TT 51: Correlated Electrons: General Theory 1

Time: Thursday 9:30–12:30 Location: H6

TT 51.1 Thu 9:30 H6

Electronic Entanglement in Late Transition Metal Oxides — •Patrik Thunström[1], Igor Di Marco[2], and Olle Eriksson[2] — [1]TU Wien, Vienna, Austria — [2]Uppsala University, Uppsala, Sweden

We present a study of the entanglement in the electronic structure of the late transition metal monoxides – MnO, FeO, CoO, and NiO – obtained by means of density-functional theory in the local density approximation combined with dynamical mean-field theory. Two main sources of entanglement are resolved. The interplay of crystal field effects and Coulomb interaction are shown to give the entanglement in CoO a particularly intricate form.

TT 51.2 Thu 9:45 H6

Interface spin polarization of Half-metal/Semiconductor heterostructures — •Andreas Held[1], Stanislav Chadov[2], Igor Di Marco[3], and Liviu Chioncel[4,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nothnitzer Str. 40, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

Half-metallic/Semiconductor interfaces (Co_2MnAl/CoMnVAl) have been recently proposed as efficient spin injectors based on Heusler materials [1]. We discuss the impact of electronic correlation within the mean field (+U) and beyond (+DMFT) upon the electronic and magnetic properties in this interface. Our results suggest that typical correlations strength encountered in the family of Heusler compounds does not lead to a dramatic depolarization effect.

[1] S. Chadov et. al. PRL 107, 047202 (2011)

TT 51.3 Thu 10:00 H6

Comparing GW+DMFT and LDA+DMFT for the testbed material $SrVO_3$ — •Ciro Taranto[1], Merzuk Kaltak[2], Nicolaus Parragh[3], Giorgio Sangiovanni[3], Georg Kresse[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have implemented the GW+dynamical mean field theory (DMFT) approach in the Vienna ab initio simulation package. Employing the interaction values obtained from the locally unscreened random phase approximation (RPA), we compare GW+DMFT and LDA+DMFT against each other and against experiment for $SrVO_3$. We observed a partial compensation of stronger electronic correlations due to the reduced *GW* bandwidth and weaker correlations due to a larger screening of the RPA interaction, so that the obtained spectra are quite similar and well agree with experiment. Noteworthily, the GW+DMFT better reproduces the position of the lower Hubbard side band.

TT 51.4 Thu 10:15 H6

Calculation of total energies and forces in correlated materials — •Ivan Leonov[1], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia

We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations. It combines *ab initio* band structure and dynamical mean-field theory and is implemented with the linear response formalism regarding atomic displacements [1,2]. We employ this approach to compute the equilibrium crystal structure and phase stability of several correlated electron materials, such as elemental hydrogen, $SrVO_3$, and $KCuF_3$. We find an excellent agreement between the results for the equilibrium atomic positions in these materials obtained from calculation of total energy and forces, respectively. The approach presented here allows one to study the structural properties of materials with strongly correlated electrons such as lattice instabilities observed at correlation induced metal-insulator phase transitions from first principles.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **101**, 096405 (2008)
[2] I. Leonov *et al.*, Phys. Rev. B **81**, 075109 (2010).

TT 51.5 Thu 10:30 H6

Effective crystal field and Fermi surface topology in correlated multi-orbital systems — Nico Parragh[1], Giorgio Sangiovanni[1], Philipp Hansmann[2], Stefan Hummel[3], Karsten Held[3], and •Alessandro Toschi[3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Centre de Physique Théorique, Ècole Polytechnique, France — [3]Institut für Festkörperphysik, Technische Universität Wien, Austria

The electronic correlation effect of enhancing/reducing the effective crystal field in multi-orbital correlated materials can be crucial in determining the topology of the Fermi surface and, hence, the physical properties of these systems. Consequently, an accurate theoretical prediction of the Fermi surface structure is a very desirable goal, in particular for the emerging field of engineering new correlated heterostructures. In this respect, however, the application of one of the most powerful ab-initio scheme, i.e. the merger between the local density approximation (LDA) and the dynamical mean field theory (DMFT), can give contractdicting results: In recent studies of Ni-based heterostructure, the predicted Fermi surface is totally different depending on whether less correleated p orbitals are or are not included in the calculation[1,2]. The LDA+DMFT model study we present here aims at a clarifying the origin of this problem and at identifying the key parameters, which control the Fermi surface properties of these systems.

