TT 90: Quantum Impurities and Kondo Physics

Time: Thursday 17:00–18:30 Location: CHE/0091

TT 90.1 Thu 17:00 CHE/0091

Unveiling local magnetic moments in copper-oxide atomic junctions — •Marcel Strohmeier[1], Samanwita Biswas[2], Wolfgang Belzig[1], Regina Hoffmann-Vogel[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

Incorporating oxygen into metallic atomic-scale junctions modifies the interatomic bonding and may even promote the formation of monoatomic chains [1]. In the specific case of copper oxide, first-principles studies have predicted the emergence of ferromagnetic ground states, attributing certain atomic configurations with spin-filtering capabilities [2]. By means of low-temperature transport measurements, we provide a series of experimental evidence indicating the presence of local magnetism in air-oxidized mechanically controllable copper break junctions. Our investigations on ultimately small contacts range from magnetotransport measurements [3] to the analysis of anomalous shot noise in the presence of strong zero-bias anomalies [4]. The analysis of the latter reveals signatures of spin-polarized currents, a finding that needs to be reconciled with the spectroscopic features being interpreted within a Kondo model [5].

[1] Thijssen et al., New J. Phys. 10, 033005 (2008)
[2] Zheng et al., J. Appl. Phys. 117, 043902 (2015)
[3] Strigl et al., Nat Commun 6, 6172 (2015)
[4] Tewari et al., Nano Lett. 18, 5217 (2018)
[5] Calvo et al., PRB 86, 075447 (2012)

TT 90.2 Thu 17:15 CHE/0091

Kondo impurities coupled to a Chern insulator — •David A. Krüger[1] and Michael Potthoff[1,2] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

We study a system consisting of two spin-$\frac{1}{2}$ impurities that are exchange-coupled to a two-dimensional Qi-Wu-Zhang Chern insulator. The interplay between the truncated Kondo effect, the truncated RKKY interaction, and the mass parameter m gives rise to a complex phase diagram comprising RKKY singlet and triplet phases, the Kondo singlet, and a partially Kondo-screened phase. Furthermore, we examine how the phase diagram depends on the coupling orbitals and the inter-impurity distance.

Using a Lanczos transformation, we map the problem to a one-dimensional chain with the impurities at the first site, which is then solved using an adaptive natural-orbital configuration-interaction technique. We also consider fictitious local magnetic fields Zeeman-coupled to the impurity spins. The field directions form a four-dimensional base manifold $\mathcal{M} \cong \mathbb{S}^2 \times \mathbb{S}^2$. The bundle of ground states over $\mathcal{M}$ can be topologically characterized by a Chern number that differs from the usual k-space Chern number and provides further insight into the limit of classical impurity spins.

TT 90.3 Thu 17:30 CHE/0091

Orbital-Selective Mott transition in a U(1) gauge model of the Kondo lattice: a Quantum Monte Carlo study — •Gaopei Pan and Fakher Assaad — University of Würzburg, 97074 Würzburg, Germany

We investigate a U(1) gauge theory formulation of the dimensional mismatch Kondo model describing a spin chain on a semi-metallic surface. Using sign-problem-free determinant quantum Monte Carlo simulations, we compute the single-particle spectra, optical conductivity, and dynamical spin structure factor of the composite fermions across a wide range of parameters.

Our results reveal a clear evolution from a Kondo-screened heavy-fermion regime to a Kondo-breakdown phase where the composite fermion spectral weight collapses. Most strikingly, the zero-frequency optical conductivity displays a sharp suppression at the breakdown point, accompanied by a redistribution of spectral weight, which cannot be explained by simple band-structure effects. Instead, the data support an interpretation in terms of an orbital-selective Mott transition, where the f-sector becomes localized while the conduction c electrons remain itinerant.

Together, these findings provide unbiased numerical evidence for a gauge-fluctuation-driven Kondo breakdown and demonstrate how composite-fermion and optical conductivity can diagnose orbital-selective Mott transition in strongly correlated metals.

