TT 55: Low-Dimensional Systems: 2D – Theory

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

TT 55.1 Wed 9:30 H 3010

Heat diffusion in the disordered Fermi and electron liquids: The role of inelastic processes — •Georg Schwiete[1] and Alexander Finkel'stein[2,3] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Texas A&M University, College Station, US — [3]The Weizmann Institute of Science, Rehovot, Israel

We study thermal transport in the disordered Fermi and electron liquids at low temperatures. Gravitational potentials are used as sources for finding the heat density and its correlation function. For a comprehensive study, we extend the renormalization group (RG) analysis developed for electric transport by including the gravitational potentials into the RG scheme. Our analysis reveals that for the disordered Fermi liquid the Wiedemann-Franz law remains valid even in the presence of quantum corrections caused by the interplay of diffusion modes and the electron-electron interaction. In the present scheme this fundamental relation is closely connected with a fixed point in the multiparametric RG flow of the gravitational potentials. For the disordered electron liquid we additionally analyze inelastic processes induced by the Coulomb interaction at sub-temperature energies. While the general form of the correlation function has to be compatible with the energy conservation, these inelastic processes are at the origin of logarithmic corrections violating the Wiedemann-Franz law. The evolution of various terms in the heat density-heat density correlation function therefore differs from that for densities of other conserved quantities, such as total number of particles or spin.

TT 55.2 Wed 9:45 H 3010

First-principles analysis of MoS_2/Ti_2C and MoS_2/Ti_2CY_2 (Y = F and OH) all-2D semiconductor/metal contacts — •Udo Schwingenschlögl[1], Li-Yong Gan[1], Yu-Jun Zhao[2], and Dan Huang[3] — [1]KAUST, Thuwal 23955-6900, Saudi Arabia — [2]South China University of Technology, Guangzhou 510640, People's Republic of China — [3]Hunan University of Arts and Science, Changde 415000, People's Republic of China

First-principles calculations are used to explore the geometry, bonding, and electronic properties of MoS_2/Ti_2C and MoS_2/Ti_2CY_2 (Y = F and OH) semiconductor/metal contacts. The structure of the interfaces is determined. Strong chemical bonds formed at the MoS_2/Ti_2C interface result in additional states next to the Fermi level, which extend over the three atomic layers of MoS_2 and induce a metallic character. The interaction in MoS_2/Ti_2CY_2, on the other hand, is weak and not sensitive to the specific geometry, and the semiconducting nature thus is preserved. The energy level alignment implies weak and strong n-type doping of MoS_2 in MoS_2/Ti_2CF_2 and $MoS_2/Ti_2C(OH)_2$, respectively. The corresponding n-type Schottky barrier heights are 0.85 and 0.26 eV. We show that the MoS_2/Ti_2CF_2 interface is close to the Schottky limit. At the $MoS_2/Ti_2C(OH)_2$ interface, we find that a strong dipole due to charge rearrangement induces the Schottky barrier. The present interfaces are well suited for application in all-two-dimensional devices.

[1] Phys. Rev. B 87, 245307 (2013).

TT 55.3 Wed 10:00 H 3010

Phase diagram of an extended quantum dimer model on the hexagonal lattice — Thiago Milanetto Schlittler[1], •Thomas Barthel[2], Grégoire Misguich[3], Julien Vidal[1], and Rémy Mosseri[1] — [1]LPTMC, Université Paris-6 — [2]LPTMS, Université Paris-Sud — [3]IPhT, CEA Saclay

We introduce a generalized quantum dimer model on the hexagonal lattice. In addition to the standard Rokhsar-Kivelson Hamiltonian, it contains a competing potential term. The phase diagram is studied by means of quantum Monte-Carlo simulations, variational ansätze and perturbation theory. The model displays a rich phase diagram and, in particular, provides a microscopic realization for the Cantor deconfinement scenario – a cascade of phases with varying flux.

TT 55.4 Wed 10:15 H 3010

The spectra of integrable staggered $sl(2|1)$ network models — •Andreas Klümper[1] and Michael Brockmann[2] — [1]Universität Wuppertal, Theoretische Physik, Gauss-Strasse 20, 42119 Wuppertal — [2]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1090 GL Amsterdam

We investigate the spectra of transfer matrices of integrable Chalker-Coddington like network models with $sl(2|1)$ symmetry and staggered $3-\bar{3}$ representations. Related to these network models are integrable superspin chains. The research on these models is motivated in general by the spin quantum Hall effect.

