TT 54: Correlated Electrons: Charge Order

Time: Friday 9:30-12:45

TT 54.1 Fri 9:30 H33

Broad-Band Noise at the Different CDW Transitions in $BaNi_2As_2 - \bullet J$ ulian Beu¹, Marvin Kopp¹, Markus König², Amir Haghighirad³, Matthieu Le Tacon³, Jure Demsar⁴, and Jens Müller¹ - ¹Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany - ²MPI CPfS, Dresden, Germany - ³KIT, Karlsruhe, Germany - ⁴Institute of Physics, JGU, Mainz

Ever since collective modes like charge (CDW) and spin density waves (SDW) have been routinely found near to or in direct competition with unconventional superconductivity in many interesting compounds, including high- T_c cuprates and iron-pnictides, the influence of these states on the superconducting phase is of interest. In this work we focus on BaNi₂As₂ (BNA), a structurally close analogue of the 122-type iron-based superconductors. In contrast to the iron-pnictides, no magnetic ordering was observed in BNA, and two different CDW phases, one incommensurate (I-CDW) and the other commensurate (C-CDW), replace a SDW phase. We investigate the charge carriers in samples of $BaNi_2(As_{1-3.5\%}P_{3.5\%})_2$ by analyzing the resistance and broad-band noise properties. The samples are structured by a FIB process with a meander current path in order to increase the absolute resistance by two orders of magnitude, making fluctuation spectroscopy possible. Our measurements reveal significant differences in the behavior of the electronic fluctuations at the two CDW formations, that show interesting connections to recent findings regarding the properties of the I-CDW in BNA [1] and our noise measurements performed on the conventional CDW system K_{0.3}MoO₃. [1] Phys. Rev. Lett. 129, 247602.

TT 54.2 Fri 9:45 H33 Visualizing *p*-Orbital Texture in the Charge Density Wave State of CeSbTe — Xinglu Que¹, Qingyu He¹, Lihui Zhou¹, Shiming Lei², Leslie Schoop³, •Dennis Huang¹, and Hidenori Takagi^{1,4,5} — ¹Max Planck Institute for Solid State Research, Stuttgart, Germany — ²Hong Kong University of Science and Technology, China — ³Princeton University, USA — ⁴University of Stuttgart, Germany — ⁵University of Tokyo, Japan

The collective reorganization of electrons into a charge density wave (CDW) inside a crystal has long served as a textbook example of an ordered phase in condensed matter physics. Two-dimensional square lattices with p electrons are well-suited to the realization of CDW, due to the anisotropy of the p orbitals and the resulting one dimensionality of the electronic structure. In spite of a long history of study of CDW in square-lattice systems, few reports have recognized the existence and significance of a hidden orbital degree of freedom. The degeneracy of p_x and p_y electrons inherent to a square lattice may give rise to nontrivial orbital patterns in real space that endow the CDW with additional broken symmetries or unusual order parameters. Using scanning tunneling microscopy, we visualize signatures of p-orbital texture in the CDW state of the topological semimetal candidate CeSbTe, which contains Sb square lattices with 5p electrons. We image atomic-sized, anisotropic lobes of charge density with periodically modulating anisotropy, that ultimately can be mapped onto a microscopic pattern of p_x and p_y bond density waves.

TT 54.3 Fri 10:00 H33

Charge Density Wave and Phonon Softening in $EuAl_4$ — •ALEKSANDR SUKHANOV¹, STEVEN GEBEL¹, ARTEM KORSHUNOV², and MAREIN RAHN¹ — ¹Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — ²Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 20018 San Sebastian, Spain EuAl₄ is a rare earth intermetallic in which competing itinerant and/or indirect exchange mechanisms give rise to a complex magnetic phase diagram, including a centrosymmetric skyrmion lattice. These phenomena arise not in the tetragonal parent structure but in the presence of a charge density wave (CDW), which lowers the crystal symmetry and renormalizes the electronic structure. Microscopic knowledge of the corresponding atomic modulations and their driving mechanism is a prerequisite for a deeper understanding of the resulting equilibrium of electronic correlations and how it might be manipulated.

In my talk, I present inelastic x-ray scattering results, which can clarify the origin of the CDW in EuAl₄.

