional system is created[3].

Crystals were grown under hydrothermal conditions. Characterization of the samples was done by magnetic measurements to determine the susceptibility and magnetic ordering. Furthermore heat capacity measurements were performed to investigate phase transitions and ordering effects at low temperature.

[1] P. A. Lee, Science 321, 1306 (2008).
[2] T.-H. Han et al., Phys. Rev. Lett. 113, 227203 (2014).
[3] S. Chu et al., Appl. Phys. Lett. 98, 092508 (2011).

TT 19.31 Mon 15:00 P2-EG

Optical conductivity of Na_2IrO_3 supporting the j=1/2 scenario — •Philipp Warzanowski[1], Nick Borgwardt[1], Maria Hermanns[2], Petra Becker[3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln

Na_2IrO_3 is widely discussed as a realization of the Heisenberg-Kitaev model with local j=1/2 moments. Challenging the j=1/2 scenario, a description in terms of quasimolecular orbitals (QMOs) with electrons delocalized over individual Ir_6 rings has been suggested [1]. Our infrared transmittance data in the vicinity of the gap for electron-hole excitations provide a litmus test for the underlying microscopic physics, since theoretical predictions based on either QMOs [2] or local j=1/2 moments [3] disagree strongly on the spectral weight of the lowest optical excitation band. We find that the spectral weight below about 0.7 eV is much smaller than reported previously, supporting the j=1/2 scenario. Moreover, we reveal a series of small absorption features around the onset of electron-hole excitations, pointing towards a mixing of electron-hole excitations with local spin-orbital excitations.

[1] I.I. Mazin *et al.*, Phys. Rev. Lett. 109, 197201 (2012)
[2] Y. Li *et al.*, Phys. Rev. B 91, 161101(R) (2015)
[3] B.H. Kim, G. Khaliullin, and B.I. Min, Phys. Rev. B 89, 081109(R) (2014)

TT 19.32 Mon 15:00 P2-EG

Pressure control of quantum magnets with heavy transition-metals — •Marian Blankenhorn[1], Tomohiro Takayama[2], Kentaro Kitagawa[3], Carl Förderer[1], and Hidenori Takagi[1,2,3] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]University of Tokyo, Tokyo, Japan

Recently, exotic quantum magnetism has been reported in $4d$ and $5d$ transition-metal oxides such as iridates, where the interplay of electron correlation and strong spin-orbit coupling leads to unconventional magnetic coupling. Such $4d$ and $5d$ oxides are regarded as weak Mott insulators produced by modest Coulomb interaction. We expect a pressure induced metal-insulator transition in a moderate pressure range, which may give rise to exotic metallic states and possible superconductivity at the critical point. One of the target materials is the 3-dimensional quantum spin liquid $Na_4Ir_3O_8$, which comprises a hyper-kagome lattice of Ir^{4+}-ions. $Na_4Ir_3O_8$ is known to be tuned into a metal by carrier doping and thus we expect that $Na_4Ir_3O_8$ can be driven into a metallic state by applying pressure. We also study honeycomb-based oxides, which are candidates for quantum spin liquids.

In order to apply high pressure up to 10 GPa, we use an opposed-anvil high pressure cell developed by Kitagawa et al. allowing electric transport measurements. We report preliminary pressure-studies on these heavy transition-metal quantum magnets and discuss the nature of exotic metallic states expected under high pressure.

TT 19.33 Mon 15:00 P2-EG

ESR study of the triangular-lattice antiferromagnet Cs_2CuBr_4 — •E. Schulze[1,2], A. N. Ponomaryov[1], J. Wosnitza[1,2], H. Tanaka[3], and S. A. Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Department of Physics, Tokyo Institute of Technology, Japan

We present high-field electron spin resonance (ESR) studies of the spin-1/2 triangular-lattice antiferromagnet Cs_2CuBr_4. The temperature dependences of ESR parameters (the effective g factor and ESR linewidth) were measured for magnetic fields applied along the three principal directions. From the angular dependence of the ESR linewidth the Dzyaloshinskii-Moriya interaction was estimated. The results are compared with the data obtained on the isostructural compound Cs_2CuCl_4.

TT 19.34 Mon 15:00 P2-EG

Density matrix embedding theory for multi-band Hubbard models — •Michael Schmid and Maria Daghofer — Universität Stuttgart

Density matrix embedding theory (DMET) [1], a recently proposed numerical method when working on many-particle systems, and its cluster formulation (CDMET) [2] are used to investigate strongly correlated electron systems such as multi-band Hubbard models. Firtst the method is tested for the single-band Hubbard model in one and two dimensions. Then we extend the method, which so far was just used to study single-band systems, to multi-band systems. We hope to get further insight into the two-band Hubbard model on a cubic lattice by using an exact diagonalization solver.

[1] G. Knizia et. al., Phys. Rev. Lett. 109, 186404 (2012)
[2] B. Zheng et. al., arXiv preprint arXiv:1608.03316 (2016)

TT 19.35 Mon 15:00 P2-EG

X-ray absorption in strong correlated high T_C superconductors — •Tobias Pitters and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien

In X-ray absorption spectroscopy, a possible process is to create a core hole an add the electron to the valence states. Theoretically, this can be treated by evaluating the one-particle Green's function in the presence of a strong potential. When modelling the antiferromagnetic parent state of high-T_C cuprate superconductors, the potential can be onsite or situated between two neighboring sites. We analyze this problem for parameter regimes relevant to cuprates and iridates using the self-consistent Born approximation.

