TT 17: Poster Session: Correlated Electrons 1

Time: Monday 15:00–18:30 Location: Poster D

TT 17.1 Mon 15:00 Poster D

Investigation of magnetic ground state of CeCoSi by means of neutron scattering — •Stanislav Nikitin[1,2], Diego Franco[3], Jae Hyeon Kwon[1], Andreas Hoser[4], Michael Koza[5], Robert Bewley[6], Christoph Geibel[1], and Oliver Stockert[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Technical University Dresden, Germany — [3]Centro Atomico Bariloche and Instituto Balseiro, Bariloche, Argentina. — [4]Helmholtz-Zentrum Berlin, Berlin, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]ISIS Neutron Source, Didcot, United Kingdom

Ce-based materials represent a rich playground for investigation of many exotic phenomena, such as heavy-fermion behavior, unconventional superconductivity, quantum criticality and so on. In this work, we explored magnetic properties of a metallic Ce-based antiferromagnet CeCoSi, which has an unusual $T-P$ phase diagram. Cerium moments order below $T_{\mathrm{N}} = 8.8$ K, however, a very moderate hydrostatic pressure of $P \approx 1.5$ GPa, stabilizes a new pressure-induced-ordered phase with significantly higher transition temperature of $T_c \approx 40$ K. Motivated by these observation, we explored magnetic structure and excitation spectra of CeCoSi by means of elastic and inelastic neutron scattering. We found that the cerium moments orders in a simple AFM structure with $\mathbf{q} = 0$. Using the results of inelastic neutron scattering and specific heat measurements we resolved the Hamiltonian of crystalline electrical field. Furthermore, we discussed a possible influence of the hydrostatic pressure on the spectra of magnetic excitations

TT 17.2 Mon 15:00 Poster D

Thermopower evolution in $Yb(Rh_{1-x}Co_x)_2Si_2$ upon $4f$ localization — •Ulrike Stockert[1], Christoph Klingner[1], Cornelius Krellner[2], Veljko Zlatić[3], Christoph Geibel[1], and Frank Steglich[1,4,5] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Physikalisches Institut, Goethe-Universität, Frankfurt/Main — [3]Department of Physics, University of Split, Croatia — [4]Center for Correlated Matter, Zhejiang University, Hangzhou, China — [5]Institute of Physics, Chinese Academy of Science, Beijing, China

$YbRh_2Si_2$ is a heavy-fermion system, which exhibits a large negative thermopower $S(T)$ with a single minimum around 80 K due to Kondo scattering from the full $4f$ multiplet. Substitution of Rh by Co leads to a strong reduction of the exchange coupling between the $4f$ and the conduction electron states and to a lowering of the Kondo scale T_{K}. This drives the system to a stable trivalent state in $YbCo_2Si_2$.

We performed thermopower measurements on $Yb(Rh_{1-x}Co_x)_2Si_2$ to study the evolution of $S(T)$ upon $4f$ localization. As T_{K} decreases with increasing x we observe the appearance of a second minimum that shifts subsequently to lower T. Simultaneously, the absolute thermopower values are strongly reduced due to the weaker exchange coupling between the $4f$ and the conduction electron states. Pure $YbCo_2Si_2$ still exhibits two minima in $S(T)$ indicative of weak residual Kondo scattering. The value at the high-T minimum is found to be proportional to the Sommerfeld coefficient for the whole series. We discuss this unexpected finding in relation to recent measurements of the valence and Fermi surface evolution with temperature.

TT 17.3 Mon 15:00 Poster D

Magnetic anisotropy in $GdRh_2Si_2$ probed by antiferromagnetic resonance — •Dieter Ehlers[1], Kristin Kliemt[2], Cornelius Krellner[2], Christoph Geibel[3], and Jörg Sichelschmidt[3] — [1]Experimentalphysik V, EKM, Universität Augsburg, 86135 Augsburg — [2]Physikalisches Institut, Goethe-Universität Frankfurt am Main, 60438 Frankfurt am Main — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden

$GdRh_2Si_2$ exhibits a complicated magnetocrystalline anisotropy [1] of well-localized Gd^{3+} moments. Below $T_{\mathrm{N}} = 107$ K [2] long range magnetic order sets in with ferromagnetic layers in the ab-plane stacked antiferromagnetically along the c-axis of the tetragonal structure. Interestingly, the strong easy-plane anisotropy allows for the observation of antiferromagnetic resonance at X- and Q-band microwave frequencies. In addition to the easy-plane anisotropy we have also quantified a weaker fourfold anisotropy within the easy plane. The obtained resonance fields are modelled in terms of eigenoscillations of the two antiferromagnetically coupled sublattices. Conversely, this model provides plots of the eigenfrequencies as a function of field and the specific anisotropy constants. An interesting perspective is the application of a similar model for understanding the magnetic ground state of the Kondo system $YbRh_2Si_2$.

[1] J. Sichelschmidt et al., Phys. Rev. B 97, 214424 (2018)
[2] K. Kliemt and C. Krellner, J. Cryst. Growth. 419, 37 (2015)

TT 17.4 Mon 15:00 Poster D

$TbRh_2Si_2$: Single crystal growth and characterization — •Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

In the last decades, many studies on RT_2Si_2 (R = rare earth, T = transition metal) ternary silicides have been made. The compounds which crystallize in the bodycentered tetragonal $ThCr_2Si_2$ structure exhibit exceptional magnetic properties such as superconductivity, valence fluctuations or the Kondo effect. In recent years, we have started to systematically investigate the magnetic properties of RRh_2Si_2 compounds, which present exciting surface properties, strongly influenced by the 4f-magetism [1]. So far, the magnetism of $TbRh_2Si_2$ has been studied on polycrystalline samples using neutron scattering [2]. The compound shows antiferromagnetic order below $T_N = 92$ K with a magnetic ordering vector k = (001). In this contribution, we present the details of the crystal growth of $TbRh_2Si_2$ single crystals by Bridgman method from indium flux. We show the results of specific heat, specific resistivity and magnetization measurements, with a focus on the magnetic transition.

[1] A. Generalov et al., Nano Lett. 17, 811 (2017)
[2] S. Quezel et al., Solid State Commun. 49, 7 (1984)

TT 17.5 Mon 15:00 Poster D

Towards crystal growth process of isotope pure $^{174}YbRh_2Si_2$ — Susanna Rongstock, •Sebastian Witt, Doan-My Tran, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

A central question in condensed matter research concerns the interplay between quantum criticality and unconventional superconductivity in strongly correlated electron systems such as heavy-electron systems. Recently, superconductivity was also discovered in the quantum-critical material $YbRh_2Si_2$ at 2 mK [1]. So far the interplay between electronic and nuclear moments of Yb and ist impact on the superconductivity is not settled. For that reason, it is essential to investigate $YbRh_2Si_2$ samples with a well-defined Yb nuclear spin, with the simplest case of ^{174}Yb which has zero nuclear spin.