TT 90.4 Thu 17:45 CHE/0091

Kondo effect competing superconductivity in Van Hove systems — •Grzegorz Michałek and Krzysztof P. Wójcik — Institute of Molecular Physics, Polish Academy of Sciences, ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

Higher-order Van Hove singularities, characterized by a power-law divergence in the electron density of states near the Fermi surface, are known to boost effects of electronic correlations and in general destabilize conventional Fermi-liquid states. We investigate the influence of such singularity on the magnetic impurity in a superconductor. In general, the Kondo effect is known to compete with superconductivity. Due to this competition, the impurity is expected to undergo a transition between the screened phase, where Kondo screening locally overcomes the superconducting pairing, and Yu-Shiba-Rusinov in-gap state formation, where impurity moment remains intact [1]. We use numerical renormalization group calculations to analyze how a singularity in the normal-state density of states influences the Kondo scale. By incorporating modified density of states into the BCS gap equation, we show the evolution of the Kondo quantum critical point with singularity exponent r.

[1] K. Satori, H. Shiba, O. Sakai, Y. Shimizu, *J. Phys. Soc. Jpn.* **61**, 3239 (1992).

TT 90.5 Thu 18:00 CHE/0091

The work distribution function of a qubit and of the Anderson impurity model — •Theodoulos Costi[1], Hoa Nghiem[2], Steven Campbell[3,4], and Andrew Mitchell[3,4] — [1]Peter Günberg Institute, Research Centre Jülich, 52428 Jülich, Germany — [2]Phenikaa Institute for Advanced Study, Phenikaa University, 12116 Hanoi, Vietnam — [3]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [4]Centre for Quantum Engineering, Science and Technology, University College Dublin, Ireland

The work distribution function (WDF) of two representative quantum impurity models, the Anderson impurity model (AIM) of strongly correlated electrons, and the Ohmic spin-boson model (SBM) of a qubit coupled to an environment, is investigated within the non-perturbative time dependent numerical renormalization group (TDNRG) approach [1]. For level quenches, the zero temperature WDF, $P(W)$, exhibits a threshold behavior above the minimum work, $W_{\min}$, taking the form $P(W) = a|W - W_{\min}|^{-(1-\alpha_{\rm OC})}$ where $\alpha_{\rm OC}$ is the Anderson orthogonality exponent. We calculate $\alpha_{\rm OC}$ analytically, finding agreement with that obtained from the TDNRG. The calculations are further validated by verifying the first three moments of the WDF and the Crooks relation. This work demonstrates the ability of the TDNRG approach to capture the quantum thermodynamics of nanoscale quantum impurity systems for strong quenches beyond the linear response regime [1].

[1] H.T.M. Nghiem, T.A. Costi, S. Campbell, A.K. Mitchell, preprint (2025)

TT 90.6 Thu 18:15 CHE/0091

Conventional and singlet-triplet Kondo effect in radical single-molecule junctions — •Elke Scheer[1], Gautam Mitra[1], Jueting Zheng[1,2], Michael Deffner[3], Karen Schaefer[3], Jonathan Z. Low[3], Luis M. Campos[4], Carmen Herrmann[4], and Theo A. Costi[5] — [1]Uni Konstanz, Germny — [2]Xiamen Univ., China — [3]Univ. Hamburg, Germany — [4]Columbia Univ., USA — [5]Research Center Jülich, Germany

The Blatter radical has been suggested as a building block in future molecular spintronic devices due to its expected long-spin lifetime [1]. Whether its radical character is maintained in single-molecule junctions depends on the environment [2]. For about 25% of single-molecule junctions investigated at low-temperature (4.2 K) we observe zero-bias anomalies that can be assigned to the Kondo effect and hence support the radical character. Additionally, a strong negative magnetoresistance is observed in junctions that do not reveal a zero-bias anomaly. By combining distance-dependent and magnetic-field-dependent measurements, quantum-chemical and quantum-transport calculations, we show that both observations can be consistently explained by a singlet-triplet Kondo model. [3,4].

[1] L. Ji et al., Adv. Mater. 32, e1908015 (2020)
[2] J. Z. Low et al., Nano Lett. 19, 2543 (2019)
[3] J. Paaske et al., Nat. Phys. 2, 460 (2006)
[4] G. Mitra et al., Chem 11, 102500 (2025)