TT 18: f-Electron Systems and Heavy Fermions II

Time: Monday 15:00–17:30 Location: H 3005

TT 18.1 Mon 15:00 H 3005

Thermodynamics of heavy fermions with crystal-field excitations and lattice coherence — •Farzaneh Zamani[1], Stefan Kirchner[2], and Johann Kroha[1,2] — [1]Physikalisches Institut and BCTP, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, China

Heavy-fermion (HF) compounds exhibit an interplay of various phenomena, including Kondo effect, lattice coherence and crystal-field (CF) splitting. It is crucial to understand the corresponding features in the thermodynamics of heavy-fermion metals, e.g., in order to separate their energy scales from quantum critical scales. However, a complete understanding has been hampered by the fact that the CF-split angular-momentum multiplets of the rare-earth ions induce multiple spectral resonances near the Fermi energy (CF satellites), which are of Kondo-like many-body origin. Thus, not only their occupation number is thermally activated, but also their spectral weight depends on temperature, leading to complex thermodynamic behavior. We clarify the many-body nature of the CF excitations. We develop the Dynamical Mean-Field Theory for the multi-orbital, CF-split Anderson lattice model, using the self-consistent slave particle technique as an impurity solver, accurate down to well below the Kondo scale. We employ a novel gauge fixing technique for fixing the U(1) gauge of the slave particle fields which enables a highly accurate calculation of the free energy and its thermodynamic derivatives. Thermodynamic and spectroscopic results for both, the multi-orbital Anderson lattice and the single-impurity case, are presented.

TT 18.2 Mon 15:15 H 3005

Kondo insulators vs. transition metal-based narrow-gap semiconductors — •Jan M. Tomczak — Institute of Solid State Physics, TU Wien, Austria

Kondo insulators display a pronounced temperature dependence in their experimental observables: An insulating low-temperature regime with an activated magnetic susceptibility gives way—above a coherence temperature—to metallic conduction and Curie-Weiss behaviour. Empirically, this crossover is strikingly akin to that found in some correlated narrow-gap semiconductors, such as FeSi and $FeSb_2$, which are based on transition metals. Here, we present realistic many-body calculations for the prototypical Kondo insulator $Ce_3Bi_4Pt_3$[1] and compare them to our previous results for FeSi[2]. We discuss simulated transport properties, as well as photoemission and optical spectra. Further, we propose a microscopic distinction between the physics of both compounds from the perspective of dynamical mean-field theory. This work was supported by the Austrian Science Fund (FWF) through project P 30213-N36.

[1] JMT, Topical Review for J. Phys.: Condens. Matter (submitted),
[2] JMT, K. Haule, G. Kotliar, PNAS 109, 3243 (2012)

TT 18.3 Mon 15:30 H 3005

Kondo-lattice ferromagnets and their peculiar order along the magnetically hard axis — •Daniel Hafner[1], Binod Rai[2], Jacintha Banda[1], Kristin Kliemt[3], Cornelius Krellner[3], Jörg Sichelschmidt[1], Christoph Geibel[1], Emilia Morosan[2], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany — [2]Physics and Astronomy Department, Rice University, Houston, Texas 77005, USA — [3]Physikalisches Institut, Johann Wolfgang Goethe-Universität, D-60438 Frankfurt am Main, Germany

We show that ferromagnetism in Ce- and Yb- based Kondo-lattice systems often aligns along the magnetically hard axis. This counter-intuitive phenomenon was believed to be a rare case, but our comparative study suggests that this is rather the common case in these materials. We discuss possible theoretical scenarios by analyzing differences and similarities between all these systems. Differences appear in properties such as Curie temperatures T_C, crystalline structures, size of the ordered magnetic moment and crystal electric field ground state. Similarities lie in a usual Kondo temperature T_K of a few Kelvin, a comparable magnetic anisotropy and a non mean-field like transition in specific heat, hinting at an important role of fluctuations.

TT 18.4 Mon 15:45 H 3005

Tracking incommensurate magnetism with Slave Boson Mean Field Theory — •David Riegler[1], Michael Klett[1], Seulgi Ok[2], Titus Neupert[2], Peter Wölfle[3], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, University of Würzburg, Germany — [2]Department of Physics, University of Zurich, Switzerland — [3]Institute for Theory of Condensed Matter and Institute for Nanotechnology, Karlsruhe Institute of Technology, Germany

Accounting for strong correlations is one of the most challenging problems in solid state physics, and has given rise to the development of a plethora of different methodological approaches. Among them, the slave boson mean field formalism has been shown to successfully describe strongly correlated electron systems such as heavy fermion physics and quantum impurity models. While DMFT is another popular method of use within the scope of these systems, the slave boson mean field method can be applied to problems beyond the reach of DMFT, and such provide an interesting complementary view. In particular, this applies to models with large Hilbert spaces, and especially the investigation of incommensurate magnetic order where the magnetic unit cell would be too large to describe it within any cluster DMFT framework. Therefore, slave boson mean field is well suited to fill a niche in contemporary methods of condensed matter physics. This talk intends to elaborate on the method of spin rotation invariant slave boson mean field theory including fluctuations around the saddle point, and its applications to the periodic Anderson model as well as the topological Kondo insulator SmB_6.

TT 18.5 Mon 16:00 H 3005

Partial Kondo screening in a frustrated Kondo lattice model — •Toshihiro Sato[1], Fakher F. Assaad[1], and Tarun Grover[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, University of California at San Diego, USA

We study a half-filled Kondo lattice model on the honeycomb lattice with geometrical frustration. The geometrical frustration adds a new competing energy scale in the Doniach phase diagram which conventionally accounts only for the competition between the RKKY interaction and the Kondo screening. Using a negative-sign-free auxiliary field quantum Monte Carlo approach, we map out the phase diagram in the presence of geometrical frustration. In addition to the conventional Kondo insulator and the anti-ferromagnetically ordered state, we provide evidence for a novel 'partial Kondo screened' phase. In this phase, the spins are selectively screened so as to alleviate frustration, and the lattice rotation symmetry is broken nematically [1].

[1] T. Sato, F. F. Assaad, T. Grover, arXiv:1711.03116 (2017)

TT 18.6 Mon 16:15 H 3005

3D topological Kondo insulators: surface band structure and space charge screening — •soroush arabi[1], francisco meirinhos[1], and johann kroha[1,2] — [1]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China

Topological Kondo insulators (TKIs) are a new class of topological insulators, emerging through the interplay of strong correlations and spin-orbit coupling. In TKIs, the bulk is a narrow band insulator due to the appearance of a localised Kondo resonance near the Fermi level and its hybridisation with the conduction band. Additionally, the strong spin-orbit coupling of the localised moments generates a nonlocal hybridisation between the local moments and the conduction band, which results in a topologically nontrivial band structure and gapless surface states [1]. In this work, we study TKIs in a slab geometry and address the problems of space charges and screening near the surfaces. The strong Kondo correlations in the 4f orbitals are treated by a layer-dependent slave boson mean field (SBMF) theory, while the Coulomb repulsion in the conduction band is described by Hartree-Fock (HF) approximation. We solve the coupled SBMF+HF theory self-consistently and thereby analyse the perseverance of topological surface states.

15 min. break.

TT 18.7 Mon 16:45 H 3005

Bulk sensitive probe of $5f$ occupation and charge density

in URu_2Si_2 and $URu_{1.7}Fe_{1.3}Si_2$ — •Martin Sundermann[1,2,3], Andrea Amorese[1,2], Hasan Yavaş[3], Pieter Glatzel[4], Maurits W. Haverkort[5], Brian Maple[6], Liu Hao Tjeng[2], and Andrea Severing[1,2] — [1]University of Cologne, Institute of Physics II, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]PETRA III, Deutsches Elektronen- Synchrotron (DESY), Hamburg, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [5]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [6]University of California, San Diego, La Jolla, California, USA