TT 19.36 Mon 15:00 P2-EG

Variational Cluster Approximation for Spin Liquids — •Teresa Schaller and Maria Daghofer — Institut für funktionelle Materie und Quantentechnologien, Universität Stuttgart, Deutschland

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of multi-band Hubbard models. The approach includes quantum fluctuations on a small cluster exactly and long-range order on a mean-field level. We will in particular investigate the filling of five electrons in the t_{2g} subshell, as it is realized in some iridium compounds. The interaction of Hund's rule and spin-orbit coupling leads to various magnetic orderings in the ground state. We present the phase diagram resulting from this competition and the impact of crystal-field splitting.

TT 19.37 Mon 15:00 P2-EG

Mean-field extension of the variational cluster approach — •Jan Lotze and Maria Daghofer — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Pfaffenwaldring 57, 70550 Stuttgart

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. Both systems must share the same two-body interactions, but may differ in one-body terms such as the kinetic hopping. Within VCA, the reference system is formed by isolated clusters. From the SFT perspective, inter-site interactions cannot be included. We propose to incorporate interactions along bonds inside the clusters exactly, while those between clusters are mean-field decoupled. Although this is an approximation, it should be controlled by the cluster-size as for pure VCA.

Results obtained for the extended Hubbard model in one and two dimensions on a square [1] and a honeycomb lattice [2] are shown.

[1] M. Aichhorn, H. G. Evertz, W. von der Linden and M. Potthoff, Phys. Rev. B **70**, 235107 (2004)
[2] M. Daghofer and M. Hohenadler, Phys. Rev. B **89**, 035103 (2014)

TT 19.38 Mon 15:00 P2-EG

Disordered Weyl spin liquids — •Kevin O'Brien, Maria Hermanns, and Simon Trebst — Universität zu Köln

Electronic Weyl semimetals have garnered considerable attention since their recent observation in TaAs and photonic materials. Here we investigate the spin analogue of the electronic Weyl semimetal – the *Weyl spin liquid*.

Such a state can be readily found in generalizations of the Kitaev honeycomb model on certain three-dimensional tricoorinated lattices. In these Weyl spin liquids, the original spin-1/2 moments form a quantum spin liquid wherein they fractionalize into gapped flux excitations of a Z2 gauge field as well as into Majorana fermions which form the gapless Weyl dispersion. One unusual aspect of the Weyl spin liquid is that it may appear under symmetry conditions which would forbid the formation of its conventional electronic counterpart, namely, with both time-reversal and inversion symmetry intact.

In this work we discuss some general properties of Weyl spin liquids as well as the impact of disorder. In particular, we investigate the effects of short- and long-range correlated disorder on the low-energy physics of these systems, and to what extent disorder is sensitive to the underlying symmetry class.

TT 19.39 Mon 15:00 P2-EG

Thermodynamics of spin fractionalization in Kitaev matter — •Tim Eschmann and Simon Trebst — Institute for Theoretical Physics, University of Cologne

The fractionalization of quantum numbers is one of the most intriguing phenomena in quantum many-body systems. Here we study the thermodynamic signatures of spin fractionalization in Kitaev models in two and three spatial dimensions by means of numerically exact quantum Monte Carlo techniques. Analytically, the fractionalization of the original spin degrees of freedom into itinerant Majorana fermions and a static $\mathbb{Z}_2$ gauge field is well understood at zero temperature and has led to a comprehensive classification of the emergent Majorana metals for a variety of two and three-dimensional lattices relevant to a number of spin-orbit dominated materials. Here, we put our focus on the physics of the $\mathbb{Z}_2$ gauge field and discuss the finite-temperature phase transitions associated with the ordering of the gauge field in three spatial dimensions.

TT 19.40 Mon 15:00 P2-EG

Spin liquids and competing magnetic orders in three-dimensional kagome magnets — •Finn Lasse Buessen and Simon Trebst — University of Cologne, Germany

One of the best experimentally established spin liquids is found in the

hyperkagome compound Na4Ir3O8 where geometric frustration is an inherent feature of its three-dimensional lattice structure of corner-sharing triangles. Here we present a detailed numerical analysis of these systems in the presence of competing nearest and next-nearest neighbor interactions using a recently developed pseudo-fermion functional renormalization group (pf-FRG) approach. We discuss why this approach allows to access the strong-coupling regime of quantum spin systems, highlight technical aspects of a state-of-the-art numerical implementation, and demonstrate its applicability for the hyperkagome systems and other three-dimensional frustrated quantum magnets.

TT 19.41 Mon 15:00 P2-EG

Spectral function of a quantum dimer model for the pseudogap metal — •Sebastian Huber and Matthias Punk — Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany

We study a quantum dimer model [1,2], which describes several key properties of the pseudogap phase of hole-doped cuprates at low hole density p. The configurations of the system are built from two species of dimers: Fermionic dimers that carry spin S = 1/2 and charge +e embedded in a neutral background of bosonic spin singlet dimers.
We compute electron spectral functions using exact diagonalization on lattices of size 6x6 and find clear signature of the so-called pseudogap at the antinode in momentum space.
In a second part we show how to implement a cluster dynamical mean-field approach in order to calculate spectral properties of the quantum dimer model with higher resolution. The cluster impurity problem is solved using the numerical renormalization group technique.

[1] D. S. Rokhsar and S. A. Kivelson, PRL 61, 20 (1988)
[2] M. Punk, A. Allais and S. Sachdev, PNAS 112, 31 (2015)

TT 19.42 Mon 15:00 P2-EG

Dynamics of a triangular spin-ladder with ring exchange — •Jonas Richter and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Ring exchange processes which become non-negligible in weak Mott insulators, typically enhance magnetic frustration and may lead to novel physics. Using linear response theory, we study the finite temperature spin and current dynamics of a triangular two-leg spin ladder with additional four-spin ring exchange which can potentially be viewed as a one-dimensional descendent of the organic Mott insulator κ-$(ET)_2Cu_2(CN)_3$. Employing complementary numerical methods, namely exact diagonalization, the Lanczos algorithm and dynamical quantum typicality, we present results for the static and dynamic structure factor, spin and energy conductivities and their corresponding Drude weights. We explore the relevant parameter space, both into the spin-Peierls as well as into the putative spin-Bose metal phase and uncover unique features in the spin dynamics which are not present for nearest-neighbor Heisenberg exchange only.

