TT 19: Correlated Electrons: (General) Theory 2

Time: Tuesday 9:30–13:00 Location: H 3010

TT 19.1 Tue 9:30 H 3010

Multiplet ligand-field theory using Wannier orbitals — •M. W. Haverkort[1], M. Zwierzycki[2], and O. K. Andersen[1] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Molecular Physics, Poznań, Poland

We demonstrate how *ab initio* cluster calculations including the full Coulomb vertex can be done in the basis of the localized, generalized Wannier orbitals which describe the low-energy density functional (LDA) band structure of the infinite crystal, *e.g.* the transition metal 3*d* and oxygen 2*p* orbitals. The spatial extend of our 3*d* Wannier orbitals (orthonormalized Nth order muffin-tin orbitals) is close to that found for atomic Hartree-Fock orbitals. We define Ligand orbitals as those linear combinations of the O 2*p* Wannier orbitals which couple to the 3*d* orbitals for the chosen cluster. The use of ligand orbitals allows for a minimal Hilbert space in multiplet ligand-field theory calculations, thus reducing the computational costs substantially. The result is a fast and simple *ab initio* theory, which can provide useful information about local properties of correlated insulators. We compare results for NiO, MnO and $SrTiO_3$ with x-ray absorption, inelastic x-ray scattering, and photoemission experiments. The multiplet ligand field theory parameters found by our *ab initio* method agree within ∼10% to known experimental values.

TT 19.2 Tue 9:45 H 3010

Quantification of correlations in quantum many-particle systems — •Krzysztof Byczuk[1], Jan Kunes[2], Walter Hofstetter[3], and Dieter Vollhardt[4] — [1]Physics Faculty, Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, 00-681 Warszawa, Poland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 53 Praha 6, Czech Republic — [3]Institut for Theoretische Physics, Goethe-Universitat, 60438 Frankfurt/Main, Germany — [4]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We introduce a well-defined and unbiased measure of the strength of correlations in quantum many-particle systems which is based on the relative von Neumann entropy computed from the density operator of correlated and uncorrelated states [1]. The usefulness of this general concept is demonstrated by quantifying correlations of interacting electrons in the Hubbard model and in a series of transition metal oxides using dynamical mean-field theory.

[1] K. Byczuk, J. Kunes, W. Hofstetter, and D. Vollhardt; arXiv:1110.3214

TT 19.3 Tue 10:00 H 3010

What do $LaCoO_3$ and ^{4}He- ^{3}He mixtures have in common? — •Jan Kuneš and Vlastimil Křápek — Institute of Physics, AS CR, Cukrovarnicka 10, Praha 6, Czech Republic

The perovskite $LaCoO_3$ has been studied for almost half a century for its peculiar magnetic and transport properties. It is generally accepted that quasi-degeneracy of a magnetic and non-magnetic multiplets is the key feature of this material, however, the understanding how it affects its physics is far from complete. We have used a two-band Hubbard model as a minimum description of a material with competing atomic states. Using the dynamical mean-field theory we have studied the temperature dependencies of the magnetic susceptibility and the one-particle spectra. At intermediate temperatures we have observed formation of a two-sublattice order, which can be understood by mapping the Hubbard model on the classical Blume-Emery-Griffiths model.

TT 19.4 Tue 10:15 H 3010

Dynamical screening effects in correlated materials — •Silke Biermann — CPHT Ecole Polytechnique, Palaiseau, France

Materials with strong Coulomb correlations are challenges for electronic structure calculations. During the last years new methods for their description have been developed. The combination of dynamical mean field (DMFT) techniques with density functional theory within the local density approximation (LDA) allows for the calculation of electronic properties of materials from first principles, taking into account the effect of arbitrarily strong Coulomb interactions. We will describe recent developments to include dynamical screening effects into such calculations [1,2]. Based on an ab initio determination of the frequency-dependent local Coulomb interactions within the constrained random phase approximation [3,4] we discuss satellite features and spectral weight transfers associated to plasmon and electron-hole excitations.

[1] M. Casula, A. Rubtsov, S. Biermann, submitted, arXiv:1107.3123
[2] Ph. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. Millis, S. Biermann, submitted, arXiv:1107.3128
[3] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein Phys. Rev. B 70, 195104 (2004).
[4] L. Vaugier, H. Jiang, S. Biermann, in preparation.