In this contribution, we report on the challenges to grow a $^{174}YbRh_2Si_2$ crystal, as the Yb-isotopes are only available as oxides and are rather expensive. We have developed a process to reduce the oxide to metallic Yb with minimal mass losses and scaled down to established crystal growth process to work with smaller total masses. The characterization of the single crystals by different methods (Laue, PXRD, resistivity, magnetization, heat capacity) partly down to low temperatures will be presented. Besides the desired compound we present the properties of a parasitic phase, (e.g. $YbRh_6Si_4$).

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

TT 17.6 Mon 15:00 Poster D

Crystal growth of the valence fluctuating system $EuPd_2Si_2$ — •Marius Peters, Eunhyung Cho, Doan-My Tran, Franz Ritter, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The study of collective phenomena raising from enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice-degrees of freedom. One system providing such a strongly coupled phase transition is $EuPd_2Si_2$ of the $ThCr_2Si_2$ structural type, showing a temperature induced valence transition of europium between the energetically vicinal valence states Eu^{2+} and Eu^{3+} at about 170K [1]. First reports on the synthesis of single crystals came up only recently [2], but a deep investigation of the valence transition in this compound is still missing. We approached the ternary Eu-Pd-Si system using differential thermal analysis to map the local composition phase diagram. We used

the Bridgman and the Czochralski method fort he successful growth of mm-sized single crystals of $EuPd_2Si_2$. In this contribution we will present chemical and structural characterization of these crystals and some preliminary physical measurements around the valence transition.

[1] E. V. Sampathkumaran et al., J. Phys. **C14**, L237 (1981)
[2] Y. Onuki et al., Philosophical Magazine **97**, 3399 (2017)

TT 17.7 Mon 15:00 Poster D

$CeRu_2P_2$ and $CeCo_2P_2$: Single Crystal Growth Methods and Physical Characterization — •Fabian Feldmann, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut Goethe Universität Frankfurt/Main

CeT_2P_2 (T = Co, Ru) are rare-earth ternary phosphides with tetragonal $ThCr_2Si_2$ type crystal structure. $CeRu_2P_2$ is an intermediate valent system [1] and $CeCo_2P_2$ is an antiferromagnet with a rather high Néel temperature $T_N = 440\,K$ [2], most likely due to an interplay of 3d and 4f magnetism.

Here, we present crystal growth methods to obtain millimeter-sized single crystals. These growths were executed with Sn-flux and self-flux with temperatures up to 1500 °C. Optical microscopy, Powder X-Ray Diffraction (PXRD), Energy Dispersive X-ray spectroscopy (EDX) and Laue method were used for chemical characterization and confirmation of single crystallinity.

In addition, we report on measurements of specific heat, magnetic susceptibility and electrical resistivity. We confirm some measurements, for instance a broad maximum in electrical resistivity at $T = 180\,K$ and metallic behavior at lower temperatures for $CeRu_2P_2$ [3]. We also show new measurements such as magnetic susceptibility of $CeCo_2P_2$, now relating to crystal orientation.

[1] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[2] Y. Tian et al. Physica B, **512**, 75-80, (2017)
[3] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)

TT 17.8 Mon 15:00 Poster D

Electrical resistivity of heavy fermion metal $YbNi_4P_2$ under high pressure — •Takaki Muramatsu[1], Owen Moulding[1], Kristin Kliemt[2], Cornelius Krellner[2], and Sven Friedemann[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

Heavy-fermion metal $YbNi_4P_2$ is a characteristic compound in terms of the magnetic property. In the tetragonal $ZrFe_4Si_2$ type crystal structure ($P4_2/mnm$), Yb ions line up to chains along *c*-axis and each chain is well separated by other chains of edge-shared Ni tetrahedra, providing quasi-one dimensional heavy-fermion system. At ambient pressure, $YbNi_4P_2$ orders ferromagnetically (FM) below $T_C = 0.17K$ [1] and the low T_C allows us to access the quantum critical point point by a combination of chemical and physical pressure [2]. In this work, we utilise physical pressure to study the interaction of magnetic moments and conduction electrons of $YbNi_4P_2$ by measuring temperature dependence of electrical resistivity.

TT 17.9 Mon 15:00 Poster D

High-field de Haas-van Alphen study of the heavy-fermion compound $CeCoIn_5$ — •J. Hornung[1,2], M. Raba[3], S. Mishra[3], D. Aoki[4], I. Sheikin[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), France — [4]Institute for Materials Research (IMR), Tohoku University, Japan

We report on de Haas-van Alphen (dHvA) measurements in the heavy-fermion compound $CeCoIn_5$ in magnetic fields up to 36 T and temperatures down to 50 mK. Compared to previous investigations, we were able to observe additional dHvA frequencies and a very diverse field dependence. While some frequencies stay unaffected by magnetic fields, like usually observed and expected, others show a strong field dependence, such as a clear discontinuity at 26.5 T with a change of the measured frequency and/or the effective mass. In addition, the spin splitting of some frequencies, already reasoned from the non-trivial temperature dependence of the dHvA amplitudes in a earlier work, could be resolved directly.

TT 17.10 Mon 15:00 Poster D

^{59}Co NMR magnetometry of the heavy-fermion compound $CeCoGe_3$ — •Sven Luther[1,2], Ilya Sheikin[3], Rikio Settai[4], Jochen Wosnitza[1,2], and Hannes Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), CNRS, Grenoble, France — [4]Department of Physics, Niigata University, Japan

The tetragonal heavy-fermion compound $CeCoGe_3$ yields, as established by thermodynamic probes, a complex magnetic phase diagram with several zero-field transitions to and between antiferromagnetically ordered phases below $T_N = 20$ K. We present a detailed, microscopic study of one of these magnetic phases via ^{59}Co ($I = 7/2$) NMR at 2 T. Here, below T_N, the symmetry breaking by magnetic order results in three inequivalent Co-sites with corresponding local sublattice magnetizations. These temperature-dependent internal fields can well be described by an Ising-type mean-field formalism. In addition to the antiferromagnetic order, which is compatible with neutron-scattering results, the analysis yields an additional uniform part, which could be induced by an unusually high polarization of hybridized conduction electrons.

TT 17.11 Mon 15:00 Poster D

Study of the low-temperature specific heat of the locally non-centrosymmetric superconductor $CeRh_2As_2$ — •Jacintha Banda, Daniel Hafner, Seunghyun Khim, Helge Rosner, Christoph Geibel, and Manuel Brando — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, we have discovered a new heavy-fermion, locally non-centrosymmetric superconductor $CeRh_2As_2$ in the $CeBe_2Ge_2$ type structure with a transition temperature $T_c \approx 0.3\,K$. We present here a comprehensive study of its low-temperature specific heat and its behaviour in a magnetic field which was applied parallel and perpendicular to the crystallographic *c*-axis. We show that a second weak phase transition can be seen in specific heat at a temperature T_0 slightly above T_c. Its field dependence is similar to that of quadrupolar phases. After having subtracted the nuclear specific heat contribution due to the quadrupolar and Zeeman terms on the arsenic nuclear spins, we present the temperature and field dependence of the electronic specific heat coefficient $\gamma = C(T,H)/T$ down to 40 mK and up to 12 T.