Location: H33

TT 54.4 Fri 10:15 H33

Charge Density Wave Quantum Critical Point under Pressure in 2H-TaSe₂ — •YULIIA TYMOSHENKO¹, AMIR-ABBAS HAGHIGHIRAD¹, ROLF HEID¹, GASTON GARBARINO², LUIGI PAOLASINI², and FRANK WEBER¹ — ¹Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — ²2European Synchrotron Radiation Facility, 71 avenue des Martyrs, CS 40220, Grenoble 38043, France

Suppression of the ordered state is one of the ways to increase the superconducting (SC) transition temperatures. Materials characterized by charge density waves (CDW) and SC are promising candidates for such studies, since both states can be associated with electron-phonon coupling. Transition metal dichalcogenides (TMD) are prominent examples of such coexisting phases, however, not all such materials show the expected behavior or possess additional mechanisms that complicate an unambiguous interpretation. Here, we report high-pressure X-ray diffraction (XRD) and inelastic X-ray scattering (IXS) measurements of a prototypical transition metal dichalcogenide 2H-TaSe₂ and determine the evolution of the CDW state and its lattice dynamics. We found that the quantum critical point (QCP) of the charge density wave is in close proximity to the reported maximum superconducting transition temperature $T_{\rm sc} = 8.2$ K. Ab-initio calculations confirm that 2H-TaSe₂ is a typical example of enhanced superconductivity with suppressed order and can serve as a textbook example for studying superconductivity near the quantum critical point of the CDW.

TT 54.5 Fri 10:30 H33

Tunable Charge Density Wave Orders in 2H-TaS₂ — •MIHIR DATE^{1,2}, JOOST ARETZ³, ENRICO DA COMO⁴, MARCIN MUCHA-KRUCZYNSKI⁴, MALTE ROESNER³, STUART S P PARKIN¹, NIELS B M SCHROETER¹, and MATTHEW D WATSON² — ¹Max Planck Institute of Microstructure Physics, Halle, Germany — ²Diamond Light Source Ltd., Didcot, UK — ³Radboud University, Nijmegen, The Netherlands — ⁴University of Bath, Bath, UK

The charge density wave (CDW) transition is an electronic instability driven by strong electron-phonon coupling, where the parent electronic band is renormalized, and shows a spectral gap. Angle-resolved photoemission spectroscopy (ARPES) has been extremely successful in identifying these spectral features, most prominently in layered van der Waals materials like 2H-NbSe₂ and TaSe₂. Surprisingly, however, until now there has not been any high-quality data reported on the 2H-TaS₂, presumably due to materials challenges. Making use of spatially resolved ARPES, we were able to overcome these challenges and measure high-quality bandstructures revealing the 3x3 commensurate charge density waves (CCDW) ground state in 2H-TaS₂. We further find variation of the stoichiometry between samples prepared by different routes, and incredibly, at a different band filling we find evidence of a new CDW order that is commensurate, but not the 3x3 reconstruction as observed in previous experiments. Our results are compared with tight-binding and ab-initio modelling which show that TaS_2 is prone to multiple instabilities that can be tuned by the band filling, with an important role played by a van Hove singularity.

TT 54.6 Fri 10:45 H33 Resistance of Vapor-Grown NbSe₂ Single Crystals under Strain — •MAIK GOLOMBIEWSKI, TIANYI XU, SIMON KNUDSEN, MICHAEL PAUL, SVEN GRAUS, TESLIN R. THOMAS, ANDREAS KREYSSIG, and ANNA E. BÖHMER — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

NbSe₂ shows a charge density wave (CDW) transition upon cooling below $T_{\rm CDW} = 32 \,\rm K$ and becomes superconducting at $T_{\rm c} = 7.2 \,\rm K$. Large NbSe₂ single crystals were grown via chemical vapor transport with iodine as transport agent. Growth conditions, such as temperature gradient, were optimized resulting in an increase in RRR. Samples were shown to have a 1:2 stoichiometry via energy-dispersive x-ray spectroscopy and the 2H-structure was confirmed by powder x-ray diffraction measurements. Temperature-dependent resistance was measured while simultaneously straining the samples using cryogenic strain and force cells. This so-called elastoresistance exhibits a minimum around $T_{\rm CDW}$. Using the force cell, large strains were applied and investigated.

We acknowledge support by the Mercator Research Center Ruhr

(MERCUR), under project number Ko-2021-0027.

TT 54.7 Fri 11:00 H33 **Fingerprints of a Charge Ice State in the Doped Mott Insulator Nb₃Cl₈ — •EVGENY STEPANOV — CNRS, Ecole Polytechnique Monolayer Nb₃Cl₈ is a textbook example of a Mott insulator [1,2]. However, little is known about its characteristics, particularly in doped regimes where the strong local correlations responsible for the Mott state are competing with significant spatial collective electronic fluctuations.**

Our many-body calculations suggest that monolayer Nb₃Cl₈ undergoes phase separation (PS) upon doping, driven by the emergence of a charge ice state [3]. In close proximity to the PS, the charge susceptibility dramatically increases and displays a distinctive bow-tie pattern in momentum space, resembling the form of magnetic susceptibility observed in spin ice states. At the same time, the effective exchange interaction between charge densities undergoes a striking transformation, acquiring a power-law dependence in real space. This dependence is reminiscent of hydrogen bonding interactions in water and serves as a hallmark of spin ice states when applied to spin degrees of freedom. These findings allow us to associate the observed PS with a charge ice state, characterized by a remarkable power-law dependence of correlations between electronic densities in real space.

While spin ice states were first experimentally realized in 1997 by Harris et al. [4], an analogue for charge degrees of freedom has remained elusive until now. Our work not only provides a theoretical description of the charge ice state but also offers compelling evidence that this novel phase can be realized in a real material.

[1] Nano Lett. 22, 4596 (2022);

[2] PRX 13, 041049 (2023);

[3] arXiv:2405.19114;

[4] PRL 79, 2554 (1997).

15 min. break

TT 54.8 Fri 11:30 H33

Non-Thermal Cavity Control of Order in Electronic Systems — •MD MURSALIN ISLAM¹, MICHELE PINI^{2,1}, RAFAEL FLORES-CALDERÓN¹, and FRANCESCO PIAZZA^{2,1} — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²University of Augsburg, Augsburg, Germany

Cavity quantum materials have emerged as a platform to study nonthermal many-body physics with applications to the control of collective electron behavior. In an electronic system coupled to cavity photons, the superconducting gap has been predicted previously to be enhanced, due to a 'Eliashberg effect' taking place due to electromagnetic fluctuations as instead of a coherent laser source [1,2]. We extend this idea for the case of charge-density-wave order and systematically derive a generalized gap equation for the non-thermal situation using field theoretical methods. This allows us to compare the modified gap equations for superconductors and charge density waves: we find that while the two equations are exactly equivalent in thermal equilibrium, they assume different forms in non-thermal settings. Our formalism also allows us to systematically investigate the role of disorder in the non-thermal enhancement of the gap in both the cases.

[1] G. M. Eliashberg, JETP Lett. 11, 114 (1970);

[2] J. B. Curtis et. al., PRL 122, 167002 (2019).

TT 54.9 Fri 11:45 H33

Disorder in Photoexcited Charge Density Wave Systems: Insights from Stochastic Resonance in Impurity Models. — •FRANCESCO VALIERA and MARTIN ECKSTEIN — Department of Physics, University of Hamburg, D-22607 Hamburg, Germany

Photoexcitation in charge density wave (CDW) systems can potentially lead to inhomogeneously disordered phases [1], where ions are displaced locally but do not achieve global ordering. In these phases, each ion moves within a local double-well potential and settles in one of the two equilibrium positions with equal probability. Similar behaviours have also been observed experimentally in VO₂ through scattering experiments [2]. A fundamental question in understanding these disordered states is identifying their signatures beyond X-ray scattering. In order to explore this, we have developed a model of a single ion embedded in a metallic host and use the semiclassical stochastic approach [3] to compute its linear response to an external probe. At low frequencies, the system exhibits a peak in the response amplitude as a function of temperature, which we attribute to stochastic resonance. The latter is typical of bistable systems that experience both periodic driving and noise and it can provide insights into the features of the local doublewell potentials and the fluctuations to which the ions are subject. [1] A. Picano et al., Phys. Rev. B 107, 245112 (2023);

[1] A. Ficano et al., Flys. Rev. B 107, 24511 [2] S. Wall et al., Science 362, 572 (2018);

[3] A. Picano et al., Phys. Rev. B 108, 035115 (2023).

11.11 (callo ct al., 1 hys. 1) 100, 000110 (2020).

