TT 5: Correlated Electrons - (General) Theory

Time: Monday 14:00–18:00 Location: H18

Invited Talk TT 5.1 Mon 14:00 H18

Time-dependent density-functional theory: the framework, applications and recent developments — •Lucia Reining — LSI, CNRS-Ecole Polytechnique, Palaiseau, France

Time-Dependent Density Functional Theory (TDDFT) [1] is used with increasing success for the ab initio description of electronic excitations, measured for example in absorption, electron-energy loss or inelastic X-ray scattering spectroscopies. In fact, TDDFT correctly covers phenomena such as classical depolarization, the Fano effect due to interference of different excitations, or the appearance of bound exciton series in the bandgap of insulators. The description of these and many other interesting effects require of course different levels of approximation, for example concerning exchange-correlation effects.

This talk will give an overview of the spirit and the fundamental ingredients of TDDFT, in comparison to the alternative description of excitation spectra through the Bethe-Salpeter Equation [2]. Different contributions will be linked to physical effects that are observed in various applications [3] including simple bulk semiconductors and insulators, but also transition metal oxides, nanostructures, or disordered systems. Some recent developments will also be presented.

[1] E. Runge and E. K. U. Gross, Phys. Rev. Lett. 52, 997 (1984).

[2] G. Onida, L. Reining, and A. Rubio, Reviews of Modern Physics 74, 601 (2002).

[3] See e.g. F. Bruneval, S. Botti, L. Reining, Phys. Rev. Lett. 94, 219701 (2005); H.-C. Weissker et al., Phys. Rev. Lett. 97, 237602 (2006).

TT 5.2 Mon 14:30 H18

Determining the ordered orbital and spin momentum as well as orbital order with the use of sum-rules in x-ray resonant scattering. — •M. W. Haverkort, C. Schüssler-Langeheine, T. Willers, and L. H. Tjeng — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Sum-rules in x-ray circular dichroism relating the integrated intensity of the x-ray absorption spectra taken with different circular polarizations to the total spin and orbital momentum are well known. Less known, but derived on the same principles, are sum rules for linear dichroism relating the absorption intensity with different linear polarizations to the orbital occupation. We extended these sum-rules, known for x-ray absorption spectroscopy, to the closely related method of resonant x-ray scattering, and show how to use this method to obtain quantitative information on charge, orbital, orbital momentum and on spin ordering even in antiferromagnetic systems. Supported by the DFG through SFB 608.

TT 5.3 Mon 14:45 H18

Kinks in the dispersion of strongly correlated electrons — •Marcus Kollar[1], Krzysztof Byczuk[1,2], Karsten Held[3], Yi-Feng Yang[3], Igor Nekrasov[4], Thomas Pruschke[5], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg — [2]Institute of Theoretical Physics, Warsaw University — [3]Max-Planck Institute for Solid State Research, Stuttgart — [4]Institute for Electrophysics, Russian Academy of Sciences, Ekaterinburg — [5]Institute for Theoretical Physics, University of Göttingen

The properties of condensed matter are determined by single-particle and collective excitations and their interactions. The coupling of two excitations may lead to abrupt changes (kinks) in the slope of the dispersion. Such kinks thus carry important information about interactions in a many-body system are of great interest, e.g., in the high-temperature superconductors. We report a novel, purely electronic mechanism yielding kinks in the electron dispersions [1]. It applies to strongly correlated metals whose spectral function shows well separated Hubbard subbands and central peak as, for example, in transition metal-oxides. The position of the kinks and the energy range of validity of Fermi-liquid (FL) theory is determined solely by the FL renormalization factor and the bare, uncorrelated band structure. ARPES experiments at binding energies outside the FL regime can thus provide new, previously unexpected information about strongly correlated electronic systems.

[1] K. Byczuk *et al.*, Preprint cond-mat/0609594.

TT 5.4 Mon 15:00 H18

Dynamical vertex approximation — a step beyond dynamical mean field theory — •Alessandro Toschi[1], Andrey Katanin[1,2], and Karsten Held[1] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institute of Metal Physics, 620219 Ekaterinburg, Russia

We have developed a new diagrammatic approach, coined "Dynamical Vertex Approximation" (DΓA), with the aim of going beyond dynamical mean field theory for strongly correlated systems, by including the effects of long-range spatial correlations. Without resorting to any finite-size cluster scheme, DΓA allows us to compute momentum dependent self-energies (and spectra), whose expressions are diagrammatically constructed starting from the two-particle irreducible local vertex. Therefore, DΓA naturally applies for studying effects of magnetic fluctuations with large correlation length in strongly correlated systems, such as the Hubbard model. Specifically, we analyze the interplay between antiferromagnetic fluctuations and the Mott metal-insulator transition in three dimensions and the formation of a pseudogap in two dimensions. The diagrammatic nature of DΓA, moreover, should allow for a generalization to the more realistic case of multi-band Hamiltonians.

