TT 6: Kondo Physics, f-Electron Systems and Heavy Fermions

Time: Monday 15:00–18:15 Location: H22

TT 6.1 Mon 15:00 H22

Zooming in on heavy fermions in Kondo lattice models — Bimla Danu[1], Zihong Liu[1], Fakher Assaad[1], and •Marcin Raczkowski[2] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

Resolving the heavy fermion band in the conduction electron momentum resolved spectral function of the Kondo lattice model (KLM) is challenging since, in the weak coupling limit, its spectral weight is exponentially small. To alleviate this limitation we consider a composite fermion operator, consisting of a conduction electron dressed by spin fluctuations that shares the same quantum numbers as the electron. Using auxiliary field quantum Monte Carlo simulations we show that for the SU(2) spin-symmetric model on the square lattice at half filling, the quasiparticle residue of the composite fermion tracks the Kondo coupling J_k. This result holds down to $J_k/W = 0.05$, with W the bandwidth, and confirms that magnetic ordering, present below $J_k/W = 0.18$, does not destroy the heavy quasiparticle. We also study the spectral function of the composite fermion in the ground state and at finite temperatures, for SU(N) generalizations of the KLM, as well as for ferromagnetic Kondo couplings, and compare our results to analytical calculations in the limit of high temperatures, large-N, large-S and large J_k.

TT 6.2 Mon 15:15 H22

Two-channel Kondo effect in locally non-centrosymmetric systems — •Daniel Hafner — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

A scalable model is presented, which shows that two-channel Kondo (2CK) physics is possible in centrosymmetric crystals, in which the spin-orbit (SO) energy splitting α of conduction electron states is stronger than the hopping parameter t between an inversion symmetric pair of them. The potential difference introduced by the SO coupling effectively suppresses the hopping and disentangles the conduction states into two channels, allowing them to independently couple to impurity spins. If the impurity sites are located on inversion centers, the identical Kondo coupling strengths lead to a symmetrical 2CK effect below the Kondo temperature T_{2CK}. Since the coupling between sectors is still present, the impurity spin is eventually fully quenched by the entangled part of the conduction electrons in a single-channel Kondo effect below T_{1CK}. For $\alpha/t > \sqrt{2}$, a temperature region $T_{2CK} > T > T_{1CK}$ with dominant 2CK physics is found. If the impurities are not located on inversion centers, the resulting channel-asymmetric 2CK model introduces a third temperature scale. Below this, each of two inversion-symmetric impurity sites is screened by one of the two channels, creating a Fermi liquid made up of two types of Kondo singlets linked by inversion symmetry. The similarity of the presented 2CK model to the well established 2CK effect in quantum dots is discussed as well as possible candidate materials like the locally non-centrosymmetric heavy-fermion superconductor $CeRh_2As_2$.

TT 6.3 Mon 15:30 H22

Spin chain on a metallic surface: Dissipation-induced order vs. Kondo entanglement — •Bimla Danu[1], Matthias Vojta[2], Tarun Grover[3], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [3]Department of Physics, University of California at San Diego, La Jolla, CA 92093, USA

We study the physics of an antiferromagnetic spin-1/2 chain Kondo coupled to a two dimensional metal as realized, for example, by depositing an array of magnetic adatoms on a metallic surface with scanning tunneling microscopy (STM) methods. Based on a field theoretical perturbative approach we show that at weak Kondo coupling this system maps onto a spin-1/2 chain coupled to a dissipative Ohmic bath. We argue that in this limit the dissipation induces long-range antiferromagnetic order along the spin chain. Using auxiliary field quantum Monte-Carlo simulations we show that the spin chain as a function of the Kondo coupling exhibits a quantum phase transition from an antiferromagnetic phase to a paramagnetic heavy fermi liquid phase. Since the heavy quasiparticle is not destroyed in the magnetic phase and at the critical point, this quantum phase transition falls in a Hertz-Millis-Moriya type quantum criticality. We discuss the relevance of our results in the context of STM experiments of magnetic adatom chains on metallic surfaces.