[1] P. Hansmann, A. Toschi, Xiaoping Yang, O.K. Andersen, and K. Held, Phys. Rev. B **82**, 235123 (2010)
[2] M. J. Han, Xin Wang, C. A. Marianetti, and A. J. Millis, Phys. Rev. Lett. **107**, 206804 (2011).

TT 51.6 Thu 10:45 H6

Quasi continuous-time impurity solver for dynamical mean-field theory with linear scaling in the inverse temperature — •Daniel Rost[1], Fakher Assaad[2], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg-University, Mainz — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg

Diagrammatic quantum Monte Carlo impurity solvers (CT-QMC) provide numerically exact solutions for dynamical mean-field theory (DMFT), at a computational cost that scales *cubically* with the inverse temperature β. In contrast, a recently proposed approach [1], based on a hamiltonian representation of the bath Green function and the BSS quantum Monte Carlo algorithm [2], scales *linearly* with β, but introduces a bias due to Trotter discretization. We present an algorithm, based on multigrid extrapolations of Green functions, that combines the advantages of both methods: (i) it retains the superior linear scaling of BSS and (ii) is free of significant Trotter errors. The accuracy of this quasi continuous-time method is established for the metal-insulator transition in the 1-band Hubbard model, in comparison with CT-QMC and exact diagonalization. We also analyze the impact of the bath discretization and conclude that the new method appears most promising for cluster DMFT studies at low temperatures.

[1] E. Khatami et al., PRE **81**, 056703 (2010); QUantum Electron Simulation Toolbox, http://www.cs.ucdavis.edu/∼bai/QUEST_public/.
[2] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).

15 min. break

TT 51.7 Thu 11:15 H6

Using Dual Bosons to go beyond EDMFT — •E.G.C.P. van Loon[1,2], A.B.J. Wilhelm[1], H. Hafermann[3], A.N. Rubtsov[4], M.I. Katsnelson[2], and A.I. Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — [2]Institute of Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]Centre de Physique Théorique, Ecole Polytechnique, CNRS, F-91128 Palaiseau Cedex, France — [4]Department of Physics, Moscow State University, 119992 Moscow, Russia

DMFT is widely used to study models of condensed matter. A problem of interacting particles is mapped onto a self-consistent impurity problem. It is exact in infinite dimension but in finite dimension it does not describe non-local effects. Dual fermions provide a way to incorporate these non-local effects beyond DMFT. Dual bosons can then be used to describe collective modes. In zeroth order, Dual Bosons correspond to EDMFT. Plasmons in Hubbard-like models can be studied using these theories. We present a new technique to use the method of Dual Bosons to self-consistently calculate the effects of these collective bosonic modes in a two dimensional Hubbard model on a square lattice. The hybridization solver from the ALPS project is used to solve an impurity model with retarded interaction. Self-energy diagrams are calculated with the resulting quantities to include non-local effects. We first present benchmark results. Then our results are compared with EDMFT results.