URu_2Si_2 goes into a nonmagnetic hidden order (HO) phase at 17.7 K and becomes superconducting below 1.5K. The order parameter of the second-order phase transition into the HO phase in URu_2Si_2 is still a mystery, despite 30 years of research. Interestingly, with applied pressure ($p \geq 0.7$GPa) the HO is replaced with antiferromagnetic order with large ordered moments of $0.4\mu_B$. This phase can also be reached by substitution of Fe on the Ru site. In the Fe substituted samples the ordered moment is even larger. Here we have addressed the questions whether the $5f$ occupation and/or the ground state wave function change with Fe substitution. We will present high energy resolution fluorescence detection M-edge and non-resonant inelastic x-ray scattering O-edge data of $URu_{1.7}Fe_{0.3}Si_2$ and compare these with results of URu_2Si_2.

TT 18.8 Mon 17:00 H 3005

High magnetic field studies on $U_2Rh_3Si_5$ — •Nico Steinki[1], Stefan Süllow[1], Marcelo Jaime[2], Franziska Weickert[2], Neil Harrison[2], Hiroshi Amitsuka[3], Michal Vališka[4], and Vladimir Sechovsky[4] — [1]IPKM, TU Braunschweig, Germany — [2]NHMFL, LANL, Los Alamos, USA, — [3]Hokkaido University, Sapporo, Japan — [4]Charles University, Prague, Czech Republic

Together with UO_2, the intermetallic $U_2Rh_3Si_5$ is a prime example of a $5f$ material exhibiting a first order magnetic phase transition [1-3]. As demonstrated by means of thermodynamic, electronic transport and neutron scattering techniques, this monoclinic system undergoes a structural transition without changing the crystallographic symmetry at $T_N = 25.6$ K. It is accompanied by one into a canted antiferromagnetically ordered state with large magnetic moments ($\mu_{ord} \sim 2.4\mu_B$), together with apparent modifications of the Fermi surface. So far, experiments have been limited to magnetic fields < 30 T, and which has hindered a better understanding of the microscopic mechanism of the phase transition in $U_2Rh_3Si_5$. Moreover, previous experiments seem to indicate that for B||a axis there is a phase boundary in the range $\sim$ 40 T. As well, the question about attaining full ferromagnetic polarization along the b axis has not been settled. Hence, in this situation we have performed high field (65 T) magnetization and magnetostriction to map out the magnetic phase diagram.

[1] B. Becker et al., Phys. Rev. Lett. **78** (1997) 1347.
[2] T. Takeuchi et al., J.A. Mydosh, Phys. Rev. B **56** (1997) 10778.
[3] R. Feyerherm et al., Phys. Rev. B **56** (1997) 13693.

TT 18.9 Mon 17:15 H 3005

Theoretical Modeling of Resonant X-Ray Emission Spectra at the Actinide $M_{4,5}$ Edges — •Jindrich Kolorenc — Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic

I discuss a theoretical description of the resonant x-ray emission spectra (RXES) that is based on the Anderson impurity model. The parameters of the model are determined from material-specific LDA+DMFT calculations. Recently, this approach was shown [1] to accurately reproduce the L-edge RXES measured in lanthanides [2]. Here, the method is extended to the M-edge spectra in actinide compounds.

The same theoretical approach applies also to the x-ray absorption spectra measured in the high-energy-resolution fluorescence-detection mode (HERFD-XAS) [3]. As an example, I investigate the origin of large variations observed among the M-edge HERFD-XAS spectra of several uranium compounds where uranium atoms are in the same oxidation state. For instance, both UO_3 and torbentite have U atoms in the U(VI) state, but the shape of their x-ray absorption spectra differs quite substantially [4,5].

[1] J. Kolorenč, Physica B (2017), DOI: 10.1016/j.physb.2017.08.069
[2] J. A. Bradley *et al.*, Phys. Rev. B **85**, 100102 (2012).
[3] K. Hämäläinen *et al.*, Phys. Rev. Lett. **67**, 2850 (1991).
[4] Y. Podkovyrina *et al.*, J. Phys.: Conf. Ser. **712**, 012092 (2016).
[5] K. O. Kvashnina, Y. O. Kvashnin, S. M. Butorin, J. Electron. Spectrosc. Relat. Phenom. **194**, 27 (2014).