TT 24: Low-Dimensional Systems: 1D - Theory

Time: Tuesday 9:30–13:00 Location: HSZ 204

TT 24.1 Tue 9:30 HSZ 204

From Luttinger liquids to Luttinger droplets using higher-order bosonization identities — Sebastian Huber[1] and •Marcus Kollar[2] — [1]Theoretical Solid State Physics, Ludwig-Maximilians-University, Munich, Germany — [2]Theoretical Physics III, University of Augsburg, Germany

The exactly solvable Tomonaga-Luttinger model describes two flavors of interacting electrons with linear dispersion in one dimension, but some of its properties are characteristic for a wider class of one-dimensional systems according to the Luttinger liquid paradigm [1]. The exact solution for linear dispersion is based on bosonization, which represents fermionic particle-hole excitations in terms of canonical bosons and maps the Tomonaga-Luttinger Hamiltonian onto a free bosonic theory. We use the framework of constructive finite-size bosonization [2] to derive explicit bosonic representations of general bilinear fermion operators including arbitrary dispersion terms. As an application, Luttinger 'droplets' with position-dependent parameters are investigated.

[1] F. D. M. Haldane, J. Phys. C: Solid State Phys. **14**, 2585 (1981).
[2] J. von Delft and H. Schoeller, Ann. Phys. **7**, 225 (1998).

TT 24.2 Tue 9:45 HSZ 204

Interplay of Site and Bond Electron-Phonon Coupling in One Dimension — •Martin Hohenadler — University of Würzburg, Germany

The interplay of bond and charge correlations is studied in a one-dimensional model with both Holstein and Su-Schrieffer-Heeger (SSH) couplings to quantum phonons. The problem is solved exactly by quantum Monte Carlo simulations. If one of the couplings dominates, the ground state is a Peierls insulator with long-range bond or charge order. At weak coupling, the results suggest a spin-gapped and repulsive metallic phase arising from the competing order parameters and lattice fluctuations. Such a phase is absent from the pure SSH model even for quantum phonons. At strong coupling, evidence for a continuous transition between the two Peierls states is presented.

TT 24.3 Tue 10:00 HSZ 204

Effective narrow ladder model for metallic atomic nanowires on semiconducting substrates — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover, Germany — [2]Universität Würzburg, Germany

We perform a systematic construction of an effective quasi-one-dimensional ladder model starting from a 3D wire-substrate model. This construction depends on an exact mapping of the full 3D wire-substrate model onto a 2D ladder model, followed by a truncation to a ladder with a limited number of legs to approximate the full wire-substrate model. For insulating (but not for metallic) substrates, ladders with at least three legs are found to give a good qualitative approximation. We discuss the influence of wire-substrate hybridization on a wire described by the 1D Hubbard model. We observe several phases such as Mott insulator, Luttinger liquid, band insulator, and Fermi liquid. The effective ladder model is suggested to describe correlation effects in systems of metallic atomic nanowires deposited on semiconducting substrates.

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TT 24.4 Tue 10:15 HSZ 204

Filling-dependent doublon dynamics in the one-dimensional Hubbard model — •Roman Rausch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg

The fate of a local two-hole doublon excitation in the one-dimensional Fermi-Hubbard model is systematically studied in the entire filling range using the density-matrix renormalization group (DMRG) and the Bethe ansatz. For strong Hubbard interaction U, two holes at the same site form a compound object whose decay is impeded by the lack of phase space. Still, a partial decay is possible on an extremely short time scale where phase-space arguments do not yet apply. We argue that the initial decay and the resulting intermediate state are relevant for experiments performed with ultracold atoms loaded into an optical lattice as well as for CVV Auger-electron spectroscopy. The discussion comprises the mixed ballistic-diffusive real-time propagation of the doublon through the lattice, its partial decay on the short time scale as a function of filling and interaction strength, as well as the analysis of the decay products, which are metastable on the intermediate time scale. The ambivalent role of singly occupied sites is key to understanding the doublon physics: For high fillings, ground-state configurations with single occupancies are recognized to strongly relax the kinematic constraints and to open up decay channels. For fillings close to half filling, however, their presence actually blocks the doublon decay. Finally, we demonstrate that the decay products as well as the doublon propagation should rather be understood in terms of Bethe ansatz eigenstates (spinons and holons).

