TT 8: CE: (General) Theory

Time: Monday 14:00–17:45 Location: H21

TT 8.1 Mon 14:00 H21

Quantum Simulations of Exotic Spin Models — •Hendrik Weimer[1], Markus Müller[2], Igor Lesanovsky[3], Peter Zoller[2], and Hans Peter Büchler[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart — [2]Institut für Theoretische Physik, Universität Innsbruck, und Institut für Quantenoptik und Quanteninformation der Österreichischen Akademie der Wissenschaften, Innsbruck — [3]School of Physics and Astronomy, The University of Nottingham

A universal quantum simulator is a controlled quantum device which efficiently reproduces the dynamics of any other many particle quantum system with short range interactions. Based on a recent proposal for a many-body with cold Rydberg atoms [1], we present an implementation of a digital quantum simulator [2]. Special focus is on the efficient simulation of Hamiltonians with local many-body interactions, including exotic spin models such as Kitaev's toric code, string nets, and lattice gauge theories. In addition, we show that the formalism also provides the simulation of dissipative terms taking the Lindblad form with many-body jump operators. These dissipative terms allow for the efficient ground state cooling and state preparation.

[1] M. Müller et al., Phys. Rev. Lett. **102**, 170502 (2009).
[2] H. Weimer et al., arXiv:0907.1657 (2009).

TT 8.2 Mon 14:15 H21

A model of charge fractionalization on the kagome lattice — •Aroon O'Brien[1], Frank Pollmann[2], Nic Shannon[3], and Peter Fulde[1,4] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [2]University of California, Berkeley, CA94720, USA — [3]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, BS8-1TL, UK — [4]Asia Pacific Center for Theoretical Physics, Pohang, Korea

Geometrically frustrated models exhibit many fascinating physical properties, one of which is the possible existence of fractionally charged excitations [1]. Such excitations may arise here as a consequence of the frustrated electronic interactions [2]. We have investigated a model of spinless fermions on the 2D kagome lattice, for which fractionally charged excitations occur in the limit of strong correlations at 1/3 filling. Here we present results for the dynamical properties of the fractional charges, as revealed by numerically calculated spectral functions. Particular focus is given to the signatures of fractional confined collective excitations observed in these spectra [3]. Recently a scheme for a quantum simulation of this model using cold atoms was proposed; we relate this to numerically calculated quantities that we argue may be measurable in optical lattice experiments [4].

[1] P. Fulde, K. Penc, N. Shannon, Ann. Phys., **11**, 892 (2002).
[2] F. Pollmann and P. Fulde, Europhys. Lett., **75**, 133 (2006).
[3] A. O'Brien, F. Pollmann and P. Fulde, to be submitted.
[4] J. Ruostekoski, Phys. Rev. Lett., **103**, 080406 (2009); J. Ruostekoski and N. Shannon, in preparation.

TT 8.3 Mon 14:30 H21

Groundstatable fermionic wavefunctions and their associated many-body Hamiltonians — •Daniel Charrier[1] and Claudio Chamon[2] — [1]Max Planck Institut für Physikkomplexer Systeme, Nöthnitzer Straße38, 01187 Dresden, Germany — [2]Physics Department, Boston University, Boston, MA

In the vast majority of many-body problems, it is the kinetic energy part of the Hamiltonian that is best known microscopically, and it is the detailed form of the interactions between the particles, the potential energy term, that is harder to determine from first principles. An example is the case of high temperature superconductors: while a tight-binding model captures the kinetic term, it is not clear that there is superconductivity with only an onsite repulsion and, thus, that the problem is accurately described by the Hubbard model alone. Here we pose the question of whether, once the kinetic energy is fixed, a candidate ground state is groundstatable or not. The easiness to answer this question is strongly related to the presence or the absence of a sign problem in the system. When groundstatability is satisfied, it is simple to obtain the potential energy that will lead to such a ground state. As a concrete case study, we apply these ideas to different fermionic wavefunctions with superconductive or spin-density wave correlations.

TT 8.4 Mon 14:45 H21

Instabilities of quadratic band crossing points — •Stefan Uebelacker[1] and Carsten Honerkamp[2] — [1]University of Würzburg — [2]RWTH Aachen

The variation of the orbital composition of bands around band crossing points near the Fermi level can generate interesting effects. In particular, rather simple interactions can give rise to the spontaneous formation of topological insulating phases (S. Raghu et al., Phys. Rev. Lett. **100**, 156401 (2008)). In contrast with Dirac points, quadratic band crossing points offer the advantage of a nonzero density of states at the crossing point, and instabilities occur already at small interaction strengths. Here, we present our results of functional renormalization group calculations for models with one and two quadratic band crossing points and discuss the possibilities for nontrivial insulating phases induced by local interactions.

