TT 2: Correlated Electrons: Electronic Structure Calculations and Other Theoretical Topics

Time: Monday 9:30–13:00 Location: H7

TT 2.1 Mon 9:30 H7

Pressure-induced spin-state ordering in Sr_2CoO_3F — •Juan Fernandez Afonso, Andrii Sotnikov, Atsushi Hariki, and Jan Kunes — Institute of Solid State Physics, TU Wien, Wien, Austria

Sr_2CoO_3F is a recently-synthesized compound that has an antiferromagnetic high-spin (HS) order at ambient pressure with a Néel temperature of 323 K. Under pressure, the HS nature of the ground-state transforms into a low-spin (LS). In this talk, we provide a theoretical analysis combining LDA+DMFT and strong-coupling effective model consistent with the experimental studies [1] that, in addition to the observed paramagnetic and antiferromagnetic regimes, points to the existence of a spin-state ordered (SSO) phase in between. This order is characterized by a checkerboard arrangement of HS and LS + IS (mixture of low- and intermediate-spin states).

[1] Y. Tsujimoto et al., Sci. Rep. 6, 36253 (2016)

TT 2.2 Mon 9:45 H7

Modeling the X-ray absorption spectra and magnetism in UGa_2 using LDA+U and LDA+DMFT — •Banhi Chatterjee and Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

We study the electronic structure and magnetic properties of the uranium inter-metallic compound UGa_2. We focus on theoretical modeling of the M-edge X-ray absorption spectra (XAS), and investigate the magnetic moments formed at the uranium atoms. Correlations between the uranium 5f electrons are considered using the static orbital-dependent LDA+U functional and the dynamical mean-field theory (LDA+DMFT). We show that the LDA+DMFT reproduces the XAS spectra more accurately than LDA or LDA+U. Distinctive spectral features are identified with atomic multiplets, which favors the localized picture of the 5f electrons in this compound. It turns out that LDA substantially underestimates the size of the magnetic moments at the uranium atoms and even LDA+U does not reach the experimental moments with reasonable values of Coulomb U. We investigate whether LDA+DMFT improves the description of the magnetic moments.

TT 2.3 Mon 10:00 H7

Efficient LDA+DMFT response functions for correlated systems — •Julian Musshoff[1,2] and Eva Pavarini[1,3] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]JARA-HPC, RWTH Aachen University, Aachen, Germany

Linear-response functions are essential for comparing theory to experiments, and yet for strongly correlated systems their calculation is very challenging. The state-of-the-art technique to calculate susceptibilities for real materials is based on the dynamical mean-field (DMFT) approach and the local-vertex approximation and its extensions. The bottleneck of this method is the calculation of 3-frequencies local susceptibilities. For this we employ an efficient scheme based on the massively-parallel general implementation of the continuous-time quantum Monte Carlo impurity solver of Ref. [1]. We explore different possible polynomial bases. To calculate lattice susceptibilities, we solve the multi-orbital and multi-site Bethe-Salpeter equation. We present results for representative orbitally ordered systems [2].

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, Phys. Rev. B **87**, (2013) 195141

[2] J. Musshoff and E. Pavarini, in preparation

TT 2.4 Mon 10:15 H7

Lattice Dynamics of Palladium in the Presence of Electronic Correlations — •Wilhelm Appelt[1,3], Andreas Östlin[2], Ivan Leonov[4,5], Michael Sekania[2,6], Liviu Chioncel[2,3], and Dieter Vollhardt[2] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, Germany — [4]Institute of Metal Physics, Yekaterinburg, Russia — [5]Materials Modeling and Development Laboratory, NUST "MISiS", Moscow, Russia — [6]Andronikashvili Institute of Physics, Tbilisi, Georgia

We compute the phonon dispersion, density of states, and the Grüneisen parameters of bulk palladium in the combined Density Functional Theory (DFT) and Dynamical Mean-Field Theory. When electronic correlations are taken into account we find a good agreement with the measured phonon spectra, and ground state properties (equilibrium lattice parameter and bulk modulus). In particular, the ground state properties are improved in comparison with DFT results. At the same time we demonstrate that the previously predicted softening of the phonon mode along the [110] direction is absent in the presence of electronic correlations.

