TT 94: Correlated Magnetism – Low-Dimensional Systems

Time: Friday 9:30–12:00 Location: HSZ/0101

TT 94.1 Fri 9:30 HSZ/0101

The zoo of states in the 2 dimensional Hubbard model — •Robin Scholle[1], Pietro Bonetti[1,2], Demetrio Vilardi[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We use real-space Hartree-Fock theory to construct a magnetic phase diagram of the two-dimensional Hubbard model as a function of temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order without biasing the system towards one of them. For an intermediate interaction strength we predominatly find Néel order close to half-filling, stripe order for low temperatures or large doping, and an intermediate region of spiral order. We then combine the approach with the functional renormalization group method and are able to access the superconducting regime. I will give a short summary of the method followed by a presentation of our current results and an outlook for possible further applications.

TT 94.2 Fri 9:45 HSZ/0101

Kondo-driven magnetic instability in Van Hove metals with sparse impurities — •Krzysztof Wójcik[1], Johann Kroha[2,3], and Peter Wahl[3,2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland — [2]Physikalisches Institut, Universität Bonn, Germany — [3]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom

We analyze a metal exhibiting a higher-order Van Hove singularity at the Fermi level and hosting sparse randomly distributed magnetic impurities. We show that a sharp resonance in the impurity local spectral density, characteristic of typical Kondo systems, is absent in the Van Hove-Kondo case. Despite the Kondo singlet ground state, the impurities contribute to total entropy and magnetization by affecting the available excited states, and below a critical temperature for any finite density of impurities these contributions dominate over those of the clean host, leading to hitherto unrecognized instabilities. An especially intriguing instability occurs in the case of a particle-hole asymmetric singularity, such as the one recently observed in $Sr_3Ru_2O_7$ [1]. In such case, despite complete Kondo screening of the impurities, the host becomes magnetically unstable due to their presence, which leads to a ferromagnetic ground state. We comment on relation to the surface magnetism observed in $Sr_3Ru_2O_7$.

[1] C. A. Marques *et al.*, *Sci. Adv.* **8**, eabo7757 (2022).

TT 94.3 Fri 10:00 HSZ/0101

Crystal structure, electronic structure and magnetism in the binary compounds Cr_3S_4 and Cr_3Se_4 — •Helge Rosner[1], Seojin Kim[1], Yurii Prots[1], Vincent Morando[2], Oksana Zaharko[2], Jörg Sichelschmidt[1], Marcus Schmidt[1], and Michael Baenitz[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, 5232 Villigen PSI, Switzerland

Cr_3X_4 (X = S, Se) crystallises in a monoclinic lattice, structurally closely related to the rhombohedral chalcogenite delafossite-like systems $AgCrX_2$. In contrast to these intrinsically semiconducting materials with a nonmagnetic monovalent cation site, in Cr_3X_4 the distorted triangular CrX_2 layers are separated by a formally trivalent and magnetic ion. In consequence, the interlayer distance is strongly reduced, making the system more three dimensional, and thus strongly increasing the magnetic ordering temperature. Here, we present a joint experimental and theoretical study of the binary material Cr_3X_4, including thermodynamic measurements, high resolution XRD, neutron scattering and density functional band structure calculations. Our data consistently demonstrate that the metallic systems undergo an antiferromagnetic ordering up to 160 K which is strongly coupled to the crystal lattice. The band structure calculations show that the conduction bands originate from strongly hybridised Cr-X states with sizeable spin-orbit interaction. In a detailed comparison, we will highlight similarities and differences between Cr_3X_4 and the chalcogenite delafossites, including samples with mixed occupation on the X site.

TT 94.4 Fri 10:15 HSZ/0101

Magnetic vector phases induced by spin-nematicity in high magnetic fields for two anisotropic quasi-1D chain compounds — •Stefan-Ludwig Drechsler[1], Lorenz Wolfram[1], Rössler Ulrich[1], Kuzian Roman[2], Klingeler Rüdiger[3], Skourskii Yurii[4], Zoghlin Eli[5], Wolter-Giraud Anja[1], Büchner Bernd[1], and Nishimoto Satoshi[1,6] — [1]IFW-Dresden, Germany — [2]DIPC, San Sebastian, Spain — [3]Heidelberg University, Germ. — [4]HLD-EMFL, Dresden, Germ. — [5]Oak-Ridge, USA — [6]TU-Dresden