TT 24.5 Tue 10:30 HSZ 204

Thermal Intra-Band Magnon Scattering in the Haldane Spin-One Chain — •Jonas Becker[1], Thomas Köhler[2], Alexander C. Tiegel[2], Salvatore R. Manmana[2], Andreas Honecker[3], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, F-95302 Cergy-Pontoise Cedex, France

We present results from a thorough evaluation of the dynamical spin structure factor of the Haldane chain at finite temperatures, based on a combination of exact numerical diagonalization, finite-temperature density-matrix renormalization group calculations and quantum Monte Carlo simulations. Simulations performed on finite open chains exhibit a sub-gap band in the thermal spin spectral function, indicative of the localized edge-modes in the Haldane chain's ground state. Furthermore, we observe the thermal activation of a distinct low-energy contribution to the spin spectral function with an enhanced spectral weight at low momenta that results from intra-band magnon scattering due to the thermal population of the single-magnon mode. These findings are discussed with respect to previous results on the spin spectral function and possible future studies on Haldane spin chain compounds based on inelastic neutron scattering experiments.

TT 24.6 Tue 10:45 HSZ 204

Photoexcitations in a 1D manganite model: From quasiclassical light absorption to quasiparticle relaxations — •Thomas Köhler[1], Sangeeta Rajpurohit[2], Ole Schumann[1], Fabian Biebl[1], Mohsen Sotoudeh[2], Stephan Kramer[3,1], Peter Blöchl[2,1], Stefan Kehrein[1], and Salvatore Manmana[1] — [1]Inst. f. Theo. Phys., U. Göttingen — [2]Inst. f. Theo. Phys., TU Clausthal — [3]Fraunhofer ITWM Kaiserslautern

We investigate the dynamics of 1D correlated systems after photoexcitation by combining ab-initio methods, time-dependent matrix product states (MPS), linearized quantum Boltzmann equations (LBE), and molecular dynamics (MD) simulations. This leads to a description spanning a wide range of time scales from femto- up to nanoseconds. We consider manganite systems in the material class $Pr_{1-x}Ca_xMnO_3$ for which we derive 1D ab-initio model Hamiltonians. At half doping, we obtain a magnetic microstructure of alternating dimers from which we derive a 1D Hubbard-type model. The dynamics is analyzed concerning the formation and lifetime of such quasiparticles via a LBE. We find that the magnetic microstructure strongly enhances the lifetime of the excitations. In this way, our work constitutes a first step to building a unifying theoretical framework for the description of photoexcitations in strongly correlated materials over a wide range of time scales, capable of making predictions for ongoing experiments investigating pump-probe situations and unconventional photovoltaics.

Financial support by DFG CRC1073 (projects B03 and C03) is gratefully acknowledged.

15 min. break.

TT 24.7 Tue 11:15 HSZ 204

Scattering of an electronic wave packet by a one-dimensional electron-phonon-coupled structure — •Christoph Brockt and Eric Jeckelmann — Leibniz Universität Hannover, Germany

We investigate the scattering of an electronic wave packet by phonons within the one-dimensional Holstein model. The electron-phonon cou-

pling is confined in a small structure between two tight-binding leads. We observe permanent energy transfer from the electron to the phonon system, transient self-trapping of the electron in the electron-phonon coupled structure and transmission resonances, that depend on the adiabaticity ratio.

A recently developed TEBD algorithm [1], that uses optimal modes [2] for the bosonic degrees of freedom, was used for this study. Analytical results are provided for a single-site electron-phonon coupled structure and for limiting cases.

Support from the DFG through the Research Unit FOR 1807 is gratefully acknowledged.

[1] C. Brockt et al., PRB **92**, 241106 (2015)
[2] C. Zhang, E. Jeckelmann, and S.R. White, PRL **80**, 2661 (1998)

TT 24.8 Tue 11:30 HSZ 204

DMRG method for the conductance of one-dimensional correlated systems — •Jan Bischoff — Leibniz Universität Hannover

We present an accurate and efficient procedure for computing the zero-temperature linear conductance of correlated one-dimensional systems using the density-matrix renormalization group (DMRG). Building on [1], we express the conductance within the linear response theory as the limits of dynamical correlation functions for finite systems. These correlation functions can be calculated with the dynamical DMRG algorithm. We have first studied non-interacting models to determine an appropriate scaling of frequency, system size, and spectral broadening by comparison with exact results. The method is demonstrated for interacting systems using the one-dimensional spinless fermion model. Our results for this lattice model agree with the field-theoretical predictions for the renormalization of the conductance in a pure Luttinger liquid as well as for the effects of an impurity in a Luttinger liquid [2]. We have found that this new approach is more efficient than a simulation of the nonequilibrium transport [3] in the linear response regime. We have also tested our approach on the Hubbard model and we plan to extend it to the problem of an interacting quantum wire connected to two broad and weakly-interacting leads.

