TT 42: Correlated Electrons: f-Electron Systems and Heavy Fermions 2

Time: Wednesday 15:00–17:45 Location: HSZ 204

TT 42.1 Wed 15:00 HSZ 204

Low-Temperature Properties of the Non-Centrosymmetric Heavy-fermion Compound $CeAl_2$ — •Christian Oberleitner, Alexander Regnat, Christian Franz, Jan Spallek, Georg Benka, Michael Petrov, Marc Wilde, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

Heavy-fermion compounds exhibit many unexpected low-temperature properties like unconventional superconductivity, non-Fermi liquid behavior or negative magnetoresistance. In this work, we report a comprehensive study of the non-centrosymmetric heavy-fermion compound $CeAl_2$ with T_N = 3.8K. The metallurgical characterization by Laue x-ray scattering and powder x-ray diffraction shows the excellent crystalline quality, which is confirmed by very high RRR values. Subsequently, magnetization, specific heat, torque magnetometry, resistivity, and Hall-effect measurements down to 200mK and up to 14T were carried out. The low-temperature measurements in the antiferromagnetic regime show complex magnetic behavior. Presumably, the Hall-effect cannot be explained by a superposition of anomalous and normal Hall-effect, which suggests a topological contribution.

TT 42.2 Wed 15:15 HSZ 204

Field-angle resolved magnetic excitations as a probe of hidden-order symmetry in CeB_6 — •Pavlo Y. Portnichenko[1], Alireza Akbari[2], Stanislav E. Nikitin[3], Alistair S. Cameron[1], Natalya Yu. Shitsevalova[4], Igor Radelytskyi[5], Astrid Schneidewind[5], Zita Hüsges[6], Jianhui Xu[6], Alexandre Ivanov[7], Jean-Michel Mignot[8], Peter Thalmeier[3], and Dmytro S. Inosov[1] — [1]TU Dresden, Germany — [2]APCTP Pohang, Korea — [3]MPI-CPfS Dresden, Germany — [4]IMPS, Kiev, Ukraine — [5]JCNS, Jülich, Germany — [6]HZB, Berlin, Germany — [7]ILL, France — [8]LLB, France

The heavy-fermion compound CeB_6 and its La-diluted alloys are among the best-studied realizations of the long-range multipolar phases, often referred to as "hidden order". Previously the hidden order in phase II was identified as primary antiferroquadrupolar and field-induced octupolar order. Here we present a combined experimental and theoretical investigation of collective excitations in the phase II of CeB_6. Inelastic neutron scattering in fields up to 16.5 T reveals a new high-energy mode above 14 T in addition to the low-energy magnetic excitations. The experimental dependence of their energy on the magnitude and angle of the applied magnetic field is compared to the results of a multipolar interaction model. We show that the rotating-field technique at fixed momentum can complement conventional INS measurements of the dispersion at constant field and holds great promise for identifying the symmetry of multipolar order parameters and the details of inter-multipolar interactions.

TT 42.3 Wed 15:30 HSZ 204

Topology in Magnetic Phases of SmB_6 — •Moritz M. Hirschmann, Huimei Liu, Andreas P. Schnyder, and Giniyat Khaliullin — Max Planck Institute for Solid State Research, Stuttgart, Deutschland

The heavy fermion compound SmB_6 is well known to be a Kondo insulator. Whereas its paramagnetic state was found to be topological, an analysis of the magnetic phases emerging in high-pressure SmB_6 considering its f-quartet ground state is still lacking. The exact magnetic order is yet unknown, therefore we discuss the two most likely magnetic structures, A-type and G-type, as well the high-field limit. We offer topological features as an experimental starting point to determine the magnetic order. With this in mind we present Dirac nodal lines for the A-type structure and Dirac points for the G-type structure. To investigate the topological properties we describe the mixed valence samarium sites with a tight-binding model and incorporate the effect of an internal magnetization. Our discussion includes symmetry arguments, Berry phases and the resulting surface states.

TT 42.4 Wed 15:45 HSZ 204

A Resonant Inelastic X-ray Scattering investigation of the 4f states in SmB_6 — •Andrea Amorese[1,2], Oliver Stockert[2], Kurt Kummer[3], Nicholas Brookes[3], Maurits Haverkort[4], Peter Thalmeier[2], Liu Hao Tjeng[2], and Andrea Severing[1] — [1]University of Cologne, Germany — [2]MPI-CPfS, Dresden, Germany — [3]ESRF, Grenoble, France — [4]University of Heidelberg, Germany

The crystal-field (CF) splitting of the $^6H_{5/2}$ Hund's rule ground state of Sm^{3+} in the strongly correlated topological insulator SmB_6 has been determined with high resolution resonant inelastic x-ray scattering (RIXS) at the Sm M_5 edge. The valence selectivity of RIXS allows isolating the crystal-field-split excited multiplets of the Sm^{3+} ($4f^5$) configuration from those of Sm^{2+} ($4f^6$) in intermediate valent SmB_6. We find that the quartet Γ_8 ground state and the doublet Γ_7 excited state are split by Δ_{CF} = 20±10meV. Considering this as an upper limit for the 4f bandwidth gives an extremely large mass renormalization from the band structure value, which can be linked to the small coefficient of fractional parentage for the hopping of the 4f electrons. The tiny band width complies with the small value of the gap and may be used to put constraints to the energies of the topological surface states. Financial support of the DFG under grant SE-1441/4-1 is acknowledged.