TT 54.10 Fri 12:00 H33

Kinetic Magnetism and Stripe Order in the Antiferromagnetic Bosonic *t-J* Model — •TIMOTHY J. HARRIS^{1,2}, ULRICH SCHOLLWÖCK^{1,2}, ANNABELLE BOHRDT^{1,2,3}, and FABIAN GRUSDT^{1,2} — ¹Ludwig Maximilian University of Munich, Munich, Germany — ²Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — ³University of Regensburg, Regensburg, Germany

Understanding the microscopic mechanisms governing the physics of doped quantum magnets is a central challenge in strongly correlated many-body physics. In this talk, I will present results that disentangle the role of particle statistics from the intrinsic physics of strong correlations in the antiferromagnetic (AFM) bosonic t-J model. Using largescale density matrix renormalization group (DMRG) calculations, we map out the T=0 phase diagram on the 2D square lattice [1]. At low doping, we find evidence of partially-filled stripe structures, reminiscent of those observed in high- T_c cuprates. As doping increases, a transition occurs to a partially-polarized ferromagnetic (FM) phase, driven by formation of Nagaoka polarons as mobile holes bind to localized FM regions. At high doping or large t/J, these polarons overlap, and the system evolves into a full-polarized ferromagnet. Our findings shed new light on the role of particle statistics in strongly correlated quantum matter, revealing connections to stripe formation and the physics of kinetic ferromagnetism. I will also discuss experimental realizations of this model using state-of-the-art quantum simulators, paving the way for future studies of doped bosonic quantum magnets. [1] T.J. Harris et al., arXiv:2410.00904 (2024).

TT 54.11 Fri 12:15 H33

SU(2) Gauge Theory for Fluctuating Stripes in the Pseudogap Regime — •MARK HENRIK MÜLLER-GROELING, PIETRO MARIA BONETTI, PAULO FORNI, and WALTER METZNER — Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

We investigate the role of charge order in a pseudogap described by an SU(2) gauge theory of fluctuating magnetic order.

The theory is based on a fractionalization of electrons into a fermionic chargon pseudospinor and a bosonic spinon, which leads to an emergent SU(2) pseudospin symmetry. In the mean-field solution of the 2D Hubbard model, which we use to describe the electrons in the copper-oxygen planes, Néel, spiral, or stripe order were observed below a density dependent transition temperature T^* [1].

Fluctuations of the spin orientation are described by a non-linear sigma model obtained from a gradient expansion of the spinon action. The spin stiffnesses are computed from a random phase approximation for the chargon susceptibility. The spinon fluctuations prevent magnetic long-range order of the electrons at any finite temperature. The phase with magnetic chargon order exhibits the most salient features characterizing the pseudogap regime in high-T_c cuprates: a strong reduction of charge carrier density, a spin gap, and Fermi arcs [2], and we set out to observe the effects of charge order in this context.

[1] R. Scholle, P. M. Bonetti, D. Vilardi, W. Metzner, PRB **108** 035139 (2023);

[2] P. M. Bonetti, W. Metzner, PRB 106, 205152 (2022).

TT 54.12 Fri 12:30 H33

Combined Cluster and Diagrammatic Method for Symmetry Broken Phases in Correlated Electron Systems — •Félix Fossati and Evgeny Stepanov — Ecole Polytechnique

In this work, we investigate dynamical symmetry breaking in correlated electron systems. To achieve this, we refine a theoretical approach called D-TRILEX [1-3], which constructs a diagrammatic expansion based on an interacting reference system, using a cluster problem as a reference. Traditional cluster methods account for short-range correlation effects within the cluster exactly but neglect correlations beyond the cluster size. Our approach addresses this limitation by self-consistently combining the non-perturbative treatment of shortrange correlations with a diagrammatic description of long-range collective electronic fluctuations. We demonstrate the effectiveness of this method by applying it to the one-dimensional Hubbard model. Our results show that the cluster extension of D-TRILEX accurately captures the transitions to the charge density wave (CDW) and bond-ordered wave (BOW) phases, which are associated with local and non-local order parameters, respectively, across various regimes of electronic interactions. This implementation provides new insights into the role of non-local interactions in dynamical symmetry breaking, establishing

D-TRILEX as a promising tool for investigating complex phases in strongly correlated systems.

- [1] E. A. Stepanov et al., Phys. Rev. B 100, 205115 (2019);
- [2] V. Harkov et al., Phys. Rev. B 103, 245123 (2021);
- [3] M. Vandelli et al., SciPost Phys. 13, 036. (2022).