TT 17.12 Mon 15:00 Poster D

Metallic 4f-electron system with a large magnetic cooling capacity — •Thomas Gruner[1], Jiasheng Chen[1], Jacintha Banda[2], Jang Dongjin[3], Manuel Brando[2], Christoph Geibel[2], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]MPI CPfS, Dresden, Germany — [3]KRISS, Daejeon, Republic of Korea

All standard cooling materials used in present day demagnetisation refrigerators for the temperature range $50\,mK < T < 2\,K$ are insulators, resulting in some problems e.g. because of their very weak low-temperature thermal conductivity. Recently, we proposed and showed that some Yb based metallic materials provide attractive alternatives [1], and ideas which meanwhile has been picked up by further research groups. In a search for even more appropriate materials we have synthesised a new Yb Heusler compound and investigated its structural, magnetic, transport and magnetocaloric properties.
Susceptibility χ(T), magnetisation $M(B)$, specific heat C(T) and resistivity ρ(T) data evidence metallic behaviour, the absence of superconductivity and a stable trivalent Yb^{3+} state, without any sign for a significant Kondo interaction. Our new compound can easily be cast into rods, making preparation of cooling pills quite simple in contrast to commonly used paramagnetic salt refrigerants. By using a demagnetisation test set-up, we demonstrate the feasibility of a simple, economically priced and durable alternative for traditional cooling devices for temperatures down to roughly 100 mK.

[1] Jang, Gruner et al.; Nature Communications; **6**, 8680 (2015)

TT 17.13 Mon 15:00 Poster D

Spin-orbit interaction and quasiparticle bands in locally non-centrosymmetric heavy-fermion systems — •Évrard-Ouicem Eljaouhari[1], Gertrud Zwicknagl[1], Seunghyun Khim[2], Manuel Brando[2], and Christoph Geibel[2] — [1]Institut für Mathematische Physik, TU Braunschweig, Braunschweig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Non-centrosymmetric heavy-fermion materials have gained much interest in the past decade. In these materials, the lack of inversion symmetry in combination with strong spin-orbit interaction and magnetic in-

teractions can lead to novel phenomena. In this poster, we present calculations of the heavy quasiparticle bands of Ce- and Yb-based heavy-fermion compounds from the tetragonal "122"-family. This class of materials comprises compounds with the inversion-symmetric $ThCr_2Si_2$ structure as well as systems with the locally non-centrosymmetric $CaBe_2Ge_2$ structure. The calculations are performed by means of the Renormalized Band method which proceeds from a Dirac relativistic description of the electronic structure and accounts for Crystalline Electric Field effects and the mass renormalisation due to strong local correlations. We discuss results for $YbIr_2Si_2$ which crystallizes in both structures depending on preparation condition. Further on, we present our new results on the new HFS $CeRh_2As_2$.

TT 17.14 Mon 15:00 Poster D

Emergence of gauge fields in the rotating polaron problem — •Mikhail Maslov, Enderalp Yakaboylu, and Mikhail Lemeshko — Institute of Science and Technology, Klosterneuburg, Austria

In a recent article [1], it was shown that in any impurity problem a many-body environment manifests itself as an external gauge field with respect to the impurity interacting with it. Here, we apply this method to the so-called rotating polaron problem, which is a quantum impurity possessing both translational and internal rotational degrees of freedom interacting with a bosonic bath [2], and study its geometric and topological properties. We show that within the perturbation theory approach in the internal angular space of the impurity the emerging gauge field corresponds to a non-Abelian magnetic monopole. Furthermore, we are able to define the second Chern number in the total coordinate of the impurity.

[1] E. Yakaboylu, A. Deuchert, and M. Lemeshko, Phys. Rev. Lett. 119, 235301 (2017)
[2] E. Yakaboylu, B. Midya, A. Deuchert, N. Leopold, and M. Lemeshko, arXiv:1809.01204 (2018)

TT 17.15 Mon 15:00 Poster D

Modeling of single impurity scattering in correlated fermionic systems — •Banhi Chatterjee[1], Jan Skolimowski[2], and Krzysztof Byczuk[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Institute of Theoretical Physics,Warsaw University, Warsaw,Poland

The one-body scattering formalism was modified [1] to describe effects of electronic correlations in many-body fermionic systems with a single impurity potential. We consider a single band model with the densities of states corresponding to Bethe, cubic and square lattice. Effects of correlations are accounted for using a model self-energy satisfying the Fermi liquid properties [2]. Here, we investigate effects of correlations on the spectral functions at the impurity site, scattering phase-shifts, and resonance energies. Depending on the geometry of the system a bound state may appear outside the continuous band for a strong enough impurity potential. However, these discrete eigen-energies are broadened when correlations are present. The bound state outside a continuum becomes a resonance-like state in correlated hosts. Our simple model can be useful in qualitative understanding of in-gap energy levels in real solids, which occur due to impurity atoms or defects with correlation Coulomb potential.

[1] K. Byczuk, B. Chatterjee, D. Vollhardt, arXiv:1807.08559, accepted for publication
[2] B. Chatterjee, K. Byczuk, JPCS: 592, 012059 (2015)

TT 17.16 Mon 15:00 Poster D

Exact Diagonalization study of large Hubbard clusters — •Mikhail Danilov[1], Sergei Iskakov[2], Malte Harland[1], Sergei Brener[1], Andrei Bagrov[3], Alexander Lichtenstein[1], and Mikhail Katsnelson[3] — [1]I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — [3]Institute for Molecules and Materials, Radboud University, 6525AJ Nijmegen, The Netherlands

Using efficient exact diagonalization scheme, we study electronic structure of 4x4 doped Hubbard cluster with realistic hopping parameters including next nearest neighbour hopping $t' = -0.3t$, which is optimal for superconducting cuprates.

To find possible candidates for superconducting regime we calculate the spectral function and network entanglement measures for different doping and Coulomb interaction.

TT 17.17 Mon 15:00 Poster D

Hydrodynamic charge and heat transport in graphene from a microscopic perspective — •Lars Fritz, Simonas Grubinskas, and Kitinan Pongsangangan — Institute for Theoretical Physics and Center for Extreme Matter and Emergent Phenomena, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

In this poster we present a description of charge and heat transport in graphene close to the Dirac point. Our starting point is microscopic and builds on a kinetic equation description, taking into account relaxation due to both interaction and disordering equal footing. Our results connect to recent experimental findings in which a strong violation of the Wiedemann-Franz law was found. We find that close to the Dirac point there is a sizeable contribution of plasmons to the heat conductivity which had not been discussed previously.

TT 17.18 Mon 15:00 Poster D

Quantum Monte Carlo simulations of quantum critical fermions — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[3], and Simon Trebst[1] — [1]University of Cologne, Germany — [2]Stanford University, USA — [3]The Weizmann Institute of Science, Israel

While quantum critical phenomena in insulators are fairly well understood, their metallic counterparts pose a substantial theoretical challenge since the order parameter fluctuations can interact with gapless excitations on a Fermi surface. When driving a metal through a phase transition, this interplay can give rise to unconventional superconductivity and "strange metal" behavior and might therefore serve as a microscopic model for some of the rich physics of high-T_c materials.