TT 8.5 Mon 15:00 H21

Electron-plasmon scattering in chiral 1D systems with nonlinear dispersion — Markus Heyl, Stefan Kehrein, Florian Marquardt, and •Clemens Neuenhahn — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics,Center for NanoScience, Ludwig Maximilians Universität München, Munich, Germany

We investigate systems of spinless one dimensional chiral electron systems occuring, e.g., in the arms of electronic Mach-Zehnder interferometers. We take into account both the curvature of the fermionic spectrum and a finite interaction range. The main observation is that due to an interplay of both, an injected high-energy fermion will scatter off plasmons (density variations) leading to an exponential decay of the single particle Green's function (GF) on top of the expected power-law decay even at zero temperature. Remarkably, it turns out that this happens in a coherent fashion, such that a monochromatic sinusoidal density pattern builds up. While one dimensional fermionic systems with linear dispersion relation are described perfectly well by means of bosonizing the system, introducing a finite curvature requires alternative techniques. Here a semiclassical ansatz for the GF is employed whose validity in the low-energy regime was shown earlier [1] and which is extended naturally. Additionally, we make use of a slightly modified version of the method proposed in [2].

[1] C.Neuenhahn and F. Marquardt, PRL 102, 046806 (2009)
[2] M.Pustilnik et al, PRL 96, 196405 (2006)

TT 8.6 Mon 15:15 H21

Fermi-edge singularity in a quantum dot — •Markus Heyl and Stefan Kehrein — Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 München

We investigate the Fermi-edge singularity problem realized in a non-interacting quantum dot. An appropriately tuned laser beam incident on the dot suddenly switches on the hybridization of a dot level with the conduction band electrons. Based on recently developed methods [1], we analytically calculate the exponent of the singularity in the absorption spectrum near the threshold and extend known analytical results [2,3] to the whole parameter regime. Furthermore, we point out that the exponent of the Fermi-edge singularity in the anisotropic Kondo model depends on anisotropy.

[1] N. d'Ambrumenil and B. A. Muzykantskii, Phys. Rev. B **71**, 045326 (2005).
[2] A. Kontani and Y. Toyozawa, J. Phys. Soc. Jpn. **35**, 1073 (1973).
[3] T. Kita, K. Ohtaka and Y. Tanabe, J. Phys. Soc. Jpn. **56**, 4609 (1987).

TT 8.7 Mon 15:30 H21

Dynamical Vertex Approximation for nanosystems — •Angelo Valli, Giorgio Sangiovanni, and Karsten Held — Institut für Festkörperphysik, TU Wien

In the spirit of Dynamical Vertex Approximation (DΓA), we propose a computational approach which assumes the locality of the n-particle fully irreducible vertex to treat nanoscopic systems. To test the reliability of our scheme, we compare it in its simplest version (n=1) to numerically exact Quantum Monte Carlo for a multi-site Anderson Impurity Model when the number of correlated atoms is small. We focus on quantities like electronic spectra and double occupancies and

compare them to alternative methods [1]. The nanoscopic DΓA has the advantage that the simulation of a much larger number of coupled nanosystems is possible than for the exact solution, e.g., an ensemble of coupled quantum dots, macromolecules, or a cluster of ad atoms on surfaces.

[1] S. Florens, PRL99, 046402 (2007)

15 min. break

TT 8.8 Mon 16:00 H21

Critical exponents and phase diagram of the Hubbard model — •Karsten Held[1], Alessandro Toschi[1], Georg Rohringer[1], and Andrey Katanin[2,3] — [1]Institute of solid state physics, Vienna University of Technology — [2]Max-Planck-Insitut für Festkörperphysik, Stuttgart — [3]Institute of metal physics, Ekaterinburg

Despite being the prototype for strongly correlated electron systems, an accurate calculation of the critical behavior of the Hubbard model was hitherto not possible. With the recently developed dynamical vertex approximation (DΓA) [1], we are finally able to include non-local correlations beyond dynamical mean field theory (DMFT) in a systematic way - on all length scales. In two dimensions, this results in a reduction of the antiferromagnetic transition temperature to $T_N = 0$ [2], in agreement with the Mermin-Wagner theorem. In three dimensions, we get a non-mean-field critical behavior, in contrast to DMFT. It agrees, at least for half filling and large Coulomb repulsion, with the Heisenberg critical exponents.

By means of DΓA, we are also able to estimate the error of DMFT. In particular, we will discuss in which regions of the phase diagram a DMFT treatment is sufficient and where non-local correlations necessarily need to be included.

[1] A. Toschi, A. A. Katanin, K. Held, Phys. Rev. B 75, 045118 (2007).