TT 42.5 Wed 16:00 HSZ 204

Partially Localized Phases in 5f Systems — •Bishal Poudel[1,2], Sébastien Burdin[1], and Gertrud Zwicknagl[2] — [1]LOMA UMR 5798, Université de Bordeaux, 33400, Talence, France — [2]Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study a generalized multi-orbital Hubbard Hamiltonian as an effective model for 5f electrons in actinide compounds. Our model assumes a large spin-orbit interaction, and includes local correlations. In our model, we use jj-scheme to classify the electronic states and due to large spin-orbit interaction the multiplet states with j = 7/2 or higher are neglected.

Here, we generalize the previous calculations [1-3] performed for 5f electrons systems using a rotationally invariant slave boson method [4] within a mean-field approximation. We analyze the phase diagram of the system at zero temperature. Varying the strength and anisotropy of the effective non-interacting electronic bandwidths, we analyze the partial -orbitally selective- localization of f electrons as well as their magnetic ordering.

[1] G. Zwicknagl, and P. Fulde, J. Phys. Condens. Matter 15, S1911 (2003).
[2] D. V. Efremov, N. Hasselmann, E. Runge, P. Fulde, and G. Zwicknagl, Phys. Rev. B 69, 115114 (2004).
[3] F. Pollmann, and G. Zwicknagl, Phys. Rev. B 73, 035121 (2006).
[4] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B 76, 155102 (2007)

TT 42.6 Wed 16:15 HSZ 204

Spectroscopic investigation of UFe_2Si_2, URu_2Si_2, UNi_2Si_2, and UPd_2Si_2: from Pauli paramagnetism to antiferromagnetism via the hidden order state. — Andrea Amorese[1,2], Martin Sundermann[1,2], Andrea Marino[2,3], Maurits Haverkort[4], Liu Hao Tjeng[2], and •Andrea Severing[1] — [1]University of Cologne, Germany — [2]MPI-CPfS, Dresden, Germany — [3]Politecnico di Milano, Milano, Italy — [4]Heidelberg University, Heidelberg, Germany

We have carried out hard x-ray photoelectron spectroscopy (HAXPES) measurements at the U 4f core level and non-resonant inelastic x-ray scattering (NIXS) at the U O4,5 edge of UT_2Si_2 compounds that all form in the tetragonal ThCr2Si2 structure but exhibit different ground state properties: UFe_2Si_2 is a Pauli paramagnet; URu_2Si_2 is the famous hidden order compound of which the order parameter is still fiercely debated despite 30 years of intense experimental and theoretical studies [1]; UPd_2Si_2 and UNi_2Si_2 are antiferromagnets with TN well above 100 K and sizeable ordered magnetic moments. We have determined the degree of the 5f-electron localization (HAXPES) as well as the symmetry of the 5f ground state wave function (NIXS [2]) across these very different compounds. This enabled us to identify their systematics and to place them in an effective Doniach phase diagram. *Financial support of the DFG under grant SE-1441/5-1 is gratefully acknowledged.*

[1] references in J.A. Mydosh and P.M. Oppeneer in Rev. Mod. Phys. 83, 1301 (2011) and in Phil. Magazine 94, 3642 (2014)
[2] M. Sundermann et al., PNAS 113, 13989 (2016)

15 min. break.

TT 42.7 Wed 16:45 HSZ 204

Metamagnetism in microstructured uranium mononitride — •S. Hamann[1,2], D. Gorbunov[1], T. Förster[1], M. König[2], A. V. Andreev[3], R. Troć[4], and T. Helm[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [3]Institute of Physics, Academy of Sciences, Prague, Czech Republic — [4]W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland

As in most $5f$ compounds, the origin of antiferromagnetism in uranium mononitride (UN) cannot be solely related to either itinerant or local behavior. While inelastic neutron scattering [1] and photoemission measurements [2] as well as bandstructure calculations suggest an itinerant nature, the recently discovered metamagnetic transition at 55 T [3] contradicts this picture. To investigate this spin-flop-like transition with transport measurements, we fabricated microstructures from single-crystalline UN using focussed ion beam technique. The gained resolution allows us to study the temperature and field-dependent Hall effect and longitudinal electrical transport in great detail.