TT 6.4 Mon 15:45 H22

Quasiparticle critical slowing down in a heavy-fermion system — •Chia-Jung Yang[1], Kristin Kliemt[2], Cornelius Krellner[2], Johann Kroha[3], Manfred Fiebig[1], and Shovon Pal[1,4] — [1]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany — [3]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, 53115 Bonn, Germany — [4]School of Physical Sciences, National Institute of Science Education and Research, HBNI, Jatni, 752 050 Odisha, India

Critical slowing down (CSD) is a universal phenomenon in phase transitions. A system, after suffering an initial perturbation, takes a very long time to return to its equilibrium state. While CSD is universally observed in the dynamics of bosonic excitations, it is not observed to occur for fermionic excitations. This is because of the half-integer nature of the fermionic spin. In this contribution, we show a fermionic CSD in the heavy-fermion (HF) compound $YbRh_2Si_2$ (YRS) by using phase-sensitive terahertz time-domain spectroscopy (THz-TDS). THz-TDS has recently been introduced as a novel tool to investigate the quasiparticle dynamics across quantum phase transition (QPT) in HF compounds [1–3]. We see that near the QPT in YRS, the build-up of spectral weight towards the Kondo temperature $T_K^* = 25\,K$ is followed by a logarithmic rise of the quasiparticle excitation rate on the heavy-Fermi-liquid side below 10 K. A critical two-band HF liquid theory shows that this is indicative of fermionic CSD, the softening of the HF quasiparticle dispersion.

TT 6.5 Mon 16:00 H22

Pressure tuning of the low-temperature states of $CeRh_2As_2$ — •Meike Pfeiffer[1], Konstantin Semeniuk[2], and Elena Hassinger[1,2] — [1]Technische Universität München, 85748 Garching, Germany — [2]Max Planck Institut für chemische Physik fester Stoffe, 01187 Dresden, Germany

$CeRh_2As_2$ is a heavy-fermion superconductor with a centrosymmetric tetragonal crystal structure lacking local inversion symmetry at the Ce sites. It presents two-phase superconductivity with an exceptionally high ratio of critical field (> 15 T) to critical temperature ($T_c = 0.3$ K). An additional phase can be observed below 0.4 K, believed to be a quadrupole-density wave (QDW) order. We conducted an electrical resistivity study of $CeRh_2As_2$ down to 30 mK applying hydrostatic pressure up to 3 GPa. We find that under pressure the Kondo coherence peak shifts linearly to higher temperature at a rate of 10 K/GPa. The QDW order is highly sensitive to lattice compression and gets fully suppressed at about 0.7 GPa. The superconducting T_c decreases with a significantly lower rate suggesting no influence of QDW on superconductivity. The upper critical fields show an anisotropic behaviour: for $H \parallel$ c it decreases, whereas for $H \parallel$ a,b it increases for pressures up to ≈ 0.9 GPa and then also decreases. We relate our observations to the change of the relevant energy scales, such as Kondo temperature, Rashba spin-orbit coupling, and interlayer hopping.

TT 6.6 Mon 16:15 H22

The quadrupole density wave and its interplay with superconductivity in $CeRh_2As_2$: A thermodynamic study — •Pavlo Khanenko[1,2], Daniel Hafner[1], Robert Küchler[1], Jacintha Banda[1], Thomas Lühmann[1], Javier F. Landaeta[1], Florian Bärtl[3], Tommy Kotte[3], Joachim Wosnitza[2,3], Christoph Geibel[1], Seunghyun Khim[1], Elena Hassinger[1,4], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence, Germany — [4]Technical University Munich, Germany

The heavy-fermion $CeRh_2As_2$ is a rare case of multi-phase supercon-

ductor (T_c = 0.26 K) located in the vicinity of a quantum critical point. Two different superconducting (SC) phases are observed for a magnetic field applied along the c-axis of the tetragonal locally-non-centrosymmetric crystalline structure. The upper critical field along c-axis ($B \parallel c$) is huge, B_{c2} = 14 T, but with field within the basal ab-plane ($B \perp c$) only a single SC phase is observed with B_{c2} = 2 T. Thermodynamic measurements have detected another non-magnetic phase transition at T_0 = 0.4 K which was interpreted as a quadrupole-density-wave (QDW) state. Here, we present new zero-field-cooled and field-cooled specific heat and thermal expansion measurements on a single crystal of $CeRh_2As_2$ with $B \parallel c$ and $B \perp c$. These allow to extend the phase diagram for $B \parallel c$ and to discuss the interplay between the SC and QDW states.