[2] A. A. Katanin, A. Toschi, K. Held, Phys. Rev. B 80, 075104 (2009).

TT 8.9 Mon 16:15 H21

Vertex Function and Dynamical Spin-Susceptibilities from DMFT — •Andreas Dolfen and Erik Koch — German Research School for Simulation Sciences and RWTH Aachen University, Germany

DMFT providing a local approximation to the electronic self-energy readily gives one-body quantities such as the Green's function. Two-body quantities like general dynamical susceptibilities are significantly harder to obtain.

Here we describe how to evaluate spin susceptibilities from an exact diagonalization impurity solver. First we construct the two-particle Green's function of the impurity model and the corresponding local irreducible vertex function. Inserting the vertex and interacting electron propagator for the lattice model into the Bethe-Salpeter equation we obtain dynamical susceptibilities. This technique allows the direct calculation of the susceptibility on the real axis.

As example, we present results for the Periodic Anderson Model.

TT 8.10 Mon 16:30 H21

LSDA+DMFT calculations of electron phonon coupling and its combination with one step model of photoemission — •Jan Minar[1], J. Braun[1], S. Mankovskyy[1], H. Ebert[1], R. Ovsyannikov[2], H. A. Duerr[2], and J. Fink[2] — [1]Dep. Chemie und Biochemie, LMU University of Munich, Germany — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

Recent developments and improvements in the resolution of angle-resolved UPS and XPS photoemission experiments require an improved (or revised) theoretical description of the photoemission process in the framework of the one-step model. In particular, the combination of the KKR band structure method with the dynamical mean field theory (DMFT) provides a quantitative interpretation of photoemission data including all matrix elements effects. Here, we present a formalism that allows to include lattice vibrations into the one-step model. In the UPS regime electron-phonon interaction is reflected by kinks and related phenomena. Calculation of the force-constant tensor within the KKR Green's function method gives access to the k-resolved Eliashberg function and an electron-phonon self-energy. This quantity can be included into the photoemission formalism. The method has been applied to angle-resolved photoemission from Ni(111) and is compared to corresponding experimental data. In contrary to the standard interpretations we found a considerable impact on the electron-phonon self-energy due to spin-flip processes that are induced by spin-orbit coupling. We also show that inclusion of correlations effects is crucial in order to describe electron phonon coupling in Ni.

TT 8.11 Mon 16:45 H21

Influence of Coulomb repulsion on the electron-phonon interaction in high-temperature superconducting copper oxides — •Giorgio Sangiovanni[1] and Olle Gunnarsson[2] — [1]Institut für Festkörperphysik, TU Wien — [2]Max-Planck Institut für Festkörperforschung, Stuttgart

The issue of how strong is the electron-phonon interaction in cuprates and how much it influences their properties is not yet settled [1-2]. Whether or not the coupling to, for instance, oxygen bond-stretching modes is sizable cannot be established with standard tools, like those based on plain Local Density Approximation, as this neglects most of the correlation effects. As several sophisticated methods for many-body calculations are now available, it turns out instead that dynamical self-energy effects strongly influence not only the interplay between an instantaneous Coulomb repulsion and a phonon-mediated retarded attraction, but also the very bare estimate of the electron-phonon matrix elements. Using Cluster Dynamical Mean Field Theory and realistic methods beyond Local Density Approximation we can study the electron-phonon interaction in cuprates in an unbiased way.

[1] R. Heid, *et al.*, PRL **100**, 137001 (2008)

[2] D. Reznik, *el al*, Nature **455**, E6 (2008)

TT 8.12 Mon 17:00 H21

Bilayer Hubbard model for ^{3}He: a cluster dynamical mean-field calculation — K.S.D. Beach[1] and •F.F. Assaad[2] — [1]Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7 — [2]Institut für theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Inspired by recent experiments on bilayer ^{3}He, we consider a bilayer Hubbard model on a triangular lattice. For appropriate model parameters, we observe a band-selective Mott transition at a critical chemical potential, μ_c, corresponding to the solidification of the fermions in the first layer. The growth of the effective mass on the metallic side ($\mu < \mu_c$) is cut off by a first order transition in which the first layer fermions drop out of the Luttinger volume and their spin degrees of freedom become locked in a spin singlet state. These results are obtained from a cluster dynamical mean-field calculation on an eight-site cluster with a quantum Monte Carlo cluster solver.
http://xxx.lanl.gov/abs/0905.1127

TT 8.13 Mon 17:15 H21

Two-particle response functions for multi-band Hubbard models — •Ernst von Oelsen[1], Jörg Bünemann[2], and Götz Seibold[1] — [1]BTU Cottbus, Lehrstuhl für Theoretische Physik, Cottbus — [2]Philipps Universität Marburg, Fