TT 59: Correlated Electrons: Quantum Impurities and Kondo Physics; Other Materials

Time: Thursday 15:00–18:30 Location: HSZ 03

TT 59.1 Thu 15:00 HSZ 03

Phase Diagram and Dynamics of an SU(N) Symmetric Kondo Lattice Model — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the interplay between Kondo screening and the magnetic RKKY interaction in an SU(N) symmetric generalization of the two-dimensional half-filled Kondo lattice model (KLM) by quantum Monte Carlo simulations with N up to 8 [1]. While the long-range antiferromagnetic (AF) order in SU(N) quantum spin systems typically gives way to spin-singlet ground states with spontaneously broken lattice symmetry, we find that the SU(N) KLM in the totally antisymmetric self-adjoint representation is unique in that for each finite N its ground-state phase diagram hosts only two phases – AF order and the Kondo-screened phase. We believe that it is the enhanced range of the RKKY interaction that is the key to stabilize antiferromagnetism at large N. Given that the range of the RKKY interaction grows as a function of N, we generically expect that the relevant physics will become more mean-field-like. A resolved abrupt jump of the coherence temperature across the phase transition for $N > 2$ supports this line of arguing and sheds new light on the rapid loss of coherence at the magnetic phase transition in heavy-fermion systems.

[1] M. Raczkowski and F. F. Assaad, arXiv:1910.07540 (2019).

TT 59.2 Thu 15:15 HSZ 03

Magnetic doublon bound states in the Kondo Lattice Model — •Roman Rausch[1], Michael Potthoff[2], and Norio Kawakami[1] — [1]Kyoto University — [2]University of Hamburg

We present a novel pairing mechanism for electrons, mediated by magnons. These paired bound states are termed "magnetic doublons". Applying numerically exact techniques (exact diagonalization and the density-matrix renormalization group, DMRG) to the Kondo lattice model at strong exchange coupling J for different fillings and magnetic configurations, we demonstrate that magnetic doublon excitations exist as composite objects with extremely weak dispersion at excitation energies of the order of 3J/2 above the ground state. They are highly stable, support a novel "inverse" colossal magnetoresistance and potentially other effects like metastable superconductivity, or cooling via quantum distillation.

[1] R. Rausch, M. Potthoff, N. Kawakami, arXiv:1909.11896

TT 59.3 Thu 15:30 HSZ 03

Genuine RKKY-Kondo quantum phase transition — •Krzysztof P. Wójcik[1,2] and Johann Kroha[1] — [1]Physikalisches Institut, Universität Bonn, Germany — [2]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Since the seminal papers of Jones and Varma, the RKKY interaction (Y) between two Kondo impurities is conventionally modeled by a Heisenberg coupling term. It gives rise to a quantum phase transition (QPT) between the Kondo and the RKKY phases in the two-impurity Kondo model. Yet, the significance of this result is still controversial. Firstly, the QPT is extremely fragile to particle-hole (PH) asymmetry, changing the QPT to a crossover in its presence. This has lead to the common belief that it cannot be realized in a realistic 2-impurity system and has made its relevance for lattice models debatable. Moreover, in the model Y and the Kondo exchange J are considered independent, although Y is genuinely generated by J, and the Kondo temperature depends on Y, as has been shown experimentally [1] and theoretically [2]. Recently, it has been proven that the QPT can be restored for weaker PH symmetry by parameter fine-tuning [3]. We revisit the problem to show by numerical renormalization group calculations that in the geometry of [1], Y induced solely by J causes the QPT for a properly symmetric case. We also discuss potential consequences of our findings for the lattice model in the context of "Kondo destruction".

[1] J. Bork *et al.*, Nat. Phys. **7**, 901 (2011).
[2] A. Nejati, K. Ballmann, J. Kroha, PRL **118**, 117204 (2017).
[3] F. Eickhoff, B. Lechtenberg, F. Anders, PRB **98**, 115103 (2018).

TT 59.4 Thu 15:45 HSZ 03

Investigation of Yu-Shiba-Rusinov states of magnetic structures on the surface of β-Bi$_2$Pd superconductor — •Stefano Trivini, Jon Ortuzar, Javier Zaldivar, and Nacho Pascual — CICnanoGUNE, San Sebastiàn, Spain

Magnetic atoms deposited on superconductors induce a pair breaking effect that reflects in intragap states known as Yu-Shiba-Rusinov (YSR) states.[1]

Through their interaction with the substrate, the atoms can be magnetically coupled between each other. This magnetic interaction is reflected in the YSR sub gap structure.[2]

While the effect of magnetic coupling of atoms in extended wires on their Kondo interaction[2] or spin excitation[2] has been previously addressed, the behavior on their YSR is still being investigated.

Here, we do atomic manipulation of magnetic adatoms on β-Bi$_2$Pd by low temperature STM, building atomically perfect magnetic structures. The YSR states can be measured by means of STS with a β-Bi$_2$Pd superconducting tip with 100 ueV energy resolution.

TT 59.5 Thu 16:00 HSZ 03

Transport in interacting quantum dots: Analytical results from the path integral approach beyond the weak tunneling regime — •Luca Magazzù and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We report on the progress in transport calculations with an analytical path integral technique applied to interacting quantum dots. Starting from the formally exact diagrammatic representation of the dot dynamics and current, a suitable parametrization of the paths of the dot variables allows to apply resummation schemes which address parameter regimes ranging from the noninteracting to the low temperature/strongly-interacting. The known analytical results are recovered in the appropriate limits.

TT 59.6 Thu 16:15 HSZ 03

Theory of scanning tunnelling spectroscopy of Co adatoms in a magnetic field: A Kondo problem of an extended impurity — •Bimla Danu[1], Fakher F. Assaad[1], and Frédéric Mila[2] — [1]Institut fur Theoretische Physik und Astrophysik, Universitat Wurzburg, Am Hubland, D-97074 Wurzburg, Germany — [2]Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The ability to build and manipulate various Kondo nano-structures has been demonstrated in many recent experiments using scanning tunneling spectroscopy (STS). For example, recent STS experiments on chains of Co adatoms have revealed a series of level crossings as a function of magnetic field. Motivated by these experimental studies, we explore the magnetic field induced Kondo effect that takes place at symmetry protected level crossings in finite Co adatom chains. In particular, we provide a quantitative theory of STS signal based on auxiliary-field quantum Monte Carlo simulations, and, show that the physics at the vicinity of level crossings is a Kondo problem of an extended Impurity.

TT 59.7 Thu 16:30 HSZ 03

Nonlinear polaron dynamics — •Tomasz Wasak, Falko Pientka, and Francesco Piazza — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A mobile impurity immersed into a degenerate Fermi system is a paradigmatic problem in many-body physics. In 2D, the impurity is dressed by particle-hole excitations and forms a new quasi-particle, called the polaron, with new dispersion relation and effective mass.

Recent observation of polaron signatures in 2D semiconductors renewed interest in this field. These systems, based on atomically thin transition metal dichalcogenides, offer promising applications in both linear and nonlinear optics, since the strongly bound excitons dominate the optical response. The presence of a bath of fermions leads to dressing of excitons resulting in the formation of exciton-polarons. These new excitations, when coupled to microcavity photons, can find applications in novel photonic devices, such as exciton-polariton lasers.

The description of the polaron physics in these systems was based on equilibrium quantum field theory or wave function techniques. However, due to finite lifetime of excitons, the system is non-equilibrium in nature, and a proper treatment is required that includes gain and loss into the theoretical description. We have developed a technique based on Keldysh non-equilibrium field-theoretical approach tailored for this open quantum system. We derived a quantum kinetic Boltzmann equation that consistently includes dissipation and drive, and allows to study the transitions between repulsive and attractive polaron branches, and non-equilibrium distributions.

