TT 10: Correlated Electrons: Other Theoretical Topics

Time: Monday 11:00–12:45 Location: HSZ/0103

TT 10.1 Mon 11:00 HSZ/0103

Two site entanglement and maximal correlations in the Hubbard model — Frederic Bippus[1], Anna Kauch[1], •Gergo Roosz[1], Christian Mayrhofer[1], Fakher Assaad[2,3], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany

The study of entanglement in strongly correlated electron systems typically requires knowledge of the reduced density matrix. Here, we apply the parquet dynamical vertex approximation to study the two-site reduced density matrix at varying distance, in the Hubbard model at weak coupling. This allows us to investigate the spatial structure of entanglement in dependence of interaction strength, electron filling, and temperature. We compare results from different entanglement measures and benchmark against quantum Monte Carlo. Using the two-site density matrix, we compute the fermionic entanglement negativity, the mutual information between the two sites. We determine the maximal correlation function between the two lattice points.

TT 10.2 Mon 11:15 HSZ/0103

Superconductor-Insulator transition in a two-orbital attractive Hubbard model with Hund exchange — •Laura Torchia and Massimo Capone — International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy

We study a two-orbital attractive Hubbard model with a repulsive Hund exchange coupling J as an idealized model for a two-band superconductor. This framework is motivated by systems where a strong isotropic electron-phonon coupling drives the on-site Hubbard repulsion U negative while leaving the exchange term unaffected. We solve the model at $T = 0$ and half-filling using DMFT, focusing on the intra-orbital singlet superconducting phase and discarding other possible instabilities, as inter-orbital pairing and a charge-density wave ordering. Already at $J = 0$, the two-orbital model features a superconductor-insulator transition as $|U|$ grows, in contrast with the single-orbital case which remains superconducting for any $U < 0$. We find that a finite J strengthens the effect of the attractive U, both in the normal state and, even more significantly, in the superconducting state. However, this pushes the system towards an effectively stronger coupling, hence to a faster transition to the insulating state.

Similarly to the Mott transition in the repulsive model, the superconductor-insulator transition here is marked by a vanishing quasi-particle weigh Z. This leads to a scenario that recalls strongly correlated superconductivity close to a Mott transition, where pairing is enhanced but phase coherence is rapidly lost, even though the present model is dominated by attractive interactions.

TT 10.3 Mon 11:30 HSZ/0103

Orbital Magnetic Field Driven Metal-Insulator Transition in Strongly Correlated Electron Systems — •Georg Rohringer[1,2] and Anton Markov[3] — [1]Theory and Simulation of Condensed Matter, Department of Physics, King's College London, The Strand, London WC2R 2LS, United Kingdom — [2]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [3]Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium

We study the effects of an orbital magnetic field on the Mott metal-insulator transition in the Hubbard-Hofstadter model. We demonstrate that sufficiently large magnetic fields induce a Mott insulator-to-metal phase transition supporting our claim with dynamical mean field theory (DMFT) numerical results. For both competing phases (metal and insulator) we observe a magnetic-field-induced metallization reflected in an enhancement of kinetic and potential energy. We demonstrate that this phenomenon originates from a field-driven redistribution of spectral weight due to the formation of magnetic minibands and the Aharonov-Bohm effect experienced by electrons virtually tunneling around an elementary plaquette. Our theoretical results might be relevant for recent experimental studies on magnetic field driven insulator-to-metal transitions in strongly correlated materials such as VO_2,λ-type organic conductors, and moiré multilayers.

TT 10.4 Mon 11:45 HSZ/0103

Probing Green's Function Zeros by Cotunneling through Mott Insulators — •Carl Lehmann[2,3,1], Lorenzo Crippa[4,2,3], Giorgio Sangiovanni[2,3], and Jan Budich[1,2,5] — [1]Technische Universität Dresden, 01069 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [4]I. Institute of Theoretical Physics, University of Hamburg, Notkestrasse 9, 22607 Hamburg, Germany — [5]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Quantum tunneling experiments have provided deep insights into basic excitations occurring as Green's function poles in the realm of complex quantum matter. However, strongly correlated quantum materials also allow for Green's functions zeros (GFZs) that may be seen as an antidote to the familiar poles and have so far largely eluded direct experimental study. Here, we propose and investigate theoretically how cotunneling through Mott insulators enables direct access to the shadow band structure of GFZs. In particular, we derive an effective Hamiltonian for the GFZ that is shown to govern the cotunneling amplitude and reveal fingerprints of many-body correlations clearly distinguishing the GFZ structure from the underlying free Bloch band structure of the system. Our perturbative analytical results are corroborated by numerical data for a one-dimensional model system consisting of a Su-Schrieffer-Heeger-Hubbard model coupled to two single-level quantum dots.