TT 19.5 Tue 10:30 H 3010

Generalized Coulomb interaction parameters for every point group symmetry — •Anna Toth[1,2], Andrey Kutepov[2], Gabriel Kotliar[2], Philipp Hansmann[3,1], Nico Parragh[1], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Vienna, Austria — [2]Department of Physics, Rutgers University, Piscataway, New Jersey, USA — [3]Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, Cedex, France

We show how to construct the independent two-electron interactions in arbitrary crystal field and for arbitrary spin-orbit coupling strength. We establish the correspondence between these interactions and the Hubbard term and Hund's rule coupling. Our scheme, which takes the point group fully into account, gives additional parameters beyond the standard Slater integrals (which describe the spherical symmetric case), or the Kanamori scheme. As an application, we determine the strength of these couplings in $BaFe_2As_2$ based on the self-consistent GW method, and give a comprehensive comparison between the different schemes.

TT 19.6 Tue 10:45 H 3010

Phase diagram of honeycomb bilayer from functional RG — •Stefan Uebelacker, Michael Scherer, and Carsten Honerkamp — Institut für Theoretische Festkörperphysik C, RWTH Aachen University, Aachen, Germany

The phase diagram for interacting electrons on the honeycomb bilayer with Bernal stacking is explored by means of the functional renormalization group. For half-filling and including a range of repulsive onsite, nearest-neighbor and next-to-nearest neighbor interaction terms we analyze the emergent instabilities and find antiferromagnetic, (modulated) charge-density-wave and quantum spin Hall order. The presented phase diagram covers the region of the bilayer graphene parameters suggested by ab initio calculations which overlaps with the phase boundary between the antiferromagnetic state and the quantum spin Hall state. We comment on the effect of small dopings and third nearest neighbor interaction.

TT 19.7 Tue 11:00 H 3010

Phase transitions of the three-state (anti-)ferromagnetic Potts model in transverse field — •Marc Daniel Schulz[1,4], Sébastien Dusuel[2], Roman Orùs[3], Julien Vidal[4], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany — [4]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

The investigation of phase transitions in two-dimensional quantum lattice systems is a challenging task. Here, we study the three-state Potts model on a two-dimensional square lattice in transverse field for antiferromagnetic and ferromagnetic coupling. To this end, we combine the methods of perturbative continuous unitary transformations (pCUT) and variational techniques using infinite projected entangled pair states(iPEPS). For the ferromagnetic coupling, we confirm the already known first-order nature of the phase transition, whereas for the anti-ferromagnetic coupling we provide strong evidence for a novel second-order phase transition compatible with the 3dXY universality class.

15 min. break.

Invited Talk TT 19.8 Tue 11:30 H 3010

Interactions and disorder in topological quantum matter — •Simon Trebst — Universität zu Köln

The emergence of topological order is one of the most intriguing phenomena in quantum many-body physics and one of possibly far reaching relevance – topological quantum matter is increasingly appreciated as possible medium for quantum computation purposes. In this talk, I will discuss the stability of topological quantum matter when considering the effects of interactions and disorder on the collective quantum state formed by a set of topological excitations, so-called anyons. In particular, I will discuss the formation of a thermal metal of Majorana fermions in a two-dimensional system of interacting non-Abelian anyons in the presence of moderate disorder. This bulk metallic phase occurs for various proposed systems supporting Majorana fermion zero modes when disorder induces the random pinning of a finite density of vortices. This includes all two-dimensional topological superconductors in so-called symmetry class D. A distinct experimental signature of the thermal metal phase is the presence of bulk heat transport down to zero temperature. I will finish by discussing implications for topological quantum computing proposals.

TT 19.9 Tue 12:00 H 3010

Robustness of a perturbed topological phase — Michael Kamfor[1], Sebastien Dusuel[2], Roman Orus[3], Julien Vidal[4], and •Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany — [2]Lycée Saint-Louis, 75006 Paris, France — [3]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany — [4]LPTMC, Université Pierre et Marie Curie, 75252 Paris Cedex 05, France

We investigate the stability of the topological phase of the toric code model in the presence of a uniform magnetic field by means of variational and high-order series expansion approaches. We find that when this perturbation is strong enough, the system undergoes a topological phase transition whose first- or second-order nature depends on the field orientation. Our work represents the first high-order series expansion for the anyonic quasi-particles of a topological phase. As a consequence, we get access to the critical properties of the perturbed toric code.