There are two kinds of integrable staggered $sl(2|1)$ models : (i) a rather well understood system based on the Temperley-Lieb algebra, (ii) a system based on the Hecke algebra and introduced by R. M. Gade in 1998. The latter model satisfies nested Bethe ansatz equations and was investigated extensively and particularly numerically by Essler, Frahm, Saleur in 2005.

We aim at an analytical treatment of the nested Bethe ansatz equations and derive a closed finite set of non-linear integral equations. These equations are well-posed and valid for any system size as well as for the largest and next-largest eigenvalues of the transfer matrix. The numerical treatment is delicate as straight forward iterations do not converge. However, the equations allow for analytical calculations of conformal properties.

TT 55.5 Wed 10:30 H 3010

Non-Fermi-liquid behavior in a 2D transport model with boson affected hopping — •Dai-Ning Cho and Steffen Sykora — Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

Charge transport mediated by excitations in a correlated background medium is a general phenomenon in condensed matter physics. A simplified model of spinless fermions which are dynamically coupled to a system of bosonic degrees of freedom has been introduced by Edwards. In our work we study the half-filled Edwards model in 2D by use of the projective renormalization method (PRM), which transforms the model Hamiltonian to a solvable effective Hamiltonian involving renormalized bosons and fermions. We find significant reduction of the one-particle spectral weight close to the charge density wave (CDW) phase, which is well-known from the 1D case. Inside this non-Fermi-liquid region an unconventional superconducting phase with s± pairing symmetry is also found. Thereby, the pairing is stabilized by strong renormalization of the charge carrier transport. We present results for the renormalized dispersions and one-particle spectral functions.

TT 55.6 Wed 10:45 H 3010

Two–parameter scaling theory of transport near a spectral node — •Andreas Sinner — Universität Augsburg

We investigate the finite–size scaling behavior of the conductivity in a two–dimensional Dirac electron gas within a chiral sigma model. Based on the fact that the conductivity is a function of system size times scattering rate, we obtain a two–parameter scaling flow toward a finite fixed point. The latter is the minimal conductivity of the infinite system. Depending on boundary conditions, we also observe unstable fixed points with conductivities much larger than the experimentally observed values, which may account for results found in some numerical simulations. By including a spectral gap we extend our scaling approach to describe a metal–insulator transition.

TT 55.7 Wed 11:00 H 3010

Composite boson mean-field theory for strongly correlated systems — •Daniel Huerga[1,2] and Jorge Dukelsky[1] — [1]Instituto de Estructura de la Materia, C.S.I.C., Madrid, Spain — [2]Institut fur Theoretische Physik III, University of Stuttgart, Stuttgart, Germany

We present a method applicable to spin and bosonic model Hamiltonians of strongly correlated systems. The method is based on the identification of clusters of the original spin and bosonic degrees of freedom as the building blocks which capture the essential quantum correlations to describe the phases emerging in the model. We present a canonical mapping which relates the original spin and bosonic operators to a new set of composite boson (CB) operators that describe the quantum states of the cluster. As the mapping is canonical, we can rewrite the original Hamiltonian in terms of CBs and approach it by standard many-body techniques, with the advantage that short-range correlations are computed exactly from the onset.

A simple Gutzwiller wave function of CBs allows us to uncover the phase diagram of two-dimensional frustrated models such as a model

of spins with ring-exchange interaction, or a system of bosons in the presence of artificial magnetic fields. A Bogoliubov approach to the CB quantum fluctuations allows us to accurately describe the recently measured Higgs and Goldstone excitation modes of a system of cold atoms loaded in a two-dimensional optical lattice. The algebraic framework set by the mapping allows for further extensions of the method.

15 min. break.

TT 55.8 Wed 11:30 H 3010

Dimensional-Crossover-Driven Mott Transition: A Variational Plaquette Study — •Benjamin Lenz[1], Salvatore R. Manmana[1], Marcin Raczkowski[2], Thomas Pruschke[1], and Fakher F. Assaad[3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37073 Göttingen, Germany — [2]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently the metal-insulator Mott transition has been studied for a quasi-two-dimensional frustrated Hubbard model with next-nearest-neighbor hopping [Raczkowski, Assaad, PRL 109 (2012)]. Following up on this CDMFT study at finite temperatures, we analyze the crossover-driven Mott transition at zero temperature by means of variational cluster approximation (VCA). Here, we focus on coupling bath sites to the correlated sites of the reference system to carefully investigate the order of the transition. The effects of this extension on the phase diagram are studied and the insulator-metal transition is found to be of first order for large and intermediate inter-chain coupling strengths. This allows us to pursue the transition to small coupling strengths where remnant 1D effects like Umklapp scattering are expected to become important.