Fortunately, certain classes of metallic quantum critical points can be analyzed by determinant quantum Monte Carlo as one can circumvent the notorious "sign problem" and retain polynomial efficiency. I will show numerically exact studies of two dimensional metals at the verge of an antiferromagnetic transition indicating Landau-damped dynamics of the order parameter and a breakdown of Fermi liquid theory. I will further demonstrate that machine learning techniques, such as quantum loop topography and convolutional neural networks, can be utilized to probe transport and identify phase transitions in such many-particle systems.

TT 17.19 Mon 15:00 Poster D

Quantum skyrmions in a triangular frustrated ferromagnet — •Vivek Lohani[1], Ciarán Hickey[1], and Achim Rosch[1,2] — [1]Institute of Theoretical Physics, University of Cologne, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, USA

Magnetic skyrmions are magnetization textures characterized by a topological winding number, initially discovered in chiral magnets. More recently, they were also predicted by Leonov and Mostovoy in a spin-1/2 Heisenberg ferromagnet with frustrated next-nearest neighbor interactions and spin-anisotropy. Their classical model predicts energetically degenerate skyrmions and antiskyrmions, and the emergence of a new zero mode, the helicity, reflecting rotation of spins around the z axis. The size of these frustration-stabilized skyrmions is also expected to be lesser than the ones found in chiral magnets. As a result, quantum properties of skyrmions might be of interest in insulating magnets at temperatures well below the bulk gap.

We investigate the existence of frustration-stabilized quantum skyrmions within a 31 site flake on a triangular lattice through exact diagonalization. We also derive the selection rules for the skyrmions in such a system. Next, we introduce a phenomenological Hamiltonian for mobile skyrmions and study couplings of the internal modes to the lowest order. This is then extended to an analysis of tunneling between skyrmions and antiskyrmions, and how the bandstructure is modified by the presence of tunneling terms, and its dependence on the number of flipped spins comprising the skyrmion.

TT 17.20 Mon 15:00 Poster D

Exotic criticality in the dimerized spin-1 XXZ chain with single-ion anisotropy — Satoshi Ejima[1], Tomoki Yamaguchi[2], Fabian H. L. Essler[3], Florian Lange[1], Yukinori Ohta[2], and •Holger Fehske[1] — [1]Institute of Physics, University Greifswald, 17489 Greifswald, Germany — [2]Department of Physics, Chiba University, Chiba 263-8522, Japan — [3]The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, UK

We consider the dimerized spin-1 XXZ chain with single-ion anisotropy D. In absence of an explicit dimerization there are three phases: a large-D, an antiferromagnetically ordered and a Haldane phase. This phase structure persists up to a critical dimerization, above which the

Haldane phase disappears. We show that for weak dimerization the phases are separated by Gaussian and Ising quantum phase transitions. One of the Ising transitions terminates in a critical point in the universality class of the dilute Ising model. We comment on the relevance of our results to experiments on quasi-one-dimensional anisotropic spin-1 quantum magnets.

TT 17.21 Mon 15:00 Poster D

Antiferromagnetic magnons with strain — •Mary Madelynn Nayga[1], Stephan Rachel[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

Motivated by recent results on strain-induced pseudo-Landau levels in graphene, nodal superconductors, and other fermionic systems, we analyze analogous scenarios in bosonic systems. We focus on magnons and provide a combined analytical and numerical study of strain effects in Heisenberg antiferromagnets. We discuss the results vis-a-vis to the graphene case.

TT 17.22 Mon 15:00 Poster D

Interchain mean-field theory for thermodynamic properties of a bimetallic ferromagnetic spin-chain compound — •Maheshwor Tiwari[1], Stefan Süllow[2], Matthias Bleckmann[2], Ralf Feyerherm[3], Wolfram Brenig[4], and Andreas Honecker[1] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France — [2]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [4]Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

Two energy scales are observed in the field-dependent specific heat of $MnNi(NO_2)_4(en)_2$, en = ethylenediamine, containing ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. $MnNi(NO_2)_4(en)_2$ orders antiferromagnetically at low temperatures in low magnetic fields, demonstrating relevant antiferromagnetic interchain coupling, with a suppression of this order already by a weak magnetic field.

Here we present numerical results for the specific heat obtained by exact diagonalization and Quantum-Monte-Carlo simulations for the alternating spin chain model, using parameters that have been derived from the high-temperature behavior of the magnetic susceptibility. The interchain coupling is included in the numerical treatment at the mean-field level. The observed strong effect of an applied magnetic field on the ordered state promises interesting magnetocaloric properties that we explore theoretically.

TT 17.23 Mon 15:00 Poster D

Strategies for the design of antiferromagnetically coupled organic spin-dimer systems — •Lars Postulka[1], Paul Eibisch[1], Ulrich Tutsch[1], Bernd Wolf[1], Martin Baumgarten[2], Kubandiran Kolanji[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe Universität, SFB/TR49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR49, D-55128 Mainz

Coupled antiferromagnetic spin-dimer systems based on stable biradicals are recognized as suitable candidates for exploring critical phenomena under well-controlled conditions. Depending on the topology of the *inter*-dimer couplings, various scenarios can be observed. The work aims at the development of novel spin-dimer systems where the *intra*- and *inter*-dimer magnetic exchange interactions can be modified in specific ways. We discuss the magneto-structural correlations of materials based on the stable radical units nitronyl-nitroxides (NN) and imino-nitroxides (IN) bridged with tolan molecules. Furthermore, using low-temperature ac susceptibility and specific heat measurements we characterize the field-induced magnetic phases of these materials and discuss their critical behavior. In addition, we present a new approach for designing the *intra*- and *inter*-molecular magnetic exchange interactions based on planar π-bridges of benzo[1,2 -*b*:4,5 -*b'*] dithiophene derivatives which connect the stable NN and IN radical units. Our results demonstrate that π-stacking of the planar bridges allows a good control of the *inter*-molecular magnetic exchange.

TT 17.24 Mon 15:00 Poster D

Strain-dependent electronic and magnetic properties of Sr_2CoIrO_6 double perovskite from DFT+U+SOC calculations — •Jiongyao Wu and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg

The electronic and magnetic properties of the double perovskite Sr_2CoIrO_6 (SCIO) are explored and compared to the end members $SrIrO_3$ (SIO) and $SrCoO_3$ (SCO) in the framework of density functional theory (DFT) including a Hubbard U term and spin-orbit coupling (SOC) with the PBEsol exchange correlation functional. While bulk SIO is metallic with a quenched spin and orbital moment, strong changes are observed for SCIO which shows insulating behavior with a band gap of ~ 200 meV and an Ir spin moment of 1.62 μ_B pointing towards a $j = 1/2$ Mott insulating state in the double perovskite. We analyze the electronic reconstruction in this system and furthermore consider the effect of strain on the electronic and structural properties of SCIO by varying the lateral lattice constant from the one of $NdGaO_3$ (compressive), through $SrTiO_3$ (unstrained) to $GdScO_3$ (tensile).

We acknowledge funding by the German Science Foundation within CRC/TRR80, project G3.

TT 17.25 Mon 15:00 Poster D

Charge-carrier doping in nickelate heterostructures — •Roberto Ortiz[1], Friederike Wrobel[1], Fanni Misják[3], Benjamin Geisler[2], Katrin Fürsich[1], Martin Bluschke[1], Enrico Schierle[4], Georg Christiani[1], Gennady Logvenov[1], Yi Wang[1], Peter van Aken[1], Bernhard Keimer[1], Ute Kaiser[3], Rossitza Pentcheva[2], and Eva Benckiser[1] — [1]Max Planck Institute, Stuttgart, Germany — [2]CENIDE, University Duisburg-Essen, Germany — [3]University Ulm, Germany — [4]Helmholtz-Zentrum, Berlin, Germany

Transition-metal oxides of the 3d series show a variety of interesting properties including robust metal-to-insulator transitions, multiferroicity and high-temperature superconductivity. One way to access these properties is to modify the charge carrier concentration by doping a particular system. In bulk materials, doping is mostly accomplished by substitution of cations, but the structural and chemical disorder generated in this way can drastically modify the electronic phase behavior and/or generate mesoscopic electronic inhomogeneities. We explore two distinctive methods of charge-carrier doping of nickelate heterostructures to investigate changes in the filling of 3d electronic states: The synthesis of $LaNiO_{2+x}$ - band-insulator superlattices by ex-situ layer-selective chemical reduction and the transfer of charge across metal-oxide interfaces in nickelate-cuprate hybrid structures.

TT 17.26 Mon 15:00 Poster D

Orbital polarization of vanadate superlattices — •Padma Radhakrishnan — Max Planck Institute for Solid State Research, Stuttgart, Germany

Rare earth vanadates (RVO_3), R- rare-earth element such as La, Y, etc have a rich phase diagram with two different spin and orbital orders depending upon the size of the lanthanide rare-earth cation [1] Heterostructuring these materials alters their structure through epitaxial strain and could further introduce spatial confinement and interface effects [2].

Multilayers of yttrium vanadate (YVO_3) with $LaAlO_3$ were grown using ultra-high-vacuum pulsed laser deposition on $NdGaO_3$ substrate. X-ray diffraction, scanning transmission electron microscopy and X-ray absorption revealed that the samples are of good quality and of pure phase. From Resonant reflectometry, depth resolved XAS profiles were obtained for the YVO_3 stack, which showed a clear modulation of the electronic structure between the interfacial and inner layers. Further, application of sum rules suggests that both types of layers have altered t_{2g} orbital occupations compared to that of bulk YVO_3, which is very likely to affect the orbital ordering and spin ordering at low temperatures.

[1] S. Miyasaka, Y. Okimoto, M. Iwama, and Y. Tokura, Phys. Rev. B, 68, 2003.

[2] E. Benckiser et al., Nature Materials, 10, 2011

TT 17.27 Mon 15:00 Poster D

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Correlated Materials — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czech Republic

We present a computational study of L-edge resonant inelastic x-ray scattering (RIXS) in 3d transition-metal (TM) oxides: NiO; $RNiO_3$; Fe_2O_3; $LaCuO_3$ and $NaCuO_2$ [1], where we em-

ploy a theoretical approach based on local density approximation and dynamical mean-field theory (DMFT). We use the Anderson impurity model (AIM) with DMFT hybridization function extended by inclusion of core orbitals. This approach enables us to describe both localized (d-d) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. We discuss the relationship of correlated $3d$ bands and fluorescencelike feature in the RIXS spectra. Our calculated results reproduce the experimental data well and RIXS can be used as a tool to study material-specific hybridization between x-ray excited TM ion and low-energy states.

[1] A. Hariki, M. Winder, J. Kuneš, Phys. Rev. Lett. **121**, 126403 (2018)

TT 17.28 Mon 15:00 Poster D

Two-dimensional electron gas at the $KTaO_3$ surface and $KTaO_3$/EuO interface — •Xue-Jing Zhang[1] and Bang-Gui Liu[2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Since the discovery of a two-dimensional (2D) electron gas at the $LaAlO_3/SrTiO_3$ interface, 2D carrier gases at such oxide interfaces and surfaces have attracted great attention because they can host many important phenomena and may produce novel functional devices. Here, we show through first-principles investigations that the surface 2D electron and hole gases in a $KTaO_3$ (KTO) thin film can be tuned by applying biaxial stress. When increasing compressive in-plane strain, the 2D carrier concentrations decrease down to zero and then a new pair of surface 2D electron and hole gases appears in which the carrier types are switched to the opposite ones. Our analysis indicates that this carrier-type switching occurs because the increasing compressive strain reverses the slope of monolayer-resolved electrostatic potential along the [001] direction. In addition, through first-principles investigations, we also study the KTO/EuO interfaces with oxygen vacancies in the KTO unit cell adjacent to EuO. We find that through interlayer exchange of the Eu-5d and Ta-5d, EuO drives the neighboring TaO_2 layer into a ferromagnetic state. These phenomena should be useful to design novel functional devices.

TT 17.29 Mon 15:00 Poster D

Tailoring $LaTiO_3$ for Mottronics — •Berengar Leikert[1], Philipp Scheiderer[1], Matthias Schmitt[1], Martin Stübinger[1], Judith Gabel[1], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Materials (RCCM), Universität Würzburg, Germany — [2]DIAMOND Light Source, Beamline I09, Didcot, England

3d transition metal oxides exhibit fascinating phenomena - absent in conventional semiconductors - like Mott insulating behaviour due to pronounced electron-electron interactions. The field of Mottronics dreams of harnessing the phase transition between the correlated metal and the Mott insulating phase of such strongly correlated materials for novel electronic devices.

We have recently demonstrated that the prototypical Mott insulator $LaTiO_3$ can undergo the band filling controlled Mott transition if it is chemically p-doped by excess oxygen during thin film growth by pulsed laser deposition. Here we report on the influence of dimensionality in the ultrathin film limit for varying doping levels by photoelectron spectroscopy, tuning the material in the generic phase diagram (correlation strength versus band filling) close to the boundary of the phase transition. Doing so the metal-insulator transition can possibly be triggered by electric field gating.

TT 17.30 Mon 15:00 Poster D

Exploring the potential gradient in the $LaFeO_3/SrTiO_3$ heterostructure by photoemission — •Martin Stübinger[1], Matthias Schmitt[1], Berengar Leikert[1], Pardeep Kumar Thakur[2], Tien-Lin Lee[2], Christoph Schlueter[3], Michael Sing[1], and Ralph Claessen[1] — [1]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom — [3]DESY Photon Science, 22607 Hamburg, Germany

In the oxide heterostructure $LaFeO_3/SrTiO_3$ (LFO/STO), the polar discontinuity between the polar LFO and the non-polar STO leads to a potential gradient in the LFO film. As opposed to the famous $LaAlO_3/SrTiO_3$ system, the built-in potential is not compensated by an electron transfer to the interface and a two-dimensional electron system does not emerge. Indeed, photovoltaic effects making use of the potential gradient to separate electrons and holes have been observed. Furthermore, different terminations of the STO substrate have been reported to change the direction of the potential. Hence, we investigated TiO_2- as well as SrO-terminated substrates. Angle-dependent photoemission was used to determine the potential gradient across the LFO film. The enhanced probing depth of hard x-ray photoemission (HAXPES) gave also access to the substrate core levels to provide a complete picture of the band alignment at the interface. Our results show an upward bending of the substrate bands toward the interface and a thickness-dependent potential gradient in the LFO film.

TT 17.31 Mon 15:00 Poster D

Magnetic anisotropy of the van der Waals ferromagnet $Cr_2Ge_2Te_6$. — •Alexey Alfonsov[1], Julian Zeisner[1,2], Sebastian Selter[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany

$Cr_2Ge_2Te_6$ compound is a quasi-two-dimensional semiconducting magnet belonging to the family of ferromagnetic layered transition metal trichalcogenides. Ferromagnetic order surviving even in the monolayer samples of these compounds renders these materials attractive for the fundamental research and for future technological applications. Such violation of Mermin-Wagner theorem is possible due to magnetic anisotropy present in these materials. Here we report an experimental study of the magnetic anisotropy in bulk single crystals of $Cr_2Ge_2Te_6$ by means of electron spin resonance (ESR) and ferromagnetic resonance (FMR) using conventional and torque-detected ESR spectrometers. Measurements were carried out in a wide frequency and temperature range, and at various angles between magnetic field and sample plane. Angular and frequency dependent measurements in the ferromagnetic phase clearly show the easy-axis type anisotropy of $Cr_2Ge_2Te_6$. Furthermore, simulation of the measured data based on a phenomenological approach yielded a precise value for the magnetocrystalline anisotropy energy density.

TT 17.32 Mon 15:00 Poster D

Charge Carrier Dynamics at the Metal-Insulator Transition in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl — •Tatjana Thomas, Harald Schubert, and Jens Müller — Institute of Physics, Goethe University Frankfurt, Germany

The organic charge-transfer salts κ-$(ET)_2X$ are intensively studied due to their interesting electronic ground states, which are usually described within an effective-dimer model. In contrast, κ-$(ET)_2Hg(SCN)_2Cl$ exhibits a metal-insulator transition at $T_{MI} \sim 30\,K$ due to charge ordering [1]. Dimerization of the ET molecules in combination with charge localization on one molecule within the dimer leads to a net dipole moment, so that the system exhibits ferroelectric order of electronic type [2]. Additional magnetic order would make the system even multiferroic, as it was recently discussed for κ-$(ET)_2Cu[N(CN)_2]Cl$ [3]. Previous works on the latter salt showed that fluctuation (noise) spectroscopy provides new insights into the low-frequency charge carrier dynamics. Here, we present recent results on κ-$(ET)_2Hg(SCN)_2Cl$, where the normalized noise power spectral density shows an increase at the charge ordering transition. At low temperatures in the ferroelectric phase, we observe a strong electric field dependence of the fluctuation spectra. An observed spectral wandering is usually a hint for spatially correlated fluctuations. Measurements of the so-called second fluctuation spectrum indeed reveal a frequency dependence below the transition, indicating a switching between metastable states.

[1] PRB **89**, 075133
[2] JPSJ **79**, 011010
[3] Nat. Mater. **11**, 755

TT 17.33 Mon 15:00 Poster D

One-dimensional spin chains in $NaCuFe_2(VO_4)_3$ studied by high-frequency ESR and static magnetization — •Florian Theuss[1], Changhyun Koo[1], Alexander N. Vasiliev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany. — [2]Lomonosov Moscow State University, Moscow, Russia

We report magnetization and high-frequency electron spin resonance spectroscopy data (HF-ESR) on the metal oxide $NaCuFe_2(VO_4)_3$. The magnetically active ions Fe^{3+} and Cu^{2+} in this compound form quasi-

one-dimensional spin chains [1]. Magnetization data confirm the evolution of long-range antiferromagnetic order below $T_N = 9.3 \pm 0.4$ K. At high temperatures, the data imply a Curie-Weiss-like behaviour with the Weiss temperature $\Theta \approx 81.2$ K. However, no AFM resonances are observed at low temperatures. Instead, the HF-ESR spectra show a single broad resonance feature without sizeable zero-field splitting. Upon heating, this resonance shifts to a smaller g-factor associated with Fe^{3+}-spins. Based on the these data, the AFM ordered phase of the compound will be discussed.
[1] A.V. Koshelev et. al., arXiv:1711.06990v1

TT 17.34 Mon 15:00 Poster D

***In−situ*-SQUID studies of Fe_3O_4 and V_2O_3 upon electrochemical lithiation** — •Lukas Deeg, Elisa Thauer, Michael Richter, and Rüdiger Klingeler — Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany

A re-usable *in-situ*-SQUID electrochemical cell for magnetisation studies during electrochemical cycling is presented. The proof of function is demonstrated by recording reversible magnetisation changes in $Li_xFe_3O_4$ nanoparticles upon electrochemical cycling. The data imply the transition from inverse spinel structure ($x = 0$) to a rocksalt phase ($x = 2$). In addition, the setup is utilised to study the effect of lithiation on the Mott-Hubbard transition in V_2O_3.

TT 17.35 Mon 15:00 Poster D

Single-crystal growth and magnetic phase diagram of Li_2FeSiO_4 — •Waldemar Hergett[1], Christoph Neef[1], Sven Sauerland[1], Martin Jonak[1], Mahmoud Abdel-Hafiez[1], Hubert Wadepohl[2], Clemens Ritter[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University — [2]Institute of Inorganic Chemistry, Heidelberg University — [3]Institut Laue-Langevin, Grenoble

By using the high-pressure optical floating-zone technique (FZ), mm-sized single crystals of γ_{II}-Li_2FeSiO_4 (space group *Pmnb*) were grown and characterized for the first time. Oriented cuboids were used for thermal expansion, specific heat, and magnetisation studies. High-resolution neutron powder diffraction experiments were performed to resolve the magnetic ground state and analyse the Li-Fe antisite disorder. The impact of different synthesis routes of the starting materials and of FZ growth parameters on the crystal quality was investigated. The single crystal structure of the *Pmnb*-polymorph was solved for the first time. Thermal expansion, magnetisation and specific heat data show a sharp λ-like anomaly associated with the onset of long-range antiferromagnetic order at $T_N = 17.0(5)$ K. Pulsed-field magnetisation studies up to 60 T enable constructing the magnetic phase diagram.

TT 17.36 Mon 15:00 Poster D

Static magnetic order in γ-Li_2FeSiO_4 as probed by ^{57}Fe Mössbauer spectroscopy — •Felix Seewald[1], Sascha Albert Bräuninger[1], Rüdiger Klingeler[2], Waldemar Hergett[2], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — [2]Kirchhoff Institute of Physics, Heidelberg University, D-69120 Heidelberg, Germany

γ-Li_2FeSiO_4 is proposed as a promising candidate material for lithium ion batteries. The Fe atoms are tetrahedrally coordinated by Oxygen. Iron has the Fe^{2+} (S=2) oxidation state and is displaced from the tetrahedron center resulting in a electric field gradient caused by the distorted tetrahedral crystal field. The Mössbauer spectrum of the powder sample shows one dominant site exhibiting magnetic order at 2.1 K and a considerable quadrupole splitting as observed at room temperature. The magnetic hyperfine field of $B = 14.7(4)$ T is oriented orthogonal to the largest principle axis of the electrical field gradient $V_{zz} = -125(3)$ V/Å^2. The isomer shift of $\delta = 1.1(1)$ mm/s is consistent with the high spin Fe^{2+} (S=2) state. We will discuss the implications of these findings on the actual magnetic structure in this system. The observed static order is in agreement with susceptibility measurements showing a transition to antiferromagnetic order below 17 K.