TT 2.5 Mon 10:30 H7

Correlated electronic structure with uncorrelated disorder — •Andreas Östlin[1], Levente Vitos[2,3,4], and Liviu Chioncel[5,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]Uppsala University, Sweden — [4]Wigner Research Center for Physics, Budapest, Hungary — [5]Augsburg Center for Innovative Technologies, University of Augsburg, Germany

We introduce a computational scheme for calculating the electronic structure of random alloys that includes electronic correlations within the framework of the combined density functional and dynamical mean-field theory. By making use of the particularly simple parameterization of the electron Green's function within the linearized muffin-tin orbitals method, we show that it is possible to greatly simplify the embedding of the self-energy. This in turn facilitates the implementation of the coherent potential approximation, which is used to model the substitutional disorder. The computational technique is tested on the Cu-Pd binary alloy system, and for disordered Mn-Ni interchange in the half-metallic NiMnSb.

TT 2.6 Mon 10:45 H7

Charge Reconstruction in Magnetic Heterostructures — •Andreas Weh[1], Liviu Chioncel[1], Ulrich Eckern[1], and Junya Otsuki[2] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics, Tohoku University, Sendai, Japan

We present a self-consistent method for using real-space dynamical mean-field theory (r-DMFT) to address local and intersite Coulomb interactions in heterostructures. The local in-plane many-body problem is solved using the continuous-time quantum Monte Carlo approach for the Hubbard model in hybridization expansion (CT-Hyb). The mean-field interlayer Coulomb potential generates a classical electrostatic problem which is solved by employing the Poisson equation for the multilayered geometry. Using this method we study half-metallic heterostructures consisting of coupled layers of single-band Hubbard models.

15 min. break.

TT 2.7 Mon 11:15 H7

The smothered phase separation - Microscopic Fermi liquid theory of the Mott transition — •Friedrich Krien[1], Erik Gerardus Cornelis Petrus van Loon[2], Mikhail Katsnelson[2], Alexander Lichtenstein[3], and Massimo Capone[1] — [1]Sissa, Trieste, Italien — [2]Radboud University, Nijmegen, The Netherlands — [3]University of Hamburg, Germany

The compressibility of the Mott insulating phase is vanishingly small, the doped Mott insulator however often exhibits a phase separation (divergence of the compressibility), which is a Pomeranchuk instability of the Fermi liquid in the charge sector. In order to better understand the counter-intuitive proximity of the two phases we calculate the two-particle Fermi liquid parameters in the DMFT approximation. Our analysis shows that the vanishing compressibility of the Mott insulator in fact requires the divergence of the charge forward scattering vertex at the Mott transition, which for finite quasi-particle weight would lead to a divergence of the compressibility. The proximity of the Mott phase is therefore connected to a tendency towards phase separation.

TT 2.8 Mon 11:30 H7

Thermodynamics of the metal-insulator transition in the extended Hubbard model — •Malte Schüler[1,2], Erik van

Loon[1,2], Mikhail Katsnelson[3], and Tim Wehling[1,2] — [1]Institut for Theoretical Physics, Universtity of Bremen — [2]Bremen Center for Computational Materials Science, Universtity of Bremen — [3]Institute for Molecules and Materials, Radboud University, Nijmegen

Due to ineffective screening, low-dimensional materials often comprise strong local and non-local Coulomb interaction at the same time. In the corresponding extended Hubbard model, nonlocal interactions can raise the order of the metal-insulator transition and under certain circumstances lead to a discontinuous first-order transition. Here, we investigate the square lattice at half filling and find a first-order transition which is far from any charge-density instability. We discuss the thermodynamics of this transition and elucidate its experimental observability based on the corresponding jump on entropy. We use the Peierls-Feynman variational principle to approximate the extended Hubbard model by an effective Hubbard model. This requires the calculation of non-local charge correlation functions for various parameters of the effective Hubbard model, which we obtain by the determinant quantum Monte Carlo method.

TT 2.9 Mon 11:45 H7

Extended Hubbard Model with nearest neighbor exchange interaction — •Edin Kapetanovic[1,2], Malte Schüler[1,2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institute for Theoretical Physics, Universtity of Bremen — [2]Bremen Center for Computational Materials Science, Universtity of Bremen

We study an extended Hubbard model (EHM) taking into account nearest neighbor direct Coulomb and exchange interactions. Whereas the simple EHM (without exchange interaction) can be mapped on a simple Hubbard model with renormalized on-site interaction $\tilde{U}$, the EHM with ferromagnetic exchange (i.e. the extended Hubbard-Heisenberg model) at half filling, allows for both, ferro- and antiferromagnetic phases, which is not captured by a simple Hubbard model. For the case of intermediate coupling strengths, which cannot be addressed by perturbation theory or similar approaches, we apply a variational scheme by mapping the EHM with exchange on an effective Hubbard model within an effective magnetic field. In the aforementioned parameter regime we find a partly magnetized phase where the kinetic energy is still significant. In contrast to the known limiting cases, a first order magnetic transition to the fully magnetized state occurs. Further study of these phenomena may provide insight on exotic magnetic phases within correlated materials. For performing the variation we rely on exact numerical solutions of the effective Hubbard model on finite clusters using determinant quantum Monte Carlo.