TT 19.43 Mon 15:00 P2-EG

Thermal transport in the Kitaev spin model — •Angelo Pidatella[1], Alexandros Metavitsiadis[2], and Wolfram Brenig[2] — [1]Institute for Theoretical Physics, Technical University of Dresden — [2]Institute for Theoretical Physics, Technical University of Braunschweig

We analyze the dynamical thermal conductivity of the Kitaev spin model on the honeycomb lattice, which constitutes an exactly solvable example for a Z_2 spin liquid. Using a mapping to Majorana particles, the thermal transport is described in terms of matter fermions interacting with a Z_2 gauge field. Findings for the transport coefficient within linear response theory will be discussed in the long wave length limit, at finite frequency, and arbitrary temperature. For the zero flux sector, analytic results will be presented, while finite flux densities will be treated numerically within a real space approach, invoking either a summation over all gauge sectors, or using an average gauge field configuration approach. Comparison with findings for the thermal transport in Kitaev spin ladders will also be provided.

TT 19.44 Mon 15:00 P2-EG

The spin-1/2 Kagome XXZ model in a field: competition between lattice nematic and solid orders — •Augustine Kshetrimayum[1], Thibaut Picot[2], Román Orús[1], and Didier Poilblanc[2] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Laboratoire de Physique Théorique, IRSAMC, CNRS and Université de Toulouse, UPS, F-31062 Toulouse, France

We study numerically the spin-1/2 XXZ model in a field on an infinite Kagome lattice. We use different algorithms based on infinite Projected Entangled Pair States (iPEPS) for this, namely: (i)an approach with simplex tensors and 9-site unit cell, and (ii) an approach based on coarse-graining three spins in the Kagome lattice and mapping it to a square-lattice model with local and nearest-neighbor interactions, with usual PEPS tensors, 6- and 12-site unit cells. We observe the emergence of several magnetization plateaus as a function of the field for different values of the anisotropy. We focus on the 1/3 plateaus using both the techniques and study the nature of its ground state as we tune the anisotropy from the Ising regime to the XY regime through the Heisenberg point and find a strong competition between lattice nematic and solid orders.

TT 19.45 Mon 15:00 P2-EG

Topological domain walls in helimagnets — •Laura Köhler[1], Jan Müller[2], Achim Rosch[2], Peggy Schönherr[3], Dennis Meier[3,4], and Markus Garst[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Cologne, Germany — [3]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [4]Department of Materials Science and Engineering, Norwegian University of Science and Technology, 7491 Trondheim, Norway

A magnetic helix arises in chiral magnetic materials with a wavelength set by the spin-orbit coupling. Using micromagnetic simulations and comparing to experimental studies on surfaces of FeGe, we show that domain walls of such helimagnetic order are distinctly different from ferromagnets and rather similar to grain boundaries of liquid crystals. Three types of domain walls are realized depending on the relative domain orientation: a curvature wall, a zig-zag disclination wall and a dislocation wall. Disclinations are vortex defects in the helix axis orientation, and they can be combined to form dislocations. We discuss the topological skyrmion charge associated with these defects, and we demonstrate that domain walls of helimagnetic order can carry a finite topological charge on average. As a consequence, they can be manipulated by spin currents and contribute to a topological Hall effect.

TT 19.46 Mon 15:00 P2-EG

Fermi surfaces of B20 compounds from Density Functional Theory and de Haas-van Alphen effect — Schorsch Michael Sauther[2], •Arthur Niedermayr[1], Matthias Dodenhöft[4], Andreas Bauer[1], Frank Freimuth[3], Bernd Zimmermann[3], Yuriy Mokrousov[3], Dirk Grundler[5], Christian Pfleiderer[1], and Marc Andreas Wilde[1] — [1]Phys.-Dep. E51, TU München — [2]Phys.-Dep. E10, TU München — [3]Peter Grünberg Institute, Jülich — [4]Phys.-Dep. E21, TU München — [5]LMGN, Lausanne

The class of chiral intermetallic compounds with cubic B20 crystal structure have attracted a lot of interest. Manganese silicide (MnSi) is a metal known for its unusual magnetic properties including a skyrmion lattice phase as well as for its strong electronic correlations and non-Fermi liquid behavior under pressure. The isostructural iron silicide (FeSi), on the other hand is commonly assumed to be a strongly correlated small-gap semiconductor at low temperature. However, the nature of the insulating state and the role of the crystal surface are not yet fully settled. We combine density functional theory (DFT) calculations and the de Haas-van Alphen (dHvA) effect in order to investigate the electronic properties of B20 compounds. First results indicate a substantial role of spin-orbit coupling for the Fermi surface properties of MnSi.

TT 19.47 Mon 15:00 P2-EG

Optical conductivity of layered ruthenates: spin-orbit and anistropic Coulomb interaction effects — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich,D-52425 Jülich, Germany

Using the LDA+DMFT approach, we calculate the in-plane and out-of-plane optical conductivity of the single-layered (Sr_2RuO_4) and double-layered ($Sr_3Ru_2O_7$) ruthenates. The calculations are performed via linear response theory and Kubo's formalism. We investigate the effects of the electron-electron interaction, the spin-orbit coupling and the low-symmetry Coulomb interaction in the optical spectra. We show that including the spin-orbit coupling improves the agreement with experimental data while the anisotropic Coulomb interaction does not change the in-plane optical spectrum. We find that, contrary to the out-of-plane conductivity, the in-plane conductivity changes con-

siderably by changing temperature and Coulomb interaction and by including the spin-orbit coupling. We explain the difference in behaviour of the in-plane and out-of-plane conductivities in terms of the corresponding non-interacting transport functions. Furthermore, we discuss the effective mass-enhancement and quasi-particle scattering rate.