TT 17.37 Mon 15:00 Poster D

The contribution of magnetic oxygen and magnetic correlations in the Mott insulator Ca_2RuO_4 — •Kevin Jenni[1], Stefan Kunkemöller[1], Yvan Sidis[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Laboratoire Léon Brillouin, CEA, Saclay

The Ruthenate system $Ca_{2-x}Sr_xRuO_4$ exhibits a variety of interesting phenomena reaching from unconventional superconductivity in Sr_2RuO_4 to a Mott-insulating state in Ca_2RuO_4. Concerning the latter, the theoretical understanding of the Mott transition in this multiband system with four electrons per Ru site is under debate to this day. There is consensus that the orbital ordering appearing in this strongly correlated material leads to an enhanced or fully occupation of the d_{xy} orbital and an occupation of the $d_{xz,yz}$ orbitals by the remaining two electrons. However, this orbital occupation only roughly corresponds to the measured ordered moment of 1.3 μ_B. To yield better insight in the exact distribution of the ordered magnetic moment over the orbitals we analyzed the magnetic form factor in detail. Our elastic neutron scattering study of an untwinned single crystal in combination with polarization analysis exposes the contribution of the apical oxygen to the ordered magnetic moment, similar to the results in $Ca_{1.5}Sr_{0.5}RuO_4$ where the p-d hybridization causes a sizeable amount of magnetic moment residing on the oxygen. Additionally we present the analysis of magnetic correlations and their dimensionality. The magnetic Bragg peak intensity vanishes rather fast above T_N = 110 K indicating a 3D correlation of the magnetic order.

TT 17.38 Mon 15:00 Poster D

Nonequilibrium Green Functions for Excited Lattice Systems—A Case Study of the Artificial Damping — •Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

The accurate description of nonequilibrium dynamics in correlated quantum-many-body systems remains to be a driving force for current research in condensed-matter physics and beyond. Among others, the nonequilibrium Green functions (NEGF) method has proven to be a powerful tool to predict quantum behavior[1], especially in the context of lattice systems[2]. Due to its two-time structure the NEGF approach gives access to two-particle and two-time observables, e.g. the double occupation and spectral properties. In 2009, von Friesen *et. al* reported the occurance of unphysical damping effects in NEGF calculations for strongly excited Hubbard clusters[3]. Since then, several ways have been proposed to overcome this deficiency by reducing the degree of selfconsistency[3,4]. Here, we focus on (time-dependent) spectral properties for finite Hubbard systems and the respective impact of both the artificial damping itself and the common methods of resolution. Furthermore, we introduce a controlled way to adjust the depth of selfconsistency based on the Dyson equation and compare its performance to previous approaches.
[1] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[2] N. Schlünzen *et al.*, Phys. Rev. B **95**, 165139 (2017)
[3] M. P. von Friesen *et al.*, Phys. Rev. Lett. **103** 176404 (2009)
[4] S. Hermanns *et al.*, Phys. Rev. B **90**, 125111 (2014)

TT 17.39 Mon 15:00 Poster D

***Ab initio* results for the dynamic structure factor of strongly correlated electrons** — Simon Groth, Tobias Dornheim, •Jan-Philip Joost, and Michael Bonitz — ITAP, CAU Kiel, Leibnizstraße 15, 24229 Kiel

The accurate description of electrons at high density and finite temperature is of paramount importance for, e.g., the understanding of astrophysical objects and correlated materials. In this context, the dynamic structure factor $S(q, \omega)$ constitutes a key quantity as it is directly measured e.g. in X-ray Thomson scattering experiments. We have recently [1] obtained the first *ab initio* results for $S(q, \omega)$ by carrying out extensive path integral Monte Carlo simulations and developing a new method for the required analytic continuation, which is based on the stochastic sampling of the dynamic local field correction $G(q, \omega)$. A particularly interesting result is the confirmation of a negative plasmon dispersion in the correlated liquid regime. This extends our recent work on the *ab initio* thermodynamic results of the warm dense electron gas [2] to dynamic quantities. These results are compared with an independent approach that is based on nonequilibrium Green functions [3].
[1] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett., in press, arxiv:1810.12776
[2] T. Dornheim, S. Groth, and M. Bonitz, Phys. Reports **744**, 1-86 (2018)
[3] N.H. Kwong and M. Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

TT 17.40 Mon 15:00 Poster D

Exact high-density limit calculation for quantum wires — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[3] — [1]Münster University of Ap-

plied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [4]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum $\epsilon_f \sim p_f^\beta$ where the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d < \beta + \alpha$ specifies systems where RPA is exact in the high-density limit. A cancellation of RPA and vertex corrections occurs up to second-order contact interaction. For finite-range potentials of cylindrical wires the structure function and correlation energy is found to be independent of the width parameter. The proposed high-density expansion agrees with diffusive Monte Carlo simulations and a fit formula is presented for the correlation energy.

[1] K. Morawetz, V. Ashokan, R. Bala, K. N. Pathak, Phys. Rev. B 97 (2018) 155147
[2] V. Ashokan, R. Bala, K. Morawetz, K. N. Pathak, Eur. Phys. J. B 91 (2018) 29, 1-7

TT 17.41 Mon 15:00 Poster D

Method for the DC-Conductance of one-dimensional correlated systems — •Jan-Moritz Bischoff and Eric Jeckelmann — Institut für Theoretische Physik, Hannover , Deutschland

We present a method for the linear DC-conductance of correlated one-dimensional lattice models[1]. Here specifically, we are interested in the conductance of Luttinger liquids. The method is based on the extrapolation of dynamical correlator functions in finite systems to the thermodynamic limit. We use a modified variant of the Density Matrix Renormalization Group(DMRG) algorithm to calculate the dynamical correlation function. We show that our method reproduces the predicted behaviour of the conductance in Luttinger liquids with impurities[1,3]. We investigate the complex behaviour of the spin and charge conductance of finite wires between leads and homogeneous electron-phonon systems.

[1] J.-M. Bischoff and E. Jeckelmann, PRB 96, 195111 (2017)
[2] C.L. Kane and M.P.A. Fisher, PRB 46, 15233 (1992)

TT 17.42 Mon 15:00 Poster D

Entanglement properties in quantum phases of the asymmetric two-leg Hubbard ladder — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Institut für Theoretische Physik, Appelstr. 2, 30167 Hannover

We investigate entanglement properties of an asymmetric two-leg Hubbard ladder that consists of one Hubbard leg and one tight-binding leg[1,2]. We use the density matrix renormalization group method to study the von Neumann entropy, central charge, Schmidt gap and entanglement spectrum for different quantum phases that appear by varying the inter-leg hopping term. We can distinguish the gapless and the correlated band insulating phases[1,2] using the entanglement properties in the ground state. The differences in entanglement properties between the Kondo-Mott and the spin-gaped Mott insulating phases[1,2] are less clear.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B 91, 155119 (2015)
[2] A. Abdelwahab and E. Jeckelmann, Eur. Phys. J. B 91, 207 (2018)

TT 17.43 Mon 15:00 Poster D

Linear-Response charge dynamics of the Hubbard model from the time-dependent Gutzwiller approximation — •Katharina Noatschk and Götz Seibold — Institut für Physik, BTU Cottbus-Senftenberg, Postfach 101344, 03013 Cottbus, Germany

The time dependent Gutzwiller approximation for the Hubbard model is obtained from the Lagrangian equation of motion for the density matrix and variational parameters. Expansion of the resulting equations up to second order in these dynamical variables yields an effective electron-boson problem where the bosons represent fluctuations of the double occupancy [1]. Within this formalism we investigate the charge excitations of the single-band Hubbard model for parameters relevant for cuprate superconducters. We also supplement the model with long-range Coulomb interaction and compare resulting excitations with experimental data from electron loss spectroscopy.

[1] J. Bünemann, M. Capone, J. Lorenzana, G. Seibold, New J. Phys., 2013

TT 17.44 Mon 15:00 Poster D

Building effective models for correlated electron systems — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

To understand strongly correlated systems, we must confront the many-body problem. Our starting point is density functional calculations for individual atoms and ions to obtain realistic basis functions and the corresponding matrix elements. In particular, we focus on the open-shell orbitals, which have the strongest correlation effects. For individual atoms and ions, we collected the Slater-Condon and spin-orbit parameters from the resulting self-consistent radial wave functions and potentials. We analyzed the trends of the parameters systematically across the periodic table, which allowed us to calculate atomic open-shell spectra in LS-, intermediate-, and jj-coupling schemes.

While atomic orbitals are mutually orthogonal within a single atom, they are, in general, non-orthogonal for atoms on different lattice sites. We studied and developed efficient multi-center integral techniques for evaluating orbital overlaps, which are essential for performing orbital orthogonalization. This allowed us to study atomic orbitals in various crystal structures. To orthogonalize the basis orbitals, we applied the Löwdin symmetric orthogonalization scheme, which minimizes the orbital modification. For the resulting orbitals, we studied the deformation due to orthogonalization and investigated the modification of the matrix elements compared with the atomic ones.

TT 17.45 Mon 15:00 Poster D

Real-Space DMFT with Classical Long-Range Coulomb Interactions: a Model Study — •Andreas Weh[1], Liviu Chioncel[1], Ulrich Eckern[1], and Junya Otsuki[2] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics, Tohoku University, Sendai, Japan

We present details of the numerical implementation of the charge self-consistent real-space dynamical mean-field theory (DMFT) for the Hubbard model considering long-range Coulomb effects at the local mean-field level. Results for spin-polarized multi-layers with different parameters are presented.

TT 17.46 Mon 15:00 Poster D

Robustness of transport and localization effects in long-range coupled spin chains — •Manuel Katzer and Alexander Carmele — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study the transport properties of a disordered Heisenberg spin chain with long-range interaction [1] to shed light on excitation localization properties in the presence of gain and dissipation. The long-range coupled chain shows nearly ballistic transport and linear response for all potential differences of the external reservoirs. In contrast, the common isotropic nearest-neighbor coupling shows negative differential conductivity and a transition from diffusive to subdiffusive transport for a far-from-equilibrium driving. For the disordered long-range coupled XXZ chain, any change in the transport behavior is independent of the potential difference and the coupling strengths of the external reservoirs and provides a robust platform to study many-body localization properties. Furthermore, we investigate the transition from a spin chain to a network of coupled harmonic oscillators [2], with nonclassical saturation effects and emerging nonlinear behavior, leading to anomalous energy transport.

[1] L. Droenner and A. Carmele Phys. Rev. B **96**, 184421 (2017)
[2] J. Huber and P. Rabl, arXiv:1807.10189

TT 17.47 Mon 15:00 Poster D

Heat transport through 1D spin chains — •Sonja Fischer and Lars Fritz — Utrecht University, Institute for Theoretical Physics, Princetonplein 5, 3584 CC Utrecht

We investigate the steady-state energy transport through a system of two coupled 1D spin chains at different temperatures. For two identical XX or Ising chains we recover the conjectured expression $J_E = \frac{c\pi}{12}(T_L^2 - T_R^2)$ for gapless chains with a conformal charge c [1] and show how this result can be generalized to non-equal chains. In addition we also consider a system with an XX chain coupled to an Ising chain, where the conjecture [1] does not apply and show that the energy transport can be controlled via a magnetic field.

[1] C. Karrasch, R. Ilan and J. E. Moore, PRB 88 195129 (2013)

TT 17.48 Mon 15:00 Poster D

Transient dynamics of the Hubbard model with nearest- and next-nearest-neighbor hopping — •Yusuf Mohammed and Alexander I. Lichtenstein — Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

We investigate the transient dynamics of the single orbital two-dimensional Hubbard model with nearest- and next-nearest-neighbor hopping. In equilibrium this model has provided a strong-coupling approach to the theory of high-temperature superconductivity as observed in copper oxides. We employ non-equilibrium cluster dynamical mean-field theory (CDMFT), using self-consistent strong-coupling perturbation theory, with the non-crossing approximation (NCA) being the lowest order. We report results for different quench protocols and driving fields.

TT 17.49 Mon 15:00 Poster D

Prescaling in a far-from-equilibrium Bose gas — Christian-Marcel Schmied[1], •Aleksandr Mikheev[2], and Thomas Gasenzer[3] — [1]christian-marcel.schmied@kip.uni-heidelberg.de — [2]aleksandr.mikheev@kip.uni-heidelberg.de — [3]t.gasenzer@uni-heidelberg.de

Non-equilibrium conditions give rise to a class of universally evolving low-energy configurations of fluctuating dilute Bose gases at a non-thermal fixed point (NTFP). While the fixed point and thus full scaling in space and time is generically only reached at very long evolution times, we here propose that systems can show prescaling much earlier, on experimentally accessible time scales. During the prescaling evolution, some well-measurable short-distance properties of the spatial correlations already scale with the universal exponents of the fixed point, while others still show scaling violations. Prescaling is characterized by the evolution obeying already, to a good approximation, the conservation laws which are associated with the asymptotically reached NTFP, defining its belonging to a specific universality class. In our simulations, we consider $N = 3$ spatially uniform three-dimensional Bose gases of labeled, e.g., by different hyperfine magnetic quantum numbers, with identical inter- and intra-species interactions. In this system, the approach of a NTFP is marked by low-energy phase excitations self-similarly redistributing towards smaller wave numbers. During prescaling, the full $U(N)$ symmetry of the model is broken, while the conserved transport, reflecting the remaining $U(1)$ symmetries, leads to the buildup of a rescaling quasicondensate distribution.