15 min. break

TT 6.7 Mon 16:45 H22

Heavy quasiparticles in Fermi surface and electronic instabilities in the heavy-fermion superconductor $CeRh_2As_2$ — •Evrard-Ouicem Eljaouhari and Gertrud Zwicknagl — Institut f. Mathemat. Physik, TU Braunschweig, Braunschweig, Germany

We present calculations of the heavy quasiparticles in the heavy-fermion compound $CeRh_2As_2$ which exhibts multi-phase superconductivity[1]. The narrow quasiparticle bands that are derived from the Ce-4f degrees of freedom are calculated by means of the Renormalized Band (RB) method. The RB scheme provides a framework for a realistic description of the coherent low-energy excitations in a Fermi liquid which combines material-specific ab-initio methods and phenomenological considerations in the spirit of the Landau theory of Fermi liquids. The central focus of the present study is the role played by the non-symmorphic lattice structure and the consequences of the Crystalline Electric Field (CEF) which removes the orbital degeneracy of the Ce 4f states. We conjecture that the quasi-quartet CEF ground state in combination with pronounced nesting features of the Fermi surface may give rise to a quadrupole density wave [2].

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[1] S. Khim et al., Science 373, 1012 (2021)
[2] D. Hafner et al., Phys. Rev. X 12, 011023 (2022)

TT 6.8 Mon 17:00 H22

Muon spin rotation/relaxation studies on the heavy-fermion superconductor $CeRh_2As_2$ — •Seunghyun Khim[1], Manuel Brando[1], Oliver Stockert[1], Christoph Geibel[1], Zurab Guguchia[2], Robert Scheuermann[2], Debarchan Das[2], and Toni Shiroka[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen PSI, Switzerland

We study magnetic and superconducting (SC) properties of the unconventional superconductor $CeRh_2As_2$ ($T_c \sim 0.3$ K) by means of muon spin rotation/relaxation (μSR) experiments. No clear evidence of oscillation is identified in zero-field μSR spectra down to 0.27 K while the relaxation rate moderately increases below $\sim$ 0.4 K. This could be associated with the suggested quadrupole-density-wave order at T_0 $\approx$ 0.4 K and the antiferromagnetic order at $T_N \approx 0.27$ K. In weak transverse-field (TF) μSR measurements, a pronounced increase in the relaxation rate was observed in the SC state. The relaxation rate (σ_s), regarded as a direct measure of the magnetic penetration depth λ ($\sigma_s \propto 1 / \lambda^2$), almost flattens below $T/T_c \sim 0.2$, being strongly indicative of suppressed quasiparticle excitations. TF-μSR measurements under 2 T reveal a power-law-like T-dependent relaxation rate in the normal state, indicating critical fluctuations. Furthermore, this relaxation rate increases with fields in both the normal and SC state, implying unusual magnetism. Our observations suggest $CeRh_2As_2$ to have a nearly fully-gapped SC behavior in the vicinity of a peculiar quantum critical point.

TT 6.9 Mon 17:15 H22

Anisotropy of resistivity and magnetotransport in $CeRh_2As_2$ — •Konstantin Semeniuk, Seunghyun Khim, and Elena Hassinger — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The recently discovered heavy-fermion superconductor $CeRh_2As_2$ exhibits an intriguing low-temperature phase diagram containing two superconducting states [1], a quadrupole density wave order [2], and an antiferromagnetic state [3]. The underlying mechanisms of such a behaviour are currently being explored. However, symmetry-induced Rashba spin-orbit effect, Kondo interaction and interlayer coupling have already emerged as the primary ingredients.

To quantify the electronic properties of the compound further, we conducted a comprehensive study of charge transport in $CeRh_2As_2$. Precise control over sample dimensions and current flow direction were achieved via focused ion beam micromachining of single crystals in a strain-free manner. Based on resistivity anisotropy measurements the three-dimensional character of the electronic structure is established. We also examine magnetoresistance and Hall effect for different orientations of magnetic field with respect to the lattice.