TT 19.48 Mon 15:00 P2-EG

Crystal structure determination of Ti-doped Ca_2RuO_4 — •Sebastian Hoffmann, Stefan Kunkemöller, Kevin Jenni, and Markus Braden — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

The crystal structure of 0, 1 and 10% Ti-doped Ca_2RuO_4 was determined by single crystal X-ray diffraction at 100K and 300K. To clarify the mechanism of superconductivity in Sr_2RuO_4, the phase diagram of $Ca_{2-x}Sr_xRuO_4$ was analysed, which possesses ferromagnetism, anitferromagnetism, superconductivity, orbital ordering and metal-insulator transitions. Sr_2RuO_4 is isostructural to the ideal tetragonal K_2NiF_4 structure with spacegroup $I4/mmm$ and non-distorted NiF_6-octahedra. The Mott insulator Ca_2RuO_4 crystallizes in the orthorhombic spacegroup $Pbca$, in which the RuO_6-octahedra are highly distorted. Upon cooling, structural changes lead to effects like the anomalous elongation of the b-lattice constant and to a shortening of the a- and c-lattice constant. These changes are accompanied by a flattening, rotation and tilting of the RuO_6-octahedra, with the tilt occuring around the b-lattice constant. In Ca_2RuO_4 there seems to be a connection of the magnetic ordering at low temperatures and the structural behaviour. Upon cooling below 110K, where antiferromagnetic order sets in, the elongation of the b-lattice constant saturates. Ti doping up to 10% seems to change the elongation from $b(300K) - b(T_N) = 0.1643$Å down to 0.0898Å. For the Ti-doped samples, the anomalous properties of Ca_2RuO_4 (relative to Sr_2RuO_4) are thus attenuated.

TT 19.49 Mon 15:00 P2-EG

Crystal growth of Ti-doped perovskite ruthenates — •Kevin Jenni, Sebastian Hoffmann, Stefan Kunkemöller, and Markus Braden — II. Physikalisches Institut, Universität zu Köln

Ruthenates of the Ruddlesden-Popper series exhibit a variety of interesting phenomena ranging from unconventional superconductivity in Sr_2RuO_4 to the Mott-insulating state in Ca_2RuO_4. Titanium doping has been found to alter dramatically the physical properties of these materials. By partially replacing the Ruthenium in the Oxygen octahedra by nonmagnetic four-valent Titanium magnetic fluctuations can be stabilized which leads to a SDW ordering in $Sr_2Ru_{0.91}Ti_{0.09}O_4$ or $Sr_3(Ru_{0.91}Ti_{0.09})_2O_7$. In $Ca_{1.78}Sr_{0.22}Ru_{0.9}Ti_{0.1}O_4$ a metal-insulator phase transition can be observed around 80 K in contrast to the undoped sample which is metamagnetic. However the availability of ruthenate crystals is limited because the growth is challenging due to the high evaporation of ruthenium up to 90% and the intergrowth of different layered ruthenates. Therefore the determination of exact growth parameters is crucial. We present the growth of single crystals of $Ca_{1.78}Sr_{0.22}Ru_{1-x}Ti_xO_4$ and $Ca_{2-x}Sr_xRuO_4$. The crystal growth was conducted by travelling floating-zone method using a Canon SC1-MDH mirror furnace yielding large crystals.

TT 19.50 Mon 15:00 P2-EG

Giant Magnetostriction, structural domain switching, and anomalous Hall effect on untwinned $SrRuO_3$ single crystals — •Danie Brüning, Stefan Kunkemöller, Markus Braden, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Deutschland

$SrRuO_3$ is the infinite-layer material of the well-known Ruddlesden-Popper series of ruthenates $Sr_{n+1}Ru_nO_{3n+1}$, which have attracted enormous interest not only due to the unconventional superconductivity in Sr_2RuO_4. Ruthenates show a large variety of physical phenomena due to electronic correlations and spin-orbit coupling. $SrRuO_3$ is the only ferromagnetic metal in this series. It is heavily studied as a conducting perovskite layer in thin films. Despite the big interest in the research of $SrRuO_3$ large and high quality single crystals became available only very recently. Our high quality cm^3 size single crystals are grown with the optical floating zone technique. From the high temperature cubic phase $SrRuO_3$ becomes tetragonal and orthorhombic via two transitions which allows for 6 twins. With uniaxial pressure applied upon cooling it is possible to untwin these crystals. We present investigations on the switching of the different structural domain states linked to a giant magnetostriction. Additionally, we analyze the anomalous Hall effect of $SrRuO_3$ and the anisotropy gap in the magnon dispersion.

Supported by the DFG via CRC 1238.

[1] S. Kunkemöller et al., Crys. Res. and Technol., 51: 299 (2016)

TT 19.51 Mon 15:00 P2-EG

"Ferroelectric" phase transition in conducting $Sr_{1-x}Ca_xTiO_{3-\delta}$ — •Dennis Finck, Steffen Harms, Xiao Lin, Christoph P. Grams, Johannes Engelmayer, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Germany

Insulating $SrTiO_3$ is a so-called quantum paraelectric close to an ferroelectric instability. On the one hand, the substitution of strontium ions by smaller and isovalent calcium ions induces a ferroelectric phase at finite temperatures. On the other hand, $SrTiO_3$ becomes metallic and even superconducting at temperatures below 1K after charge carrier doping [1].