[1] T. M. Holden *et al.*, Phys. Rev. B. **30**, 1 (1984)
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[3] K. Shrestha *et al.*, Scientific Reports **7**, 1 (2017)

TT 42.8 Wed 17:00 HSZ 204

Crystallographic structure and magnetism of UNi_4B — •Jannis Willwater[1], Stefan Süllow[1], Milan Klicpera[2], Michal Valiska[2], Vladimir Sechovsky[2], Bachir Ouladdiaf[3], and Hiroshi Amitsuka[4] — [1]IPKM, TU Braunschweig, Germany — [2]Department of Condensed Matter Physics, Charles University, Czech Republic — [3]Institut Laue-Langevin, France — [4]Department of Condensed Matter Physics, Japan

The frustrated intermetallic magnet UNi_4B has been reported to crystallize in a hexagonal crystallographic structure and to exhibit a peculiar type of partial magnetic order at low temperatures. Recently, synchrotron x-ray diffraction data have indicated that the structure is orthorhombic and not hexagonal. The best description of the crystal structure at 300 K was obtained with the space group 63 (*Cmcm*). In this situation, to understand the nature of the magnetic transitions at low temperature, it requires the determination of the low temperature crystallographic symmetry. Therefore, we have studied a ^{11}B enriched single crystal UNi_4B, here using elastic neutron scattering. In our experiment, various structural Bragg peaks forbidden for the *Cmcm* symmetry have been detected and indicate that the symmetry of the crystal structure is even lower. From fits to our data, we have obtained the best description of the structure with the orthorhombic space group 25 (*Pmm2*). Further we have detected various magnetic Bragg peaks and established their temperature dependence.

TT 42.9 Wed 17:15 HSZ 204

Terahertz conductivity of heavy-fermion systems from time-resolved spectroscopy — •C.-J. Yang[1], S. Pal[1], F. Zamani[2], K. Kliemt[3], C. Krellner[3], O. Stockert[4], H. v. Löhneysen[5], J. Kroha[2], and M. Fiebig[1] — [1]ETH Zürich, Switzerland — [2]University of Bonn, Germany — [3]Goethe-University Frankfurt, Germany — [4]MPI CPfS Dresden, Germany — [5]KIT Karlsruhe, Germany

Ultrafast, phase-sensitive terahertz (THz) spectroscopy has recently been introduced as a novel tool to investigate the quasiparticle (QP) dynamics across the quantum phase transition in heavy-fermion compounds [1,2]. The incident THz pulse with a spectral range of 0–3 THz creates collective intraband excitations within the heavy band as well as resonant interband transitions between the hybridizing heavy and light parts of the conduction band. The latter break the Kondo singlet and thus lead to a time-delayed echo-like response [1,2]. By contrast, the intraband excitations leave the heavy quasiparticles intact and are expected to be Fermi-liquid Drude response. Our time-resolved phase-sensitive measurements of the electric field response enables us to separate both types of excitations by their delay time and to derive their individual contributions to the THz optical conductivity. While the Kondo-breaking interband transitions create no Drude peak, the intraband excitations recover the Drude response as expected. It is thus possible to separate strongly and weakly correlated electronic contributions to the optical conductivity.

[1] C. Wetli *et al.*, Nat. Phys. **14**, 1103 (2018)
[2] S. Pal *et al.*, PRL **122**, 096401 (2019)
[3] C.-J. Yang *et al.*, under prep. (2019)

TT 42.10 Wed 17:30 HSZ 204

Resonant X-Ray Emission Spectra: Effects of the Final-State Core Hole — •Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

The resolution of the x-ray absorption spectroscopy is fundamentally limited by the life-time broadening of the core hole created in the absorption event. When the absorption is detected by monitoring a particular core-to-core emission process of filling the created hole (for instance, the 3d → 2p transition in the case of lanthanide L edges), the broadening is reduced and it is determined by a considerably longer life time of the shallower 3d hole remaining in the final state [1]. This is not always the whole story – there can be a sizable exchange interaction between the final-state core hole and some partially filled valence shell (this would be the 4f shell in the lanthanide example). The exchange interaction causes multiplet splitting that reduces the resolution again and potentially even introduces spurious features to the deduced absorption spectra. I will discuss these effects theoretically using the atomic model and the Anderson impurity model. I will show under which simplifying conditions the many-body part of the problem reduces to evaluation of a propagator of the final-state core hole, a quantity that is measured by the x-ray photoemission.

[1] K. Hamalainen, D. P. Siddons, J. B. Hastings, L. E. Berman, Phys. Rev. Lett. **67**, 2850 (1991).