TT 19.10 Tue 12:15 H 3010

Supersymmetry in Rydberg-dressed lattice fermions — •Hendrik Weimer[1], Liza Huijse[1], Alexey Gorshkov[2], Guido Pupillo[3], Peter Zoller[4], Mikhail Lukin[1], and Eugene Demler[1] — [1]Physics Department, Harvard University, Cambridge, MA, USA — [2]IQI, Caltech, Pasadena, CA, USA — [3]University of Strasbourg, Strasbourg, France — [4]University of Innsbruck and IQOQI, Innsbruck, Austria

Supersymmetry is a powerful tool that allows the characterization of strongly correlated many-body systems, in particular in the case of supersymmetric extensions of the fermionic Hubbard model [1]. At the same time, these models can exhibit rich and exotic physics on their own, such as flat bands or exponentially large ground state degeneracy. We show that such lattice models can be realized with Rydberg-dressed fermions in optical lattices. Strong interactions within the ground state manifold of the atoms can be realized by admixing a weak contribution of a highly excited Rydberg state [2]. By tuning the experimental parameters away from the supersymmetric point, it is possible to assess the validity of a supersymmetric approach to strongly correlated electrons in a systematic way.

[1] P. Fendley, K. Schoutens, J. de Boer, PRL **90**, 120402 (2003).
[2] J. Honer, H. Weimer, T. Pfau, H. P. Büchler, PRL **105**, 160404 (2010).

TT 19.11 Tue 12:30 H 3010

Application of wave function based electron correlation methods to van der Waals bound crystals — •Carsten Müller[1] and Denis Usvyat[2] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin Takustr. 3, Berlin, 14195, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Regensburg Universitätsstr. 31, Regensburg, 93040, Germany

The treatment of van der Waals bound systems, such as molecular crystals is a remains challenging in theoretical solid state chemistry. In these systems, electron correlation is crucial and HF or standard DFT functionals often fail to produce reliable cohesive energies. On the other hand, common implementations of wave function based post-HF methods, such as MP2 or Coupled Cluster theory, suffer from an unfortunate scaling with system size, and are difficult to adopt to periodic systems.

In our investigations we have combined the Method of Increments, which is one type of local correlation method, with embedded cluster calculations to investigate physisorption Ar fcc and the CO_2 crystal at the LMP2 and LCCSD(T) levels. First, periodic LMP2 calculations were performed to obtain appropriate parameters for the size of the excitation domains and to assess the convergence of the incremental expansion. Then different schemes for the embedding of the finite clusters were assessed for their influence on the convergence behavior of the incremental expansion. And finally calculations at the LCCSD(T) level and with larger basis sets were used to obtain the cohesive energy of Ar fcc and CO_2 with benchmarking quality.

TT 19.12 Tue 12:45 H 3010

Temperature evolution of phonon spectra of elemental iron near the α-γ phase transition — •I. Leonov[1], A. I. Poteryaev[2,3], V. I. Anisimov[2], and D. Vollhardt[1] — [1]TP III, Center for Electronic Correlations and Magnetism, Uni Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]Institute of Quantum Materials Science, Yekaterinburg, Russia

We present results of a theoretical investigation of the electronic and lattice dynamical properties of elemental iron at finite temperatures obtained within dynamical mean-field theory implemented with the frozen-phonon method [1]. This approach allows us to compute correlation induced lattice transformations and their temperature evolution. We find that electronic correlations are important to explain the lattice stability of iron at the bcc-fcc phase transition. We notice a weak anomaly in the transverse T_1 acoustic mode in the Γ-N direction of the bcc phase. This behavior can be ascribed to a dynamical precursor effect of the bcc-to-fcc phase transition and is found to occur above the Curie temperature. Upon further heating, the bcc phase becomes dynamically unstable due to the T_1 mode near the N point. By contrast, the fcc lattice is found to be dynamically stable in a broad temperature range, including temperatures above and below the bcc-fcc phase transition temperature. Our results for the structural phase stability and lattice dynamical properties of iron are in good agreement with experiment.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **106**, 106405 (2011); I. Leonov *et al.*, arXiv:1110.0439 (2011).