[1] J. Landaeta et al., Phys. Rev. X, accepted (2022)
[2] D. Hafner et al., Phys. Rev. X **12**, 011023 (2022)
[3] M. Kibune et al., Phys. Rev. Lett. **128**, 057002 (2022)

TT 6.10 Mon 17:30 H22

Influence of substrate clamping in epitaxial $EuPd_2Si_2$ thin films — •Sebastian Kölsch[1], Cornelius Krellner[1], Hans-Joachim Elmers[2], and Michael Huth[1] — [1]Goethe Universität, Frankfurt (Main) — [2]Johannes Gutenberg-Universität, Mainz

Europium-based ternary compounds, which crystallize in the tetragonal $ThCr_2Si_2$ structure, reveal a variety of interesting phenomena, which are attributed to strong electronic correlations and a competition between Kondo effect and the RKKY interaction. Recently $EuPd_2Si_2$ gained increased interest due to a temperature-driven valence transition from nearly Eu^{2+} above 200 K to Eu^{3+} below about 50 K. This rapid but continuous change of the Europium mean valence is accompanied by a relative change of the $EuPd_2Si_2$ a lattice constant by about -2 % reflecting the strong coupling of lattice and electronic degrees of freedom. For epitaxial thin films of this material the underlying substrate has to be taken into account. In this case the change of the lattice constants due to clamping to the substrate impacts the possible thermal expansion of the corresponding in-plane components. So far research has focused on optimizing single crystal growth conditions under different doping scenarios to tune the system into a critial endpoint. Epitaxial thin films instead offer the possibility to strain-engineer this correlated system by appliying biaxial strain to the thin film material upon cooling.

Here we present for the first time the successful growth of $EuPd_2Si_2$ as epitaxial thin film and report our recent results regardings its clearly distinct properties as compared to single crystals.

TT 6.11 Mon 17:45 H22

Theory of valence-band photoemission from Am metal — •Jindrich Kolorenc — Institute of Physics (FZU), Czech Academy of Sciences, Praha, Czech Republic

The 5f states in americium metal are generally agreed to be localized, similar to 4f states in lanthanides, being in a well-defined $5f^6$ configuration (Am^{3+}). In the same time, the valence-band photoemission spectrum [1,2] cannot be interpreted as a single set of multiplet transitions ($5f^6 \rightarrow 5f^5$) like in lanthanides [3], and a second set of multiplets ($5f^7 \rightarrow 5f^6$) has to be introduced [4]. Two mechanisms were suggested as a possible origin of these additional transitions: (i) Am^{2+} layer forming at the surface of the sample or (ii) a second screening channel for the 5f hole created during the photoemission process, with the second mechanism later determined as more likely [2]. Up to now, there does not seem to be a quantitative theory that would substantiate these empirical ideas. The best attempt to date [5] combined the DFT+DMFT method with a generalized Hubbard-I impurity solver, which reproduced the $5f^7 \rightarrow 5f^6$ part of the spectrum well, but it also generated a spurious 5f intensity at the Fermi level. Here I report a DFT+DMFT study employing a more accurate impurity solver (exact diagonalization) and demonstrate the mechanism leading to the $5f^7 \rightarrow 5f^6$ multiplets in the Am PES spectra.

[1] J. R. Naegele *et al.*, Phys. Rev. Lett. **52**, 1834 (1984)
[2] T. Gouder *et al.*, Phys. Rev. B **72**, 115122 (2005)
[3] J. K. Lang *et al.*, J. Phys. F: Met. Phys. **11**, 121 (1981)
[4] N. Mårtensson *et al.*, Phys. Rev. B **35**, 1437 (1987)
[5] A. Svane, Solid State Commun. **140**, 364 (2006)

TT 6.12 Mon 18:00 H22

Kondo systems with periodically driven dipole transitions — •Michael Turaev and Johann Kroha — Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany

In this work, we study the effects of light irradiation on a magnetic impurity. The impurity is modelled by the single impurity Anderson model where the local impurity is coupled to the conduction electrons via dipole coupling. Therefore, the application of a strong laser field

induces a time-periodic hybridization. This can be treated within Floquet Green's function method combined with the slave boson noncrossing approximation [1]. What we see is that the Kondo peak is robust against small driving strengths, and then it gets strongly suppressed when the driving strength increases. However, we find that the destruction of the Kondo effect occurs much faster in terms of driving strength compared to a situation where the energy level of the impurity is itself driven independently.

[1] B. H. Wu and J. C. Cao, Physical Review B81, 085327 (2010)