TT 5.5 Mon 15:15 H18

Nature and order of orbital-selective Mott transitions — •Nils Blümer[1] and Krunoslav Požgajčić[2] — [1]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [2]Institut für Theoretische Physik, J.W. Goethe-Universität, 60438 Frankfurt

Motivated by experiments on $Ca_{2-x}Sr_xRuO_4$, numerous theoretical studies have recently explored the possible occurence of orbital-selective Mott transitions (OSMTs) in multi-band Hubbard models with orbital-dependent hopping amplitudes. By now, consensus has been reached that (within dynamical mean-field theory, DMFT) a sequence of two orbital-selective transitions occurs generically in the two-band case – even in the case of Ising-type Hund rule couplings. However, the precise nature and thermodynamic order of each of these transitions (which may be different for $T>0$ and $T=0$) have remained controversial.

In order to address these issues, we directly compute first derivatives of the free energy within DMFT using quantum Monte Carlo (QMC) simulations at $T>0$ and selfenergy functional theory (SFT) at $T=0$. High precision is achieved in QMC by using analytic high-frequency corrections and in SFT by including multiple bath sites per orbital, respectively, and checked by comparisons of SFT data with $T \to 0$ extrapolated QMC results.

TT 5.6 Mon 15:30 H18

Ab-initio wavefunction-based methods for solids: correlation corrections to the band structure of oxide compounds — •Liviu Hozoi, Uwe Birkenheuer, and Peter Fulde — Max-Planck-Institut fuer Physik komplexer Systeme, 01187 Dresden

We apply ab-initio wavefunction-based methods to the study of correlation effects on the band structure of oxide compounds. We choose MgO as a prototype closed-shell system. As a zeroth-order approximation, we compute first the Hartree-Fock (HF) bands and the (localized) Wannier orbitals associated with these. The HF data for the infinite crystal is transferred then to a quantum chemical program and used as input for the construction of embedded clusters. Correlation effects on the fundamental band gap and on band widths are computed by using a quasiparticle picture and a local Hamiltonian approach. For the (N-1)/(N+1) valence and conduction band states, we found that relaxation and polarization effects associated with the on-site and nearest-neighbor ligand electron shells account for 40% of the difference between the HF and experimental gaps. Long-range polarization effects bring also large corrections. Within the approximation of a dielectric continuum, these corrections amount to 50% of the difference between the HF and experimental gap values. Whereas correlation effects are important for estimating band gaps, we found that they produce only minor changes on the HF band widths, at least in this material. The results show that our approach, based on a transparent formalism and well-controlled approximations, is able to provide a good understanding of the major effects that determine the electronic band structure.

15 min. break

Invited Talk TT 5.7 Mon 16:00 H18

Electronic Correlations in Electron-Transfer Systems — •Ralf Bulla[1], Sabine Tornow[1], and Frithjof Anders[2] — [1]Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg — [2]Fachbereich 1, Universität Bremen

Electron transfer processes play an important role in a variety of physical, chemical, and biological systems. Already the transfer of a single electron from the donor to the acceptor can be viewed as a complicated many-body problem, due to the coupling of the electron to the infinitely many environmental degrees of freedom, usually described as a bosonic bath. Here we focus on the quantum mechanical modelling of *two*-electron transfer processes and the influence of the Coulomb interaction between the electrons. It turns out that electronic correlations significantly influence the dynamics of the electron transfer process. We identify situations under which concerted transfer of the two electrons occurs, in contrast to a stepwise single-electron transfer. Calculations are performed using the non-perturbative numerical renormalization group approach for both equilibrium and non-equilibrium properties.

TT 5.8 Mon 16:30 H18

Charge transfer through DNA and peptides: The role of electron correlations — •Sabine Tornow[1], F. Anders[2], and R. Bulla[1] — [1]Theoretical Physics III,Center for Electronic Correlations and Magnetism,University of Augsburg — [2]Institute of theoretical physics,University of Bremen

In nature charges are transferred trough proteins or DNA over large distances. To describe the real time dynamics of the charges we consider a dissipative extended Hubbard model. The environment is modelled similar as in a spin boson model. In the nuclear tunnelling regime we calculate the time dependent populations with the time-dependent Numerical Renormalization Group. We found a considerable difference between single and multiple charge dynamics.