We report and analyze pulsed high-field data near quasi saturation and low-T thermodynamic ones for Li_2CuO_2 up to 60 T and reanalyze the organic ladder compound verdazyl β-2,3,5 (V) measured at stationary fields below 12 T [1] exhibiting both cusps in the magnetic susceptibilities χ at low-T pointing to field induced magnetic vector phases due to the presence of spin nematicity according to a scenario proposed in [2] making visible the otherwise difficult to detect tensorial nematic order parameter. The symmetric and/or antisymm. spin symmetry as well as a subtile interplay of ferromagnetic (FM) and anti-FM couplings are essential for the appearance of 2-magnon bound states supported by the XYZ magnetism observed for Li_2CuO_2 and the low-symmetry crystalline structure for V, resp. For the former we report specific heat data at ambient field pointing possibly to the onset of a Bose condensation below 1 K of 3-magnon bound states as suggested in [3].

[1] H. Yamaguchi *et al.*, J. Phys. Soc. Jpn. **87**, 043701 (2018).
[2] A. Smerald *et al.*, Phys. Rev. B **91**, 174402 (2015).
[3] C. Agrapidis *et al.*, Phys. Rev. Res. **7**, 043051 (2025).

TT 94.5 Fri 10:30 HSZ/0101

Spins in Rotation: Probing anisotropy in $YbAlO_3$ — •Lipsa Behera[1,2], Javier Landaeta[2], Konstantin Semeniuk[2], and Elena Hassinger[3] — [1]Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids — [3]Karlsruhe Institute of Technology

$YbAlO_3$ is an example of a quasi-one-dimensional S=1/2 spin-chain system with weak Ising-like interchain coupling. It has an interesting phase diagram for H//a with an anti-ferromagnetic order below 0.9 K, a field induced longitudinal spin-density wave phase, and a transverse anti-ferromagnetic state. It enters the field polarized state at 1.15 K. Here we present magnetic AC susceptibility measurements performed under rotation at 25 mK to study how sample misalignment influences the phase diagram and critical fields. We find that rotating towards the c-axis leaves the overall phases unchanged, with only the critical fields shifting to higher values. Rotation towards the b-axis, on the other hand produces some interesting results. A splitting of the susceptibility maxima (corresponding to the transition to the fully polarized state) is observed. This suggests the presence of two independent sublattices. Some critical fields move to lower values indicating more stability in the transverse direction. These results hold the potential to highlight intriguing quasi-1D physics.

15 min. break

TT 94.6 Fri 11:00 HSZ/0101

Magnetic characterization of the spin-ladder magnet $Bi_2CuO_3(SO_4)$ — •Rodolfo A. Rangel Hernandez[1], Alexander A. Tsirlin[1], Victoria Ginga[1], Kirill Povarov[2], and Sergey Zvyagin[2] — [1]University of Leipzig, Leipzig, Germany — [2]Helmholtz-Zentrum, Dresden-Rossendorf, Dresden, Germany

We present the first comprehensive magnetic characterization of $Bi_2CuO_3(SO_4)$, a spin-ladder magnet with ferromagnetic rungs and antiferromagnetic legs. Heat-capacity, susceptibility and magnetization measurements reveal characteristic signatures of a gapped low-dimensional quantum magnet. Ab initio DFT+U calculations, together with a Wannier-function analysis and quantum Monte Carlo (QMC) simulations, are used to describe the magnetism of the ladder. By fitting the experimental susceptibility with QMC, we estimate a spin-gap of $\Delta \approx 20$ K and the leading exchange couplings to be $J' \approx$ -208 K (rung) and $J \approx 243$ K (leg). Additionally, electron spin resonance confirms an extrinsic nature of the susceptibility upturn at low temperatures. Our result establishes $Bi_2CuO_3(SO_4)$ as a new realization of a spin-ladder with ferro- and antiferromagnetic interactions and provide reliable microscopic parameters for future research.