[1] D. Bohr, P. Schmitteckert, and P.W. Wölfle, Europhys. Lett., 73, 246 (2006)
[2] C.L. Kane and M.P.A. Fisher, PRB 46, 15233 (1992)
[3] M. Einhellinger, A. Cojuhovschi, and E. Jeckelmann, Phys. Rev. B 85, 235141 (2012)

TT 24.9 Tue 11:45 HSZ 204

Thermal transport in Kitaev–Heisenberg ladders — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study the finite temperature thermal transport properties of a Kitaev–Heisenberg two leg ladder, as a minimum quasi one–dimensional representative of the corresponding two–dimensional model on a Honeycomb lattice. In the absence of Heisenberg interactions, we find that the pure Kitaev ladder is an ideal heat insulator at all temperatures. This is a direct consequence of the fractionalization of spin degrees of freedom which acts as a thermally activated disorder leading to localization. On the other hand, Heisenberg interactions restore DC conductivity, driving the system into a conducting state where transport is mediated by triplon excitations. We primarily rely on numerical techniques, namely exact diagonalization and the quantum typicality.

TT 24.10 Tue 12:00 HSZ 204

Nonequilibrium energy dynamics in the spin-$\frac{1}{2}$ XXZ chain — •Younes Javanmard[1], Soumya Bera[1], and Jens H. Bardarson[1,2] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Department of Theoretical Physics, KTH Royal Institute of Technology, Stockholm, Sweden

We study the real-time dynamics of spin-$\frac{1}{2}$ XXZ chains out of thermal equilibrium using time evolving block decimation algorithms. We consider both integrable and non-integrable systems at and away from half-filling, focussing on the analysis of the time-dependent behavior of the local energy density profile and current.

TT 24.11 Tue 12:15 HSZ 204

Microscopic Analysis of 1D Lattice Models for Synthetic Helical Liquids — •Lorenzo Pastori and Jan Carl Budich — Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

Helical liquids exhibiting spin-momentum locking are known to appear at the edges of 2D time-reversal invariant topological insulators. Here we investigate various Fermi-Hubbard models for 1D lattice systems where synthetic helical liquids can be realised. In such models the low-energy physics around the Fermi points can be described in terms of emergent helical Luttinger liquid behaviour. Using density matrix renormalisation group techniques, we quantitatively analyse the presence of spin-momentum locking, i.e. the key hallmark of helical liquids, by studying ground state spin-spin correlation functions.

TT 24.12 Tue 12:30 HSZ 204

Role of Cu 4*d* and O 3*p* orbitals in the many-body wavefunction of corner-sharing cuprates — •Nikolay A. Bogdanov[1], Giovanni Li Manni[1], Sandeep Sharma[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University Chemical Laboratory, Cambridge, U.K.

Electronic and magnetic properties of one- and two-dimensional cuprates have been investigated for several decades but are still not fully understood. We study the electronic structure of the undoped Sr_2CuO_3 and La_2CuO_4 corner-sharing cuprates with state-of-the-art wavefunction-based *ab initio* calculations. We find that in order to obtain reasonable agreement with the experimentally observed large magnetic exchange couplings for these compounds, it is necessary to go beyond multiband models containing only Cu 3*d* and O 2*p* bands. To capture the orbital breathing effects it is necessary to extend the model space with diffuse Cu 4*d* and O 3*p* orbitals. For a Cu-O-Cu unit this leads to a problem of 24 electrons in 26 orbitals that can't be solved with conventional methods. In our study we employ full configuration interaction quantum Monte Carlo (FCIQMC) and density matrix renormalization group (DMRG) techniques to tackle this problem.

TT 24.13 Tue 12:45 HSZ 204

Topological mirror insulators in one dimension — •Alexander Lau[1], Jeroen van den Brink[1,2], and Carmine Ortix[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany — [3]Institute for Theoretical Physics, Utrecht University, Netherlands

In the context of novel topological states of matter protected by crystalline symmetries, we show that the presence of mirror symmetry leads to a new class of time-reversal invariant topological insulators in one dimension. These *topological mirror insulators* are characterized by a nontrivial $\mathbb{Z}_2$ topological invariant defined in terms of the partial polarization, which we show to be quantized in the presence of a 1D mirror point. Their hallmark is an odd number of electronic integer end charges at the mirror-symmetric boundaries of the system.

We check our findings against spin-orbit coupled Aubry-André-Harper models which realize this novel topological state of matter. The presented models could be realized, for instance, in cold-atomic Fermi gases loaded in periodic optical lattices.