TT 10.5 Mon 12:00 HSZ/0103

Conformal elastic zero modes at isostructural transitions — •Lars Franke[1], Nick Sander[1], and Markus Garst[1,2] — [1]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

In correlated materials the coupling of the itinerant electrons to the crystal lattice can induce an isostructural instability where the bulk modulus vanishes. This occurs for example at the endpoint of a line of first order Mott metal-insulator transitions or metamagnetic transitions [1]. Interestingly, at such an isostructural instability the acoustic phonons remain non-critical and their velocities are finite. Consequently, the isostructural transition is a genuine mean-field transition without critical microscopic fluctuations. Nevertheless, we demonstrate that four elastic macroscopic zero modes exist. In addition to a soft mode given by a macroscopic volume change, there are three further zero modes corresponding to special conformal transformations. We discuss the consequences for the critical dynamics close to isostructural instabilities as well as realizations in dilational metamaterials.

[1] M. Zacharias, L. Bartosch, M. Garst, PRL 109 (2012) 176401

TT 10.6 Mon 12:15 HSZ/0103

Stabilization of sliding ferroelectricity through exciton condensation — •Matteo D'Alessio[1,2], Daniele Varsano[2], Elisa Molinari[1,2], and Massimo Rontani[2] — [1]University of Modena and Reggio Emilia, Department of Physics, Informatics and Mathematics, Modena, Italy — [2]CNR Nanoscience Institute, Modena, Italy

Sliding ferroelectricity is a phenomenon that arises from the insurgence of spontaneous electronic polarization perpendicular to the layers of two-dimensional (2D) systems upon the relative sliding of the atomic layer constituents. Because of the weak van der Waals (vdW) interactions between layers, sliding and the associated symmetry breaking can occur at low energy cost in materials such as transition-metal dichalcogenides. Here we discuss theoretically this phenomenon by focusing on a prototype structure, the WTe2 bilayer, where sliding ferroelectricity was first experimentally observed. We compute the significant energy band renormalizations of the ground state induced by excitonic effects and show that in the case of bilayer WTe2 - as long as exciton coherence survives - relevant modifications result in the energetics of the system that contribute to stabilize ferroelectricity upon sliding displacement of the layers. We thus show that electron-hole interaction effects can play an important role in sliding ferroelectricity, where they have been neglected up to now.

TT 10.7 Mon 12:30 HSZ/0103

Ising Spin-Orbit Coupling in Three Dimensions — •Tonghua Yu, Eli Gerber, and Benjamin Wieder — Institut de Physique Théorique, Université Paris-Saclay, CEA, CNRS, F-91191 Gif-sur-Yvette, France.

Ising-type spin-orbit coupling (SOC) that produces out-of-plane spin polarization has been extensively explored in nonmagnetic two-dimensional (2D) materials, and has been shown to give rise to intriguing phenomena such as Pauli-limit-violating and spin-triplet superconductivity, SOC-polarized (interacting) topological bands, and high-performance nonvolatile valley spin valve. For 2D systems lying in the xy-plane, Ising SOC enforces that the bulk is nearly S_z-symmetric, in sharp contrast to systems dominated by Rashba or Dresselhaus SOC. Though all known examples of Ising SOC occur in 2D mono- or few-layer systems, there is no mathematical obstruction that restricts three-dimensional (3D) crystals from exhibiting nearly perfect (Ising-like) SOC textures. Using Green's functions and the projected spin spectrum applied to first-principles calculations, we identify 3D materials with Ising SOC that do not decompose into simple van der Waals layers of 2D Ising SOC materials, and we characterize their associated topological properties. Our calculations expand the class of Ising SOC materials and reveal new venues for spintronics and unconventional superconductivity.