TT 94.7 Fri 11:15 HSZ/0101

Symmetry-Protected Topological Phase Diagrams of Dimerized Heisenberg Ladders — Tim Obrock and •Anas Abdelwahab — Leibniz Universität Hannover, Institute für Theoretische Physik, Hannover, Germany

We present symmetry-protected topological phase diagrams of unfrustrated dimerized spin-$\frac{1}{2}$ ladders with perpendicular ($J_\perp$) and diagonal (J_d) rung couplings, studied as a function of dimerization (δ) and inter-wire coupling strength. For two perpendicularly coupled wires, our results reproduce the established picture from previous studies: antiferromagnetic rungs yield a trivial spin-0 phase, while ferromagnetic rungs drive the system into the Haldane symmetry-protected topological phase at small $|\delta|$, with critical lines converging to the dimerized spin-1 chain limit for $J_\perp \ll -1$.

For three perpendicularly coupled wires, earlier work has shown that antiferromagnetic rungs drive a transition from trivial ($\delta > 0$) to Haldane ($\delta < 0$). Under ferromagnetic rungs, the system approaches the dimerized spin-$\frac{3}{2}$ chain limit for $J_\perp \ll -1$, exhibiting a sequence of trivial*Haldane*trivial*Haldane phases as δ evolves from 1 to -1.

Extending beyond these previous studies, we analyze the case of two and three diagonally coupled wires. For two wires, antiferromagnetic rungs produce a Haldane region bounded by $|\delta| \approx J_d/2$, containing the exact spin-1 chain limit at $J_d = 1$ and $\delta = 0$, while ferromagnetic rungs keep the system trivial. For three diagonally coupled wires, our results reveal a phase diagram with trivial and topological phases but without an apparent spin-chain limit.

TT 94.8 Fri 11:30 HSZ/0101

Self-consistent mean-field theory and continuous unitary transformations for ordered quantum antiferromagnets with long-range interactions — •Maximilian Bayer[1], Dag-Björn Hering[2], Vanessa Sulaiman[2], Götz Uhrig[2], and Kai Schmidt[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Condensed Matter Theory, Technische Universität, Dortmund, Germany

We investigate the antiferromagnetic Heisenberg model on a square lattice in the presence of algebraically decaying long-range interaction. The model is first studied using a fully self-consistent mean-field treatment going beyond linear spin-wave theory. We discuss the challenges and solutions to obtain numerical results of these long-range interacting systems using functional self-consistency equations familiar to the superconducting gap equation and a parametrisation using Epstein-zeta functions to capture the long-range behaviour without truncation in the system size. In a next step we go beyond the mean-field level and apply continuous similarity transformations (CST) in momentum space. The associated flow equations are truncated in the scaling dimension to capture consistently quantum fluctuations in the ordered phase in the same manner as for the case of nearest-neighbor interactions [1]. Our aim is to understand the one-magnon dispersion at low and high energies including the fate of the characteristic roton minimum.

[1] M. Powalski, G.S. Uhrig, K.P. Schmidt, PRL 115, 207202 (2015)

TT 94.9 Fri 11:45 HSZ/0101

Electric-field-driven flat band in a distorted generalized sawtooth chain — •Vadim Ohanyan[1,2], Lusik Amiraghyan[1,3], Michael Sekania[4,5], and Marcus Kollar[6] — [1]Laboratory of Theoretical Physics, Yerevan State University, 1 Alex Manoogian, 0025 Yerevan, Armenia — [2]CANDLE, Synchrotron Research Institute, 31 Acharyan Str., 0040 Yerevan, Armenia — [3]Institute of Applied Problems of Physics, 25 Hr. Nersisyan St, Yerevan 0014, Armenia — [4]Rechenzentrum, University of Augsburg, 86135 Augsburg, Germany — [5]Andronikashvili Institute of Physics, Javakhishvili Tbilisi State University, Tamarashvili str. 6, 0177 Tbilisi, Georgia — [6]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We investigate flat magnon bands in a sawtooth chain where symmetric exchange, DM interaction, and axial anisotropy differ on each side of the triangular plaquette. When the DM terms arises from the Katsura-Nagaosa-Balatsky (KNB) magnetoelectric mechanism, the corresponding DM coefficients become functions of the electric field and the lattice geometry. This dependence is governed by two bond angles, which become inequivalent under a distortion of the triangular plaquette. We derive the conditions under which an electric field, aligned along the lattice bonds, drives the one-magnon spectrum into a flat-band regime. The distortion angle dependence of the saturation field is examined as well. We construct a mapping from flat-band solution obtained for a general DM interaction into those arising from its KNB-induced form.