TT 55.9 Wed 11:45 H 3010

Ground state phase diagram of the bilayer square lattice at half filling — •Michael Golor[1], Timo Reckling[1,2], Laura Classen[2], Michael M. Scherer[2], and Stefan Wessel[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen — [2]Institut für Theoretische Physik, Universität Heidelberg

We employ a combination of functional renormalization group calculations and projective determinantal quantum Monte Carlo simulations to examine the Hubbard model on the square lattice bilayer at half filling. We obtain a comprehensive account on the ground state phase diagram with respect to the extent of the system's metallic and (antiferromagnetically ordered) Mott-insulating as well as band-insulating regions. We discuss the difficulty in exploring the weak-coupling regime with quantum Monte Carlo and identify the non-interacting system's Fermi surface as its origin.

TT 55.10 Wed 12:00 H 3010

FRG study of the Hubbard model on the bilayer square lattice — •Timo Reckling[1,2], Michael M. Scherer[2], and Laura Classen[2] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen University, 52056 Aachen, Germany — [2]Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany

We study Hubbard model on the bilayer square lattice at and away from half filling as a model unifying various aspects of the physics of two-dimensional correlated fermions. We discuss on-site and interlayer density-density interactions by means of an unbiased functional renormalization group approach. This allows us to deduce the emergent order without previous assumptions about its nature and symmetry and can therefore be used to establish the appearance of spin and charge density wave ordering, as well as two types of superconductive instabilities away from half filling.

TT 55.11 Wed 12:15 H 3010

Mott physics in the half-filled Hubbard model on a family of vortex-full square lattices — •Dominik Ixert[1], Fakher Assaad[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik 1, TU Dortmund, D-44221 Dortmund, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the half-filled Hubbard model on a one-parameter family of vortex-full square lattices ranging from the isotropic case to weakly coupled Hubbard dimers. The ground-state phase diagram consists of four phases: A semimetal and a band insulator which are connected to the weak-coupling limit, and a magnetically ordered Néel phase and a valence bond solid (VBS) which are linked to the strong-coupling Mott limit. The phase diagram is obtained by quantum Monte Carlo (QMC) and continuous unitary transformations (CUTs). The CUT is performed in a two-step process: Nonperturbative graph-based CUTs are used in the Mott insulating phase to integrate out charge fluctuations. The resulting effective spin model is tackled by perturbative CUTs about the isolated dimer limit yielding the breakdown of the VBS by triplon condensation. We find three scenarios when varying the interaction for a fixed anisotropy of hopping amplitudes: (i) one direct phase transition from Néel to semimetal, (ii) two phase transitions VBS to Néel and Néel to semimetal, or (iii) a smooth crossover from VBS to the band insulator. Our results are consistent with the absence of spin-liquid phases in the whole phase diagram.

[1] D. Ixert, F. F. Assaad, and K. P. Schmidt,
PRB **90**, 195133 (2014).

TT 55.12 Wed 12:30 H 3010

Entanglement properties of one- and two-dimensional quantum Ising and XXZ spin-1/2 models — •Briiissuurs Braiorr-Orrs[1], Michael Weyrauch[1], and Mykhailo Rakov[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany — [2]Kyiv National Taras Shevchenko University, 64/13 Volodymyrska st., 01601 Kyiv, Ukraine

Entanglement properties of 1D (spin rings) and 2D (on a square lattice) spin-1/2 quantum Ising and XXZ models are investigated. Numerical methods (MPS in 1D and TERG and CTMRG in 2D) with imaginary-time evolution are used to model the ground state of the studied models. Different entanglement measures, such as one-site entanglement entropy, one-tangle, concurrence of formation and assistance, negativity and entanglement per bond are calculated and their 'characterizing power' to determine the phase transition is compared. A special emphasis is made on the connection of the symmetry properties of the ground states and the entanglement properties of the states.

TT 55.13 Wed 12:45 H 3010

Lattice Conformal Blocks and Topological Phases — •Roberto Bondesan — THP, Cologne, Germany

Conformal blocks are holomorphic building blocks of correlation functions of 2D conformal field theories. The Moore-Read approach relates these objects to the ground state wave functions in the fractional quantum Hall effect. In this talk I will present a lattice perspective on this approach. In particular I will discuss how to use vertex models of statistical mechanics to achieve a tensor network states description of strongly interacting chiral topological phases.