TT 68: Correlated Electrons: (General) Theory 1

Time: Wednesday 15:00–18:15 Location: H 3010

TT 68.1 Wed 15:00 H 3010

Ab-initio study of the finite temperature magnetism in iron and nickel — Michael Karolak[1], •Andreas Hausoel[1], Ersoy Sasioglu[2], Alessandro Toschi[3], Andrey A. Katanin[4], Karsten Held[3], Alexander Lichtenstein[5], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Peter Grünberg Institut, Forschungszentrum Jülich — [3]Institute of Solid State Physics, TU Wien — [4]Institute of Metal Physics, Ekaterinburg — [5]Institut für Theoretische Physik, Universität Hamburg

The calculation of the ferromagnetic transition temperature of itinerant ferromagnets like iron and nickel has been a very hard problem for theory ever since. This is due to the interplay between strong local interactions and the itinerant character of the electrons. Here we show fully ab-initio DFT+DMFT calculations for bcc-iron and fcc-nickel, using the numerically exact Continuous Time Quantum Monte Carlo method in hybridization expansion. We consider the full cubic Coulomb interaction from cRPA and discuss the effects of different commonly used approximations, i.e. density-density and Slater-Kanamori. This way we obtain the best ab-initio estimates of the transition temperatures of iron and nickel one can achieve with static interactions and neglecting non-local spatial correlations.

TT 68.2 Wed 15:15 H 3010

La_2NiTiO_6: A 3D $S = 1$ fcc Heisenberg antiferromagnet — Michael Karolak, •Martin Edelmann, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The double perovskite La_2NiTiO_6 is identified as an interesting $S = 1$ quantum antiferromagnet on a three-dimensional fcc sublattice. By means of Density Functional Theory (DFT) in combination with Dynamical Mean Field Theory (DMFT) it is demonstrated that this material is a high-spin d-electron system deep in the Heisenberg limit and established that its paramagnetic Mott phase persists down to low temperatures not because of frustration effects but rather for the strong coupling physics. The strong-coupling nature is assessed from a multi-orbital DFT+DMFT analysis of the energetic balance between the ordered and disordered phase, which reveals a kinetic-energy-driven ordering. La_2NiTiO_6 emerges thus as a paradigmatic realization of a spin-triplet Mott insulator[1].

[1] M. Karolak, M. Edelmann, and G. Sangiovanni, arXiv:1407.2255 (2014).

TT 68.3 Wed 15:30 H 3010

Multi-orbital GW+(E)DMFT investigation of strongly correlated materials — •Lewin Boehnke[1], Fredrik Nilsson[2], Ferdi Aryasetiawan[2], and Philipp Werner[1] — [1]University of Fribourg, Switzerland — [2]Lund University, Sweden

The merits of the combination of the GW-formalism for non-local self-energy effects and (extended) dynamical mean field theory (E)DMFT to rigorously incorporate local fluctuations have been realized more than a decade ago [1], yet the numerical obstacles finding physically sound approximations for the respective parts prevented a broad adaption.

Previous approaches a GW+(E)DMFT treatment of strongly correlated multi-orbital electron systems employed various degrees of approximation for the DMFT impurity problem, the self-consistency and the interface of the two complementary methods.

We use suitable continuous time (CT-Hyb) solvers to deal with the frequency dependance of the impurity interaction and a fitted Matsubara-axis formulation of the GW-algorithm to examine the multi-orbital perspective to material investigations.

[1] Biermann, Aryasetiawan, Georges, PRL **90** (2003)

TT 68.4 Wed 15:45 H 3010

Electron correlation at the interface : A charge self-consistent DFT+DMFT approach. — •Sumanta Bhandary[1], Zhicheng Zhong[2], Liang Si[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria — [2]Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have employed a method to describe the interplay between structural distortion and induced charge as well as orbital degrees of freedom in a self-consistent way by combining density functional theory (DFT) and dynamical mean field theory (DMFT)[1]. The scheme involves solution of the full system in a local density approximation (Wien2K) followed by a wannier projection on correlated sub-bands (Wannier90). The impurity problem is treated with DMFT by employing continuous time quantum monte carlo (CT-QMC) method in the hybridization expansion (w2dynamics). The correlation induced correction to the charge density is incorporated in the total charge, which is obtained over a self-consistent loop of DFT and DMFT. The thin layer of $SrVO_3$ (SVO) on $SrTiO_3$ (STO) undergoes a Mott-Hubbard transition due to the spontaneous orbital symmetry breaking [2]. In contrast to SVO, there is a significant charge transfer between the layers of $SrRuO_3$.

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[1] F. Lechermann *et al.* PRB 74, 125120;
L. V. Pourovskii *et al.* PRB 76, 235101.
[2] Z. Zhong *et al.* arXiv:1312.5989.

TT 68.5 Wed 16:00 H 3010

Charge self-consistent DFT+Many-body with a flexible self-energy representation — •Christoph Piefke, Malte Behrmann, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

Starting from ab initio density functional theory in its local density approximation (DFT/LDA), strongly correlated electron systems are investigated using a combination of different self-energy approximations in a charge-self-consistent approach. After identifying a correlated subspace via projections onto localized orbitals [1], a multi-orbital Hubbard-Hamiltonian, including spin-flip-, pair-hopping- and spin-orbit-coupling-terms, is introduced. Fed with parameters from experiment, this operator gives rise to a self-energy-correction, which can be treated in different approximations, e.g. by taking it as the orbital occupation times interaction strength (Hartree-Fock, HF) or by mapping the interactions onto an itinerant quasiparticle part and localized bosonic degrees of freedom (e.g. Rotationally Invariant Slave-Boson Mean-Field theory, RISB-MF [2,3]). The correction flows back to LDA. We report, how this approach fits in the landscape of available techniques for strongly correlated electron systems and explore its chances and limits in the context of realistic strongly correlated materials.

[1] B. Amadon, F. Lechermann, A. Georges, F. Jollet, T.O. Wehling, and A.I. Lichtenstein, PRB **77**, 205112, (2008)
[2] T. Li, P. Wölfle, and P. J. Hirschfeld, PRB **40**, 6817 (1989)
[3] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, PRB **76**, 155102, (2007)

TT 68.6 Wed 16:15 H 3010

Optimal bath discretization for exact diagonalization solvers of Anderson impurity models — •Malte Schüler[1,2], Christian Renk[1,2], and Tim Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

Exact diagonalization (ED) solvers of the Anderson impurity model (AIM) provide access to real frequency spectral properties and work in presence of arbitrarily complex Coulomb interactions, spin-orbit coupling and at low temperatures. Due to Hilbert space constrains the non-interacting bath of the AIM has however to be discretized, which is the main approximation within ED approaches and gives rise to ambiguities. We present a method which finds optimal parameters of the discretized model. Optimal means that the resulting density matrix represents the density matrix of the full model as closely as possible. This is accomplished by using a variational principle. We show benchmark results and comparisons to other discretization schemes and solvers like CT-QMC as well as first results on realistic 5-Orbital impurity models. Orbital occupancies, local spin moments and thermodynamic properties are well described within this variational ED approach.

15 min. break.

Topical Talk TT 68.7 Wed 16:45 H 3010

Structural Stability and Lattice Dynamics of Correlated Electron Materials — •Ivan Leonov — TP III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

I will discuss a computational scheme for the investigation of complex correlated electron materials which is able to treat atomic displacements, and hence structural transformations, caused by electronic correlations. It combines ab initio band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. This approach is employed to compute the electronic structure and phase stability of several correlated electron materials. In particular, we study the cooperative Jahn-Teller effect in paramagnetic $KCuF_3$, the electronic properties and lattice dynamics of Fe at the bcc-fcc phase transition as a function of temperature, the electronic state and structural stability of V_2O_3 at the Mott-Hubbard metal-insulator transition, and the electronic structure and phase stability of FeSe. Our results for the equilibrium crystal structure, phase stability, and lattice dynamics are in quantitative agreement with experimental data. We find that electronic correlations are important to explain the lattice stability of correlated materials. We also present our recent results obtained by the LDA+DMFT approach implemented with the linear-response formalism regarding atomic displacements which makes it possible to evaluate the interatomic forces and, thereby, determine the atomic displacements. Our results show an overall good agreement between the total energy and force computations of the equilibrium atomic positions.

