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.

TT 6: Nanoelectronics III - Molecular Electronics

Time: Monday 14:00–17:00 Location: H19

TT 6.1 Mon 14:00 H19

Electron transport through organic molecules and the influence of adsorbates on the conductance of aluminium contacts — •F. Pauly[1,2], S. Wohlthat[1,2], J. Viljas[1,2], M. Häfner[1,2], J.C. Cuevas[1,2,3], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe — [3]Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid

In the first part of this talk we will analyze the electrical conductance properties of a series of organic molecules. This series comprises molecules with different numbers of phenyl rings and modified side groups [1]. For these oligophenylenes we investigate the changes in the conductance due to both varied molecule lengths and different bonding positions within our newly developed DFT transport program [2,3]. As a second application of our method we study the transport properties of atomic-sized aluminium contacts in the presence of oxygen molecules, namely O, O_2, and O_3. In particlar we analyze the evolution of the transport characteristics for increasing electrode distances, simulating the opening of a break junction [4].