15 min. break.

TT 59.8 Thu 17:00 HSZ 03

Unusual phase boundary of the magnetic-field-tuned valence transition in $CeOs_4Sb_{12}$ — •Kathrin Götze[1], Matthew Pearce[1], Paul Goddard[1], Marcelo Jaime[2], M. Brian Maple[3], Kalyan Sasmal[3], Tatsuya Yanagisawa[4], Alix McCollam[5], Thomas Khouri[5], Pei-Chun Ho[6], and John Singleton[2] — [1]University of Warwick, Coventry, UK — [2]National High Magnetic Field Laboratory, Los Alamos, USA — [3]University of California, San Diego, USA — [4]Hokkaido University, Sapporo, Japan — [5]High Field Magnet Laboratory (EMFL), Nijmegen, NL — [6]California State University, Fresno, USA

The H-T phase diagram of the filled skutterudite $CeOs_4Sb_{12}$ was mapped out in magnetic fields up to 60 T by resistivity, magnetostriction, and MHz conductivity. The semimetallic low-H, low-T L phase and the metallic high-H, high-T H phase are separated by a valence transition which – opposing the “elliptical” text-book behaviour for which $H^2 \propto T^2$ – exhibits a boundary with an almost wedge-like shape with a non-monotonic gradient that alternates between positive and negative. We ascribe the unusual behaviour of the phase boundary at low T to the presence of additional energy scales associated with a quantum critical point. Field-dependent, increasing effective masses derived from quantum oscillations close to the intersection of L, H and the ordered spin-density wave phase are interpreted as indicators of this quantum criticality. The high-T, low-H portion of the phase diagram may instead be associated with the proximity of $CeOs_4Sb_{12}$ to a topological semimetal phase induced by uniaxial stress.

TT 59.9 Thu 17:15 HSZ 03

Controlling electronic phases in an excitonic insulator by cryogenic scanning tunneling microscopy — •Qingyu He[1], Xinglu Que[1], Alexander Yaresko[1], Andreas Rost[1,3], Masahiko Isobe[1], Tomohiro Takayama[1], Lihui Zhou[1], and Hidenori Takagi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan — [3]University of St. Andrews, St. Andrews, England

The excitonic insulator is a long conjectured correlated electron phase stabilized by weakly screened electron-hole interactions. Recent intensive studies have established Ta_2NiSe_5 as one of the most promising candidate materials. The precise control of a many-body electronic phase with an external handle is both challenging and interesting. In our study, we realized a full and controllable phase tuning of Ta_2NiSe_5 from the excitonic insulator ground state to a zero-gap semiconductor state by using a tip of scanning tunneling microscope. Such dramatic reconstruction of electronic states proves the many-body nature of the gap in Ta_2NiSe_5, and is consistent with excitonic insulator behavior.

TT 59.10 Thu 17:30 HSZ 03

Ab-initio study of the possible excitonic insulator Ta_2NiSe_5. Investigating the electronic properties of the structural transition and its excitonic features — •Lukas Windgaetter[1], Simone Latini[1], Hannes Huebener[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA

The excitonic insulator is a theoretically predicted phase in which a condensate of bound electron hole pairs is the electronic groundstate of the crystal. Recently Ta_2NiSe_5 has been proposed as a promising candidate material with many experiments hinting towards the existence of such an excitonic insulating phase. However, it is still under debate whether the high temperature phase is semi-metallic or a small gap semiconductor and how the pure structural transition which accompanies the excitonic transition affects the materials properties. To settle these questions a thorough theoretical study using ab-initio methods is needed. We present DFT and GW calculations for the high-temperature orthorhombic phase as well as for the low temperature monoclinic phase of Ta_2NiSe_5. We show that our results suggest, that the high temperature phase starts from a semi-metallic groundstate which becomes a semiconductor in the low temperature phase after undergoing the structural phase transition. Furthermore we investigate the phonon spectrum and identify a soft phonon mode in the high temperature phase which drives the structural transition.