TT 5.9 Mon 16:45 H18

Competition of Pomeranchuk instability and superconductivity — •hiroyuki yamase and walter metzner — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

We analyze a mean-field model of electrons on a square lattice with two types of interaction: forward scattering favoring d-wave Fermi surface symmetry breaking (Pomeranchuk instability) and a BCS interaction driving d-wave superconductivity. Tuning the interaction parameters a rich variety of phase diagrams is obtained. If the BCS interaction is not too strong, Fermi surface symmetry breaking is obtained around van Hove filling, and coexists with superconductivity at low temperatures. In the presence of a paring gap it is easier to realize Fermi surface symmetry breaking via a continuous phase transition at low temperatures than without. For a relatively strong BCS interaction, Fermi surface symmetry breaking can be limited to intermediate temperatures, or can be suppressed completely by pairing.

TT 5.10 Mon 17:00 H18

Nonequilibrium functional renormalization group for interacting fermionic quantum systems — •Severin Jakobs[1], Volker Meden[2], and Herbert Schoeller[1] — [1]Institut für Theoretische Physik A, RWTH Aachen, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Germany

We extend the functional renormalization group to the treatment of fermionic quantum systems within Keldysh formalism, providing a unified approach to equilibrium and nonequilibrium situations. To this end we introduce an imaginary frequency cut-off to the relevant fermi functions. In case of nonequilibrium, the flow parameter is furnished with additional real components corresponding to the different chemical potentials involved. Applying our method to nonlinear transport through an interacting quantum wire with two contact barriers, we find that nonequilibrium induces a change of the scaling exponents.

TT 5.11 Mon 17:15 H18

Konkurrenz von Supraleitung und Ladungsordnung im zweidimensionalen Holstein-Modell — •Steffen Sykora, Arnd Hübsch und Klaus Becker — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Wir untersuchen die gegenseitige Beeinflussung von Supraleitung und Ladungsordnung im zweidimensionalen Holstein-Modell mit Hilfe einer neuartigen projektiven Renormierungsmethode (PRM). Ausgangspunkt ist ein effektiver Hamiltonoperator, der Ordnungsparameter für eine mögliche Ladungsordnung und für Supraleitung enthält. Durch schrittweises Eliminieren der Elektron-Phonon-Wechselwirkung werden die Ordnungsparameter und auch die elektronischen und phononischen Anregungsenergien renormiert. Es zeigt sich, dass bei hinreichend starker Kopplung ein Übergang von einer supraleitenden zu einer ladungsgeordneten Phase auftritt.

TT 5.12 Mon 17:30 H18

Constructing an exact CSL Hamiltonian — •Ronny Thomale[1], Darrell Schroeter[2], Eliot Kapit[3], and Martin Greiter[1] — [1]Institut für Theorie der Kondensierten Materie, D 76128 Karlsruhe — [2]Department of Physics, Occidental College, Los Angeles, CA — [3]Department of Physics, University of Chicago, Chicago, IL

We construct a Hamiltonian that singles out the chiral spin liquid on a square lattice with periodic boundary conditions as the exact and, apart from the two-fold topological degeneracy, unique ground state. The model provides a framework to study spinon excitations and the fractional statistics they obey in two dimensions, an issue of interest to the fields of topological quantum phases, high-T_c superconductivity, and quantum computing.

TT 5.13 Mon 17:45 H18

Magnetic phases of the t-J model at low doping — •Juergen Falb, Marcello Barbosa da Silva Neto, and Alejandro Muramatsu — Institut für Theoretische Physik III, Universitaet Stuttgart, D-70550 Stuttgart, Germany

Based on the method of Dirac quantization for constrained systems, we set up a path integral for the t-J model. Spin degrees of freedom result in a unimodular vector field while dopant holes are spin 1/2 fermions. The constraint against double occupancy can be solved exactly by choosing spin quantization axes of the dopant holes that follow the local direction of the spins. Assuming a staggered spin field leads to staggered spinless fermions. A gradient expansion of the t-t'-t"-J model in the low doping limit leads to a CP^1 model with a coupling to the gauge fields different from 1. The possible magnetic phases in parameter space will be discussed.