TT 38: Correlated Electrons: Low-dimensional Systems - Models 1

Time: Thursday 9:30–13:00 Location: HSZ 301

TT 38.1 Thu 9:30 HSZ 301

Thermally Activated Peierls Dimerization in Ferromagnetic Spin Chains — •Jesko Sirker[1], Alexander Herzog[1], Andrzej M. Oles[1,2], and Peter Horsch[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland

We demonstrate that a Peierls dimerization can occur in ferromagnetic spin chains activated by thermal fluctuations [1]. The dimer order parameter and entanglement measures are studied as functions of the modulation of the magnetic exchange interaction and temperature, using a spin-wave theory and the density-matrix renormalization group. We discuss the case where a periodic modulation is caused by spin-phonon coupling and the case where electronic states effectively induce such a modulation. The importance of the latter for a number of transition metal oxides is highlighted.

[1] Phys. Rev. Lett. 101, 157204 (2008)

TT 38.2 Thu 9:45 HSZ 301

A real-time study of diffusive and ballistic transport in spin-1/2 chains using the adaptive time-dependent DMRG method — •Stephan Langer[1], Fabian Heidrich-Meisner[1], Jochen Gemmer[2], Ian McCulloch[3], and Ulrich Schollwoeck[1] — [1]Institut für Theoretische Physik C, RWTH Aachen University, Germany — [2]Institut für Theoretische Physik, Universität Osnabrück, Germany — [3]The University of Queensland, Brisbane, QLD 4072, Australia

We study spin transport and dynamics in one-dimensional quantum spin-1/2 systems at zero temperature. Using the time-dependent adaptive Density Matrix Renormalization Group (DMRG) method, we follow the time evolution of the magnetization starting from inhomogeneous initial states. Our goal is to distinguish between ballistic and diffusive transport. This is achieved by looking at the long-time behavior of the spatial variance of the magnetization, where, for instance, a quadratic increase in time is indicative of ballistic transport. Applying this to the spin-1/2 XXZ chain, we confirm the established picture of ballistic transport in the critical phase. In the massive phase, strong perturbations are required to drive the dynamics, which show diffusive behavior. Then we turn to two non-integrable models, the two-leg spin-ladder and the frustrated spin chain, for which we find diffusive behavior in all massive phases, but ballistic transport in the gapless phase of the frustrated chain. Since our analysis does not rely on linear-response theory, we can explore the full range of perturbation strength, and, in particular, out-of-equilibrium physics.

TT 38.3 Thu 10:00 HSZ 301

Ground State Properties of the 1D t-J Model with Density Matrix Renormalization Group — •Alexander Moreno[1], Alejandro Muramatsu[1], Salvatore Manmana[2], and Reinhard Noak[3] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institute of Theoretical Physics, Condensed Matter Theory, Lausanne, Switzerland — [3]Philipps Universität Marburg, Germany

We study the ground state properties of the one-dimensional t-J model by using the Density Matrix Renormalization Group (DMRG). On the basis of spin-spin, density-density, and pairing correlation functions we study the possible phases, like Luttinger liquid, superconducting, spin-gap and phase separated regions and clarify the contradictions between different studies[1-3].

[1] M. Ogata, M. U. Luchini, S. Sorella, and F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).

[2] C. S. Hellberg and E. J. Mele, Phys. Rev. B. **48**, 1 (1993).

[3]M. Nakamura, K. Nomura, and Kitazawa, Phys. Rev. Lett. **79**, 3214 (1997).

TT 38.4 Thu 10:15 HSZ 301

Local density of states of 1D Mott insulators and CDW states with a boundary — •Dirk Schuricht[1], Fabian H. L. Essler[1], Akbar Jaefari[2], and Eduardo Fradkin[2] — [1]The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK — [2]Department of Physics, University of Illinois at Urbana-Champaign, USA

We determine the local density of states (LDOS) of one-dimensional incommensurate charge density wave (CDW) states in the presence of a strong impurity potential, which is modeled by a boundary[1]. We find that the CDW gets pinned at the impurity, which results in a singularity in the Fourier transform of the LDOS at momentum $2k_F$. At energies above the spin gap we observe dispersing features associated with the spin and charge degrees of freedom respectively. In the presence of an impurity magnetic field we observe the formation of a bound state localized at the impurity. All of our results carry over to the case of 1D Mott insulators by exchanging the roles of spin and charge degrees of freedom. We discuss the implications of our result for scanning tunneling microscopy experiments on spin-gap systems such as two-leg ladder cuprates.