TT 2.10 Mon 12:00 H7

Lefschetz thimbles approach for the sign problem in Hubbard model away of half-filling — •Maksim Ulybyshev[1], Christopher Winterowd[2], and Savvas Zafeiropoulos[3] — [1]Institut für Theoretische Physik, Julius-Maximilians-Universität, 97074 Würzburg, Germany — [2]University of Kent, School of Physical Sciences, Canterbury CT2 7NH, UK — [3]Institute for Theoretical Physics, Universität Heidelberg, Philosophenweg 12, D-69120 Germany

Quantum Monte Carlo simulation of the Hubbard model away of half filling suffer from the sign problem which makes the method almost inapplicable in this case. We applied the Lefschetz thimble approach to the Hubbard model on hexagonal lattice with chemical chemical at van Hove singularity. In this method the integration contour for continuous auxiliary fields is shifted into complex space. There are optimal manifolds ("Lefschetz thimbles"), where fluctuations of the phase of the Monte Carlo weight are substantially suppressed. Thus the sign problem is also suppressed and can be dealt with using conventional reweighting technique. Thimbles are attached to saddle points of the action in complex space. Thus the algorithm includes the search for these saddle points and also the special methods for sampling over curved surfaces in complex space. We made the practical implementation of the above mentioned algorithms, suitable for the Hubbard model, and estimated the complexity of the residual sign problem. We also show that it is possible to manipulate the saddle points of the action using different versions of the Hubbard-Stratonovich transformation, thus also changing the complexity of the sign problem.

TT 2.11 Mon 12:15 H7

From gapped Goldstone to Higgs modes in excitonic magnets — •Jan Kuneš[1], Dominique Geffroy[1,2], Josef Kaufmann[1], Atsushi Hariki[1], Andreas Hausoel[3], and Patrik Gunacker[1] — [1]TU Wien, Austria — [2]Masaryk University, Brno, Czechia — [3]Univesity of Würzburg, Germany

We present a dynamical mean-field study of dynamical susceptibility in two-orbital Hubbard model across the exciton condensation transition. We observe appearance of Goldstone modes consistent with the broken symmetries. Reducing continuously the symmetry of the Hamiltonian we open gaps in the Goldstone modes. Upon increasing the amplitude of the symmetry breaking terms the character of the gapped modes smoothly changes from gapped Goldstone modes to Higgs amplitude fluctuations. Another notable observation is a qualitative change of the dynamical spin structure factor upon exciton condensation, which may be used as an experimentally accessible probe of the spin-triplet exciton condensate.

[1] Geffroy et al., arXiv:1808.08046

TT 2.12 Mon 12:30 H7

A Fractionalized Metal in a Falicov-Kimball Model — •Martin Hohenadler and Fakher Assaad — Universität Würzburg

Quantum Monte Carlo simulations are used to reveal two different metallic regimes in a 2D spinful Falicov-Kimball model with a three-body interaction. For weak to intermediate coupling, gapless single-particle excitations are consistent with a Fermi liquid. In contrast, for strong coupling, metallic behavior is observed despite the absence of quasiparticles. This regime can be understood using the concepts of orthogonal metals and fractionalization. Interesting connections to lattice-gauge and slave-spin theories are highlighted.

TT 2.13 Mon 12:45 H7

Fluctuation effects at the onset of the $2k_F$ density wave order in two-dimensional metals — •Jachym Sykora[1], Tobias Holder[2], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100

We analyze quantum fluctuation effects at the onset of charge or spin density wave order in two-dimensional metals with an incommensurate $2k_F$ wave vector. We distinguish two cases where the ordering vector connects either a single pair of hot spots on the Fermi surface or two pairs of hot spots. For both cases we evaluate the self-energy to leading order in fluctuation expansion (one loop). For the case of single pair of hot spots we find anomalous frequency scaling and a divergent renormalization of Fermi velocity. However this one loop result is found to not be self-consistent casting doubt on the existence of such a quantum critical point. The case of two pairs of hot spots also exhibits non-Fermi liquid behavior, however of a weaker kind and is the subject of current investigation.