Therefore the question arises what happens when both effects are combined. Here, we provide experimental evidence for a polar ground state also in the metallic compound. As mobile charge carriers screen the electric polarization, it is technically not possible to directly measure ferroelectricity. Thus, our conclusion ist based on measurements of sound velocities and thermal expansions.

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] B. S. de Lima, M. S. da Luz, F. S. Oliveira, L. M. S. Alves, C. A. M. dos Santos, F. Jomard, Y. Sidis, P. Bourges, S. Harms, C. P. Grams, J. Hemberger, X. Lin, B. Fauqué, and K. Behnia,
Phys. Rev. B **91**, 045108 (2015)

TT 19.52 Mon 15:00 P2-EG

Impact of electron doping on thermodynamic and transport properties of the magnetoelectric antiferromagnet $EuTiO_{3-\delta}$ — •Johannes Engelmayer, Christoph Grams, Xiao Lin, Joachim Hemberger, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Various perovskite titanates $ATiO_3$ are known to undergo ferroelectric phase transitions, e.g., for $A = \mathrm{Ba, Pb, Cd}$. In contrast, $CaTiO_3$ and $SrTiO_3$ show quantum paraelectric behavior, that is, ferroelectric long-range order is suppressed by quantum fluctuations. In addition, the insulating $SrTiO_3$ becomes metallic upon electron doping via oxygen deficiencies ($SrTiO_{3-\delta}$ with $\delta > 0$) and even shows superconductivity for certain carrier concentrations. The rare-earth titanate $EuTiO_3$ is similar to $SrTiO_3$. Both, Eu^{2+} and Sr^{2+} have the same ionic radii, but Sr^{2+} is nonmagnetic while Eu^{2+} has a large magnetic moment of $7\mu_B$. Below $T_N = 5.5$ K the localized 4f moments order antiferromagnetically in a G-type configuration. While stoichiometric $EuTiO_3$ is semiconducting, metallic behavior can be induced by oxygen deficiencies, similar to $SrTiO_{3-\delta}$. Here, we present a detailed characterization of $EuTiO_{3-\delta}$ with $-10^{-2} \leq \delta \leq 10^{-2}$ based on field- and temperature-dependent measurements of magnetization, specific heat, and thermal expansion. Moreover we use resistivity and permittivity measurements as complementary methods to investigate the magnetoelectric properties, since the conductivity of the samples covers 17 orders of magnitude.

TT 19.53 Mon 15:00 P2-EG

Correlating paramagnetic spin centers in the 'nonmagnetic' $5d^4$ compound Ba_2YIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Franziska Hammerath[1], Gizem Aslan Cansever[1], Tushar Dey[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden,D-01171 — [2]Institut für Festkörperphysik, Technische Universität Dresden,D-01062

We will present the electron spin resonance results of the double perovskite Ba_2YIrO_6. This material provides a playground to examine the magnetic interactions in a 5d transition metal oxide with strong spin-orbit coupling. Theory predicts that due to the strong spin-orbit coupling this $5d^4$ iridate should be in a nonmagnetic state. However, static magnetic and NMR measurements evidence the occurrence of paramagnetic spin centers that are correlated at low temperatures. To obtain deeper insight into the magnetic properties of Ba_2YIrO_6 ESR measurements of a polycrystalline sample were carried out for several temperatures and frequencies. This enables to quantify several different paramagnetic spin centers. Two of them correspond to S=1/2 with the g-factor g=1.99 and g=1.90, and the third one to S=3/2 with g=1.49. An overview of the possible origins for the different spin cen-

ters and their relevance to the unexpected magnetism of this compound will be shown on this poster.

TT 19.54 Mon 15:00 P2-EG

NMR Investigation of Ir-based Double Perovskites — •Margarita Iakovleva[1,2,3], Evgeniia Vavilova[3], Hans-Joachim Grafe[1], Manna Kaustuv[4], Michael Vogl[1,2], Tusharkanti Dey[5], Sabine Wurmehl[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Zavoisky Physical-Technical Institute, Kazan, Russia — [4]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [5]Universität Augsburg, Augsburg, Germany

Iridium based double perovskites are unique materials where Coulomb repulsion, strong spin-orbit coupling, exchange interaction and crystal field have comparable energy scales. The interplay between all of these interactions and correlations may lead to the emergence of novel electronic and magnetic states. In this work we report the ^{139}La nuclear magnetic resonance (NMR) results on the double perovskite compounds La_2MIrO_6 with magnetic and nonmagnetic ions at the M position (M = Co, Cu, Zn). Nuclear relaxation rate ${T_1}^{-1}$ measurements in La_2CuIrO_6 show the peak at $T \approx 74$ K that is the signature of a magnetic transition. Moreover with further decreasing the temperature the T-dependence of ${T_1}^{-1}$ shows the shoulder at $T \approx 60$ K that can be associated with a cooperative ordering of the transverse moments. In case of La_2CoIrO_6 the ${T_1}^{-1}$ measurements do not show any anomalies at T below the ordering temperature. Our investigation has revealed complex magnetic interactions in the compound where strongly spin-orbit coupled 5d transition metal ions coexist with strongly correlated spin-only 3d (Co, Cu) and non-magnetic Zn ions.