TT 59.11 Thu 17:45 HSZ 03

Zeeman spin-orbit coupling and magnetic quantum oscillations in an antiferromagnetic organic metal — Florian Kollmannsberger[1,2], Michael Kunz[1,2], Werner Biberacher[1], Pavel Grigoriev[3], Revaz Ramazashvili[4], Hideki Fujiwara[5], and •Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]L. D. Landau Institute for Theoretical Physics, Chernogolovka, Russia — [4]Laboratoire de Physique Théorique, Université de Toulouse, Toulouse, France — [5]Osaka Prefecture University, Osaka, Japan

We employ the layered organic antiferromagnetic (AF) superconductor κ-$(BETS)_2FeBr_4$ as an exemplary system for revealing theoretically predicted [1] Zeeman spin-orbit coupling (SOC). This novel type of SOC has been proposed as a generic feature of antiferromagnetic metals producing several unusual effects. In particular, it should lead to spin degeneracy of Landau levels, which can be probed by magnetic quantum oscillations [2]. To this end, we have carried out detailed studies of the magnetic quantum oscillations in the low-field, AF, as well as in the high-field, paramagnetic (PM) states of κ-$(BETS)_2FeBr_4$. We have found that the spin-splitting effect on the oscillation amplitude, observed in the PM state, completely disappears in the AF state [3]. We interpret this result as a direct signature of the Zeeman SOC.

[1] R. Ramazashvili, Phys. Rev. Lett. **101**, 137202 (2008).
[2] V.V. Kabanov et al., Phys. Rev. B **77**, 132403 (2008).
[3] R. Ramazashvili et al., arXiv:1908.01236 (2019).

TT 59.12 Thu 18:00 HSZ 03

LDA+DMFT view on electronic structure and magnetism of UGa_2 — •Banhi Chatterjee and Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Whether the uranium 5f electrons are closer to being localized or itinerant in the intermetallic compound UGa_2 is still debated. The experimental magnetic moments are large, approximately 3 μ_B, favoring the localized picture. LDA severely underestimates the moments. Although the moments are enhanced within LDA+U, they do not reach the experimental value for a reasonably large U [1]. We investigate if the picture can be improved within LDA+DMFT using exact diagonalization as the impurity solver. We can reproduce the recently measured x-ray absorption spectra at the uranium M edge better than LDA+U [1]. Distinctive spectral features are identified as fingerprints of the localized 5f electrons. We can further recover the experimental valence band photoemission spectra. We present two different formulations of the theory: In LDA+DMFT the polarization is induced only to the 5f states by means of a polarized self-energy, in LSDA+DMFT all states are allowed to polarize. It turns out that neither of the methods gives satisfactory magnetic moments without *ad hoc* manual intervention in tuning the spin polarized double counting.

[1] A. V. Kolomiets, M. Paukov, J. Valenta, A. V. Andreev, K. Kvashnina, F. Wilhelm, A. Rogalev, D. Drozdenko, P. Minarik, J. Kolorenc, B. Chatterjee, M. Richter, L. Havela (in preparation).

TT 59.13 Thu 18:15 HSZ 03

Metal-to-insulator transition in a Dirac semimetal: the case of $BaNi_xCo_{1-x}S_2$ — Benjamin Lenz and •Michele Casula — Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

We study the mechanism behind the metal-to-insulator transition in the correlated $BaNi_xCo_{1-x}S_2$ series, by using advanced many-body first-principles methods, such as a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

The $BaNi_xCo_{1-x}S_2$ family, first considered as a potential candidate for high-temperature superconductivity, has seen a renewed attention for its fascinating spin properties. $BaNiS_2$ is a Dirac semimetal, with 4 Dirac cones lying at the Fermi level, and with strong spin-orbit coupling, placing it close to a topological phase.

Rationalizing its phase diagram as a function of doping and temperature offers a unique opportunity to understand the interplay between topology and correlation in an experimentally accessible situation.