TT 68.8 Wed 17:15 H 3010

Correlated metal - Mott insulator heterostructures: real space dynamical mean-field study — •Karol Makuch and Krzysztof Byczuk — Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Motivated by recent experiments on transition metal oxide interfaces we study models of heterostructures with strong electronic correlations. In particular, we investigate a layer of a Mott insulator sandwiched between two semi-infinite correlated metals. The width of a layer varies from one to many lattice constants. The system is described by the Hubbard model on a simple cubic lattice with the position dependent Hubbard interaction. Properties of the system are investigated within the real space dynamical mean-field theory with the continuous time quantum Monte Carlo solver created in our group. Proximity effects and structures of local excitations in different parts of the system are described.

TT 68.9 Wed 17:30 H 3010

Fluctuation diagnostics of the electron self-energy: Origin of the pseudogap physics — Olle Gunnarsson[1], Thomas Schäfer[2], James Le Blanc[3,4], Emanuel Gull[4], Jaime Merino[5], Giorgio Sangiovanni[6], Georg Rohringer[2], and •Alessandro Toschi[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]IFP, Vienna University of Technology, Austria — [3]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [4]Department of Physics, University of Michigan, Ann Arbor, USA — [5]Departamento de Física Teórica de la Materia Condensada, IFIMAC Universidad Autónoma de Madrid, Spain — [6]Institute of Physics and Astrophysics, University of Würzburg, Germany

We demonstrate how to identify which physical processes dominate the low-energy spectral functions of correlated electron systems. We obtain an unambiguous classification by analysing the equation of motion for the electron self-energy in its charge, spin and particle-particle representations. Our procedure is then employed to clarify the controversial physics responsible for the appearance of the pseudogap in correlated systems. We illustrate our method by examining the attractive and repulsive Hubbard model in two-dimensions. In the latter, spin fluctuations are identified as the origin of the pseudogap, and we also explain why d-wave pairing fluctuations play a marginal role in suppressing the low-energy spectral weight, independent of their actual strength.

TT 68.10 Wed 17:45 H 3010

Excitonic condensation of strongly correlated electrons — •Jan Kunes — Institute of Physics, ASCR, Prague, Czechia

Instabilities of the two-band Hubbard model in the vicinity of the spin-state transition are investigated using the dynamical mean-field theory. Excitonic condensation is found to be the leading instability in a part of the parameter space [1]. The complex nature of the exitonic order parameter allows several phases to be realised. We show that by doping away from half-filling all the symmetry allowed phases can be realised and investigate their physical properties [2,3].

[1] J. Kunes and P. Augustinsky, Phys. Rev. B 89, 115134 (2014)
[2] J. Kunes and P. Augustinsky, arXiv:1405.1191
[3] J. Kunes, arXiv:1410.5198

TT 68.11 Wed 18:00 H 3010

Dynamical electronic correlations in nanostructures — •Angelo Valli[1,2], Giorgio Sangiovanni[3], Alessandro Toschi[2], Massimo Capone[1], and Karsten Held[2] — [1]Democritos National Simulation Center, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (IOM) and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy — [2]Vienna University of Technology, Vienna, Austria — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

The understanding and control of strong electronic correlation effects represents one of the most challenging research topic of modern solid state physics. Thanks to the refined ability to manipulate matter down to the nanoscale, we are nowadays able to explore electronic correlations within an artificial experimental environment. Moreover, the intrinsic high tunability of nano- and heterostructures hints at the fascinating possibility to directly control quantum phenomena. The experimental progress call for a deeper understanding of many-body effects on the nanoscale beyond paradigmatic models. To this end, we employ state-of-the art many-body methods within the reference frame of the dynamical mean-field theory and its extensions, in order to describe electronic, magnetic, and transport properties of nanoscopic systems. Among the applications, we explore the role of dynamical electronic correlations in carbon-based systems, ranging from few atoms molecules to graphene nanoflakes.