[1] D. Schuricht, F. H. L. Essler, A. Jeafari, and E. Fradkin, Phys. Rev. Lett. **101**, 086403 (2008).

15 min. break

TT 38.5 Thu 10:45 HSZ 301

Temperature dependent optical conductivity in frustrated chain cuprates near the ferromagnetic-spiral critical point — •Stefan-Ludwig Drechsler[1], Jiri Malek[1,2], Satoshi Nishimoto[1], Helge Rosner[3], Ulrike Nitzsche[1], Roman Kuzian[1,4], and Helmut Eschrig[1] — [1]IFW-Dresden, Germany — [2]Inst. Phys. ASCR, Czech Republic — [3]MPI-CPfS Dresden, Germany — [4]Inst. of Mat. Sci. Problems, Kiev, Ukraine

The optical conductivity $\sigma(\omega)$ [1] and the loss function of EELS are calculated at finite temperature T for CuO_2 chain clusters within a five-band O2pCu3d-Hubbard model using exact diagonalizations and the DMRG-technique. Data at $T = 300$ K for Li_2CuO_2 are reanalyzed within this approach. The relative weights of Zhang-Rice singlet and triplet charge excitations near 2.7 and 4 eV, respectively, depend strongly on T, and a rather dramatic dependence of $\sigma(\omega)$ on the ratio of the 1^{st} to 2^{nd} neighbor exchange integrals is predicted. From our results information about exchange interactions for frustrated edge-shared cuprates can be obtained from T-dependent optical spectra. The obtained exchange integrals compare well with results of LDA+U calculations. Our results are also relevant for magnetically weakly coupled unfrustrated wide-gap insulators in general.

[1] J. Málek *et al.*, PRB **78** 060508(R) (2008).

TT 38.6 Thu 11:00 HSZ 301

Density Matrix Renormalization Group in the Heisenberg picture — •Michael Hartmann[1,2,3], Javier Prior[2,3], Stephen Clark[4], and Martin Plenio[2,3] — [1]Technische Universität München, Physik Department, 85748 Garching, Germany — [2]Institute for Mathematical Sciences, Imperial College London, United Kingdom — [3]QOLS Blackett Laboratory, Imperial College London, United Kingdom — [4]Clarendon Laboratory, University of Oxford, United Kingdom

In some cases the state of a quantum system with a large number of subsystems can be approximated efficiently by the density-matrix renormalization group (DMRG), which makes use of redundancies in the description of the state. Here we show that the achievable efficiency can be much better when performing DMRG in the Heisenberg picture (H-DMRG), as only the observable of interest but not the entire state is considered. In some non-trivial cases, H-DMRG can even be exact for finite bond dimensions.

TT 38.7 Thu 11:15 HSZ 301

Disorder-induced stabilization of pseudogap in the electronic spectral density of the two-dimensional Anderson-Hubbard model — •Prabuddha Chakraborty[1,2], Simone Chiesa[2], Richard Scalettar[2], and Warren Pickett[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]University of California, Davis, CA 95616, USA

In this talk, we present the observation of a pseudogap in the electronic spectral density in the two-dimensional Anderson-Hubbard model on a square lattice. We show the behaviour of the pseudogap when the electronic density, the disorder strength and the Hubbard correlation are varied. In particular, we show that the disorder stabilizes the pseudogap across a wide range of electron densities and correlation strengths. The numerical methods we use are exact diagonalization and Determinant quantum Monte Carlo. We also demonstrate that our observations are completely consistent with recent experimental results on disordered high temperature Cuprate superconductors.

TT 38.8 Thu 11:30 HSZ 301

Correlation and impurities in carbon nanotubes: A DMRG approach — •Alexander Struck[1], Sebastian A. Reyes[1,2], and Sebastian Eggert[1] — [1]Department of Physics and Reserch Center OPTIMAS, Univ. Kaiserslautern, Kaiserslautern, Germany — [2]Departamento de Física Pontificia Universidad Católica de Chile, Santiago de Chile, Chile

Carbon nanotubes (CNTs) are well suited to study strong electronic correlations in quasi-one-dimensional systems experimentally and theoretically. Of particular interest is the interplay of interactions between the conducting electrons and impurities in the nanotube. Impurities include the boundaries of short tubes as well as structural imperfections such as the Stone-Wales lattice distortion. Interactions can lead to different phases of the electron liquid, depending on their range and strength, and can produce quasi-localized ground states of e.g. the Mott insulator type or a charge density wave. In this talk, we introduce effective lattice models to describe armchair and zigzag nanotubes with different types of impurities at low energies. The models are quasi-one dimensional and allow straightforward use in 1D techniques like the density-matrix renormalization group (DMRG). We discuss impurity effects in armchair CNTs and the influence of electron-electron interaction using DMRG calculations.