TT 51.8 Thu 11:30 H6

Non-perturbative precursors of the Mott-Hubbard transition at the two-particle level — •Thomas Schaefer[1], Georg Rohringer[1], Karsten Held[1], Olle Gunnarsson[2], Sergio Ciuchi[3], Giorgio Sangiovanni[4], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Universita degli Studi de l'Aquila, L'Aquila, Italy — [4]Institute of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Amongst plenty other successes, DMFT is able to cover the Mott-Hubbard metal-to-insulator transition (MIT), which is an intrinsic non-perturbative phenomenon. At the MIT the local spin susceptibility diverges, following Curie's law in the insulating phase, whereas the local charge susceptibility remains finite at the transition [1]. However, these divergencies are not the only hallmarks of the MIT at the two-particle level. In fact, the first non-perturbative precursors of the MIT can be identified well inside the metallic phase in the frequency structures of the irreducible vertex functions [2,3]. The strong enhancements of the irreducible vertex functions, characterising this precursor, stem from local scattering processes and can be traced up to the limit of high temperatures (i.e. the atomic limit).

[1] A. Georges et al., Rev. Mod. Phys. 68, 13-125 (1996)
[2] G. Rohringer et al., Phys. Rev. B 86, 125114 (2012)
[3] T. Schaefer et al., in preparation (2012)

TT 51.9 Thu 11:45 H6

Non-perturbative derivation of effective models using graph-based continuous unitary transformations — •Kris Cöster and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I , TU Dortmund, 44221 Dortmund, Germany

Unitary transformations are an essential tool in many-body physics mapping the original model to a simpler effective model in a better suited basis. One way to schematically derive such unitary transformations is given by the so-called continuous unitary transformations (CUTs). For lattice models of finite dimension, these CUTs can be combined with graph theory to capture all zero-temperature fluctuations within a controlled spatial range (gCUTs) providing a robust non-perturbative scheme to derive effective low-energy models when at least one degree of freedom is gapped. This method has already been succesfully applied to various systems and the aim is to increase both the understanding and the accuracy of this novel tool. To this end we introduce a general recipe on each graph respecting all symmetries of the graphs. Furthermore, an intuitive truncation on each graph is gained. One particular challenge for gCUTs is that the graphs typically have less symmetries than the full lattice model. The impact of this reduced symmetry on the effective low-energy Hamiltonian is studied focussing on possible remedies. These aspects are tested for one-dimensional and two-dimensional quantum spin systems.

TT 51.10 Thu 12:00 H6

Revealing the breakdown of spin-charge separation in spin-imbalanced fermions in one dimension using quench dynamics — •Michael Sekania[1] and Paata Kakashvili[2] — [1]Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, Germany — [2]Department of Physics and Astronomy, Rutgers University, USA

Recently, spin-imbalanced fermions in one dimension have attracted considerable attention both theoretically and experimentally. This system was successfully simulated using ultracold atoms in optical lattices. The phase diagram was measured and found to be in agreement with exact analytical calculations. It was also established theoretically that the spin-charge separation, an important property of Luttinger liquids, is absent. Low-energy bosonic excitations do not carry spin and charge separately due to the interaction between spin and charge degrees of freedom. Based on our numerical (time-dependent Density-Matrix Renormalization Group method) and analytical calculations (Bethe Ansatz, Bosonization) on the Hubbard model, we propose quench experiments which not only reveal the breakdown of spin-charge separation but also make it possible to study the so called "string" bound states in this system.

TT 51.11 Thu 12:15 H6

Conserved quantities of SU(2)-invariant interactions for correlated fermions and the advantages for quantum Monte Carlo simulations — Nicolaus Parragh[1], Alessandro Toschi[2], Karsten Held[2], and •Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Deutschland — [2]Institut für Festkörperphysik, Technische Universität Wien, Vienna, Österreich

In the context of realistic calculations for strongly correlated materials with d or f electrons the efficient computation of multi-orbital models is of paramount importance. Here we introduce a set of invariants for the SU(2)-symmetric Kanamori Hamiltonian, which allows us to massively speed up the calculation of the fermionic trace in hybridization-expansion continuous-time quantum Monte Carlo algorithms. We show that by exploiting this set of good quantum numbers the study of the orbital-selective Mott transition in systems with up to seven correlated orbitals becomes feasible.

[1] N. Parragh, A. Toschi, K. Held, and G. Sangiovanni, Phys. Rev. B **86**, 155158 (2012)