TT 19.55 Mon 15:00 P2-EG

Microstructuring Quantum Materials — •Toni Helm, Maja Bachmann, Kimberly Modic, Kent Shirer, Markus König, Sebastian Seifert, Nabhanila Nandi, Andrew Mackenzie, and Philip Moll — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

In 'Quantum materials', non-trivial quantum mechanics leads to unusual physical properties that promise the potential to improve our understanding of many body quantum states as well as to spark ideas for novel electronic applications exploiting these unusual properties. Our research focuses on the mesoscale physics of quantum matter, in particular topological matter, unconventional superconductors and magnetic metals when their dimensions become comparable to their relevant length scales on the micron and sub-micron level. We develop techniques based on focused ion beam (FIB) micromachining to fabricate mesoscopic devices from single crystals. We showcase three examples of the wide range of materials and applications approachable by microstructuring: We show (1) how Fermi arc surface states contribute to the charge transport in microstructures of the Dirac semimetal Cd_3As_2 on length scales smaller than the mean-free-path; (2) how a subtle phase transition just above the superconducting transition changes the electronic structure in the quasi-1D metal $Ta_4Pd_3Te_{16}$, revealed by resistivity anisotropy measurements on the micron-scale and (3) how micro-channels of ultra-pure metals with electron-electron scattering such as $PdCoO_2$ can lead to hydrodynamic corrections to the standard ballistic transport.

TT 19.56 Mon 15:00 P2-EG

Cantilever-based torque magnetometry for de Haas-van Alphen experiments on correlated metals — •Marc Andreas Wilde, Schorsch Michael Sauther, Arthur Niedermayr, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany

Cantilever-based torque magnetometers have been optimized to measure the quantum oscillations of the magnetization, i.e., the de Haas-van Alphen (dHvA) effect in both correlated bulk metals and low-dimensional electron systems. For strongly correlated bulk metals the focus of the sensor and readout design is on a compact, rotatable and Millikelvin-compatible setup that fits into the bore of standard high-field superconducting solenoids. For low-dimensional systems highest sensitivity due to the inherently small signal strength is a prerequisite. We present specific implementations based on capacitive readout and fiber-optical interferometry and discuss their advantages and limitations in the context of dHvA experiments on correlated metals. In particular when large bulk crystals are not available, position readout techniques that do not scale with the sensor size are shown to be advantageous.

TT 19.57 Mon 15:00 P2-EG

Experimental determination of the Fermi surface in transition metal diborides — •Schorsch Michael Sauther[1], Matthias Dodenhöft[1], Matthias Brasse[1], Stephan Gerhard Albert[1], Jan Kuneš[2], Andreas Bauer[1], Alexander Regnat[1], Olga Young[3], Uli Zeitler[3], Christian Blum[4], Sabine Wurmehl[4,5], Dirk Grundler[6], Christian Pfleiderer[1], and Marc Andreas Wilde[1] — [1]Physik-Department, TU München — [2]Institute of Physics, Academy of Sciences, Prag — [3]HFML-EMFL, Radboud University, Nijmegen — [4]IFW, Dresden — [5]Institut für Festkörperphysik, TU Dresden — [6]LMGN, IMX, STI, EPF Lausanne

Transition metal diborides exhibit a variety of ground states including BCS superconductivity and complex forms of magnetic order. For a detailed understanding of the magnetic and electronic properties a comprehensive picture of the Fermi surface (FS) is a prerequsite. For the itinerant antiferromagnet chromium diboride (CrB_2), e.g., the intricate interplay between FS properties and the complicated magnetic order is not yet fully understood [1]. We employ torque magnetometry at low temperatures down to 0.3 K and in high magnetic fields up to 35 T to measure the quantum oscillations of the magnetization, i.e., the de Haas-van Alphen (dHvA) effect. Combined with density functional theory (DFT) calculations, the dHvA effect is a powerful tool that allows determination of the FS properties. We present recent results on CrB_2 and further isostructural diborides.

[1] M. Brasse *et al.*, Phys. Rev. B **88**, 155138 (2013)

TT 19.58 Mon 15:00 P2-EG

Electrochemical Characterization and Valence Tuning of Lithium Nitridometallates — •Elisa Thauer[1], Alex Ottmann[1], Christoph Neef[1], Manuel Fix[2], Anton Jesche[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Experimentalphysik VI, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

The electrochemical properties of lithium metal nitrides $Li_2Li_{1-x}M_xN$ with M = Fe or Ni and of Li_3N are investigated by cyclic voltammetry and galvanostatic cycling. Based on these results, the lithium content and thus the valence of the transition metal ions is altered electrochemically. In addition to XRD studies on the electrochemically treated materials, the effect of delithiation on the magnetic properties is studied by means of SQUID magnetometry. For $Li_{2.7}Fe_{0.3}N$, electrochemical tuning yields suppression of the initial hard magnetic ground state. In the case of $Li_{2.6}Ni_{0.4}N$, the paramagnetic response diminishes upon delithiation. Finally, we show perspectives for delithiation procedures in Li_3N.

TT 19.59 Mon 15:00 P2-EG

Growth of stoichiometric $LaTiO_3$ thin films by pulsed laser deposition — •Philipp Scheiderer, Matthias Schmitt, Alex Gössmann, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Oxide heterostructures exhibit fascinating properties, e.g., the coexistence of superconductivity and ferromagnetism at the interface of $LaAlO_3/SrTiO_3$, but the extraordinary electronic properties of transition metal oxides (TMOs) caused by electron correlation yet wait to be fully harnessed. The Mott insulator $LaTi^{3+}O_3$ (LTO) is a prototypical material for such strongly correlated TMOs, which can be prepared by pulsed laser deposition. However, in order to obtain stoichiometric LTO strongly reducing growth conditions are required since the thermodynamically stable bulk phase is the oxygen-rich band insulator $La_2Ti_2^{4+}O_7$.

We therefore systematically study the impact of oxidizing and reducing background atmospheres and the oxygen out diffusion from the substrate into thin LTO films. *In situ* x-ray photoelectron spectroscopy of films prepared on STO reveals overoxidation due to oxygen outdiffusion from the STO substrate, which can be partially suppressed by introducing a $LaAlO_{3-x}$ (LAO) buffer layer. Further control over the oxygen stoichiometry is gained by the use of $DyScO_3$ substrates, presumably due to the lower mobility of oxygen. Overoxidation during storage in air can be prevented by introducing a LAO capping layer of a few unit cells thickness, acting again as a diffusion barrier for oxygen.