15 min. break.

TT 38.9 Thu 12:00 HSZ 301

Quantum oscillations from Fermi arcs — •Heidrun Weber[1,2] and Marcel Franz[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T 1Z1

When a metal is subjected to a strong magnetic field B, nearly all measurable quantities exhibit oscillations periodic in $1/B$. Such strong quantum oscillations represent a canonical probe of the Fermi surface, a defining property of a metal. We will discuss a new mechanism for quantum oscillations which requires only finite segments of a Fermi surface to exist, terminated by a pairing gap. We consider a real-space version of a BCS-like model Hamiltonian, whose hopping amplitude includes the usual Peierls factor and whose superconducting order parameter takes into account the existence of an Abrikosov vortex lattice. By a fully quantum mechanical treatment of the model we show that the density of states at the Fermi level exhibits an oscillatory behavior. Our results reconcile the recent breakthrough experiments showing quantum oscillations in a cuprate superconductor $YBa_2Cu_3O_{6.51}$, with a well-established result of many angle resolved photoemission (ARPES) studies which consistently indicate Fermi arcs - truncated segments of a Fermi surface - in the normal state of cuprates.

TT 38.10 Thu 12:15 HSZ 301

Momentum dependence of the spin-susceptibility in two dimensions: nonanalytic corrections in the Cooper channel — Stefano Chesi[1], •Robert Zak[1], Pascal Simon[1,2,3], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Laboratoire de Physique et Modelisation des Milieux Condenses, CNRS and Universite Joseph Fourier, BP 166, 38042 Grenoble, France — [3]Laboratoire de Physique des Solides, CNRS UMR-8502 Universite Paris Sud, 91405 Orsay Cedex, France

We consider the effect of rescattering of pairs of quasiparticles in the Cooper channel resulting in the strong renormalization of second order corrections to the spin susceptibility in a two-dimensional electron system. We use the Fourier expansion of the scattering potential in the vicinity of the Fermi surface to find that each harmonic becomes renormalized independently. Since some of those harmonics are negative, the slope of the spin susceptibility is bound to be negative at small momenta, in contrast to the lowest order perturbation theory result, which predicts a positive slope. We present in detail an effective method to calculate diagrammatically corrections to the spin susceptibility to infinite order.

TT 38.11 Thu 12:30 HSZ 301

Quantum Hall ferromagnetic states and spin-orbit interactions in the fractional regime — •Stefano Chesi and Daniel Loss — Department of Physics, University of Basel, CH-4056 Basel, Switzerland

The competition between the Zeeman energy and the Rashba and Dresselhaus spin-orbit couplings is studied for fractional quantum Hall states. A transition of the spin-polarization direction is predicted to occur at a small value of the Zeeman energy. For a given fractional state, the phenomenon can be accurately described in the perturbative limit of high magnetic fields. We consider the Laughlin wavefunctions and the Pfaffian state as specific examples and show that this phenomenon allows one to obtain valuable information about the nature of the correlated ground-state, and in particular about its pair-correlation function. We discuss indications of non-analytic features around the fractional states and include significant effects of the nuclear bath polarization in the relevant regime of temperatures and magnetic fields.

TT 38.12 Thu 12:45 HSZ 301

Weak-coupling CT-QMC and it's application to the Peierls transition in the quarter filled Holstein model. — •Fakher F. Assaad and Thomas C. Lang — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

After briefly reviewing the weak coupling CT-QMC approach we show how to generalize it to include phonon degrees of freedom[1]. The efficiency of this approach is tested in the framework of the one-dimensional Holstein model at quarter-band filling. We show that for adiabatic phonons, a phase transitions from a Luttinger to Luther Emery liquid is triggered by the electron phonon coupling. The Luther-Emery phase is characterized by dominant $2k_f$ charge correlations[2]. Those results stem from a detailed study of the temperature dependence of the single particle spectral function, the optical conductivity, as well as charge and spin dynamical structure factors.

[1] F.F. Assaad and T. Lang, Phys. Rev. B 76, 035116 (2007)
[2] F.F. Assaad, Phys. Rev. B 78, 155124 (2008).