TT 19.60 Mon 15:00 P2-EG

Synthesis and Characterization of $La_{2-2x}Sr_{1+2x}Mn_2O_7$ thin

films — •Florian Hollemann, Marius Keunecke, Vladimir Roddatis, Daniel Steil, Stefan Mathias, and Vasily Moshnyaga — Georg-August-Universität Göttingen

Perovskite oxides are an intriguing material system showing effects like superconductivity, CMR, metal-insulator transitions. These effects are related to the strong interaction between charge, spin, orbit and lattice degrees of freedom. Because of the inherent 2D structure the layered manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ is attractive as a model system for low-dimensional physics and can serve as a playground to study these interactions. We fabricated Ruddlesden-Popper phase (n=2) $La_{2-2x}Sr_{1+2x}Mn_2O_7$ thin films on LSAT(001) substrates using metalorganic aerosol deposition (MAD), with and without atomic layer epitaxy (ALE). For bulk systems the phase diagram is well known, but for thin films it is not yet completely reported. Our aim is to develop a thin film phase diagram by varying the doping x and characterising the electrical and magnetic behavior by using SQUID and PPMS. The structural quality and phase purity was checked using the in-situ-ellipsometry, XRR, XRD, AFM and TEM.

TT 19.61 Mon 15:00 P2-EG

Emergence of hydrodynamic long-time tails from noisy Boltzmann equations — •Philipp Weiss, Jonathan Lux, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

When an interacting quantum system undergoes a quantum quench, we expect that the system will ultimately reach thermal equilibrium. Local equilibrium is established by scattering of quasiparticles on intermediate time scales. However, global equilibration requires diffusive transport of conserved quantities resulting in a slow algebraic relaxation towards thermal equilibrium. Phenomenologically, the final state of the relaxation can be described by fluctuating hydrodynamics. But, how does this irreversible dynamics emerge from the unitary time-evolution of a closed quantum system?

Here, we address this question within a quantum-kinetic approach. Even on the level of the Boltzmann equation an additional noise term is required to reproduce the algebraic long-time behavior. In a first step, we show that fluctuating hydrodynamics can be derived from the fluctuating Boltzmann equation. Similarly, we aim to derive a "noisy quantum-Boltzmann equation" which mimics the hydrodynamic fluctuations on the quantum level. A possible derivation starts from a modified Keldysh-Dyson equation, supplemented by a noise term. Such an equation defines a noise-dependent Green's function. Following this route, we have to ensure that averaging of "noisy Green's functions" reproduces the exact higher-order correlation functions.

TT 19.62 Mon 15:00 P2-EG

Pumping approximately integrable systems — •Florian Lange, Zala Lenarcic, and Achim Rosch — Universität zu Köln

Weak perturbations can drive an interacting many-particle system far from its initial equilibrium state if one is able to pump into degrees of freedom approximately protected by conservation laws. This concept has for example been used to realize Bose-Einstein condensates of photons, magnons, and excitons. Integrable quantum systems like the one-dimensional Heisenberg model are charac- terized by an infnite set of conservation laws. Here we develop a theory of weakly driven integrable systems and show that pumping can induce huge spin or heat currents even in the presence of integrability breaking perturbations, since it activates local and quasi-local approximate conserved quantities. The resulting steady state is qualitatively captured by a (truncated) generalized Gibbs ensemble with Lagrange parameters that depend on the structure but not on the overall ampli- tude of perturbations or on the initial state. We suggest to realize novel heat or spin pumps using spin-chain materials driven by THz radiation.

TT 19.63 Mon 15:00 P2-EG

A simple tensor network algorithm for 2d steady states — •Augustine Kshetrimayum[1], Hendrik Weimer[2], and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Insitut für Theoretische Physik, Leibniz Universität Hannover, AppelStrasse 2, 30167 Hannover, Germany

We present a tensor network algorithm that approximates steady-states of 2d quantum lattice dissipative systems in the thermodynamic limit. The implementation of our method is remarkably simple and efficient. We prove the validity of the approach by computing the steady states of a dissipative quantum Ising model, relevant to address controversies in dissipative systems of interacting Rydberg atoms, and benchmark our simulations with a variational algorithm based on product and correlated states. Our method is the first implementation of the calculation of steady states in 2d for quantum lattice systems with tensor networks.

TT 19.64 Mon 15:00 P2-EG

Real-time dynamics in the two-dimensional Kondo-lattice model with classical spins — •Lena-Marie Gebauer — I. Institut für Theoretische Physik, Universität Hamburg

The two-dimensional ferromagnetic Kondo lattice with localized spins coupled to a system of non-interacting conduction electrons is the prototypical model for layered manganites and can be simulated using ultracold fermions trapped in optical lattices. Here, we present a quantum-classical hybrid theory for the thermodynamics and the real-time dynamics of the model where the spins are treated as classical degrees of freedom.

The equilibrium phase diagram is derived and found to agree well with previous classical Monte-Carlo data [2]. It comprises different phases, an antiferromagnet at half-filling as well as ferromagnetic, incommensurate and phase-separated states. We study the exact real-time dynamics initiated by different parameter quenches.

[1] M. Sayad, M. Potthoff, New J. Phys. 17 (2015) 113058
[2] S. Yunoki et al., Phys. Rev. Lett. 80, 845 (1998)

TT 19.65 Mon 15:00 P2-EG

First-principles molecular transport calculation — •Michael Rumetshofer, Gerhard Dorn, Lilia Boeri, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We have performed a first-principles calculation of the charge transport through a benzene-1,4-dithiol (BDT) molecule contacted by two semi-infinite gold chains. Density Functional Theory, within the plane-wave pseudopotential method, is used to calculate the electronic band structure. Transforming the Kohn-Sham eigenvalues and eigenfunctions to a real-space basis of maximally localized Wannier functions allows extracting a tight-binding Hamiltonian to describe the transport system. Strong electron correlations are included on the BDT molecule using an extended Hubbard model, similar to [1]. Non-equilibrium Green functions are then used to calculate the charge transport through the BDT molecule. It turns out that in the case of single gold chains as leads, the transport properties are determined only by the orbitals coupling to the gold s-orbitals. Therefore transport through the benzene p_z-orbitals is suppressed.

[1] D. A. Ryndyk, A. Donarini, M. Grifoni, K. Richter, Phys. Rev. B 88, 085404 (2012).

TT 19.66 Mon 15:00 P2-EG

Non-equilibrium steady states of the ionic Hubbard model in strong electric fields — •Yusuf Mohammed and Martin Eckstein — Max Planck Research Department for Structural Dynamics, Hamburg, Germany

We investigate the transport properties and non-equilibrium steady state phases of the dissipative ionic Hubbard model driven by an electric field. In the ionic Hubbard model, metallic behavior is enhanced by a competition of band insulating and Mott insulating behavior. The system is analyzed by means of the inhomogeneous dynamical mean-field theory (DMFT), using the iterated perturbation theory as impurity solver. The steady states of this model are accessed directly through the Keldysh contour formalism. We report results at half-filling for different interaction strengths, temperatures and geometries.

TT 19.67 Mon 15:00 P2-EG

Time propagation of systems with long range interaction in the framework of matrix product states — •Lars-Hendrik Frahm, Maximilian Hollstein, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg

The framework of matrix product states (MPS) has been seen to be more than just a compact technique to describe correlations in the density matrix renormalization group (DMRG) method. Among many other applications, MPS also turned out to allow for an efficient treatment of time-dependent systems. In this contribution, we benchmark the time-dependent MPS concept for systems with long range interaction (e.g. molecules). This type of system is especially challenging to approach since there is no fundamental law that guarantees a proper MPS representation (like there is for ground states in 1D local

systems). We discuss how to capture the necessary correlations with truncated MPS and how this truncation influences the time evolution after a quench. We compare our results to the time-dependent multi-reference configuration interaction singles (TDMRCIS) method, which is able to capture all correlations but only in a specific subspace of Hilbert space.

TT 19.68 Mon 15:00 P2-EG

Ultrafast dynamics of correlated fermions in lattice systems: Spectral properties — •Jan-Philip Joost, Niclas Schlünzen, and Michael Bonitz — CAU Kiel, Germany

The spectral properties of the infinite 1D Hubbard chain in the ground state can be described exactly by the Bethe ansatz [1]. However, for higher dimensional systems or the description of dynamical processes this spectral analysis becomes a challenging task. The nonequilibrium Green functions [2] (NEGF) approach grants easy access to the time-resolved spectral properties of extended and strongly correlated systems and is therefore well-suited to fill this gap [3]. Here, we present time-dependent and spatially resolved results for the spectral function and the dispersion relation of 1D and 2D systems in the ground state as well as for various nonequilibrium excitations. From a methodological point of view we compare different many body approaches, including the second Born, T-matrix and the third order approximation.

[1] F. H. L. Essler *et al.*, *The One-Dimensional Hubbard Model* (Cambridge University Press, 2005)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] N. Schlünzen *et al.*, Phys. Rev. B **93**, 035107 (2016)

TT 19.69 Mon 15:00 P2-EG

The 1D Anderson model revisited: Low-frequency behavior of the optical conductivity — •Tim Breidenbach and Robin Steinigeweg — University Osnabrück

We study the low-frequency dependence of the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ of the one-dimensional Anderson model, i.e., for non-interacting spin-less fermions in a random on-site potential. Using the method of exact diagonalization and dynamical quantum typicality, we calculate the real-time decay of the current autocorrelation function and obtain $\mathrm{Re}\,\sigma(\omega)$ by the Fourier transform of long-time data. We particularly variate the strength of disorder to determine low-frequency power laws at finite temperatures and in finite systems as well as the range of validity of Mott's law. Our results may shed light on corresponding studies in the many-body case, e.g., [1].

[1] R. Steinigeweg *et al.*, Phys. Rev. B **94**, 180401(R) (2016)

TT 19.70 Mon 15:00 P2-EG

Nonequilibrium dynamics of correlated fermions in lattice systems: A benchmark analysis of the nonequilibrium Green functions approach — •Niclas Schlünzen[1], Jan-Philip Joost[1], Fabian Heidrich-Meisner[2], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]LMU München, Germany

The nonequilibrium dynamics of correlated fermions in lattice systems are of high current interest in the communities of both condensed matter and ultacold atoms. While there is a very fruitful progress in present experiments (e.g. Ref. [1]), the theoretical description constitutes a challenging task, especially in the regime of strong coupling and higher dimensions. Recently, two-dimensional quantum simulations of the expansion of fermions based on nonequilibrium Green functions[2] (NEGF) have been presented[3] that showed excellent agreement with the experiments. We present a benchmark analysis of the NEGF approach compared to results of the numerically accurate density matrix renormalization group (DMRG) method[4], which predominantly has been limited to one dimenional systems. The results indicate that NEGF can compete for weak to intermediate coupling strengths while being easily extendable to higher dimensions, larger system sizes and longer propagation times.

[1] U. Schneider *et al.*, Nat. Phys. **8**, 213 (2012)
[2] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[3] N. Schlünzen, S. Hermanns, M. Bonitz, and C. Verdozzi, Phys. Rev. B **93**, 035107 (2016)
[4] N. Schlünzen *et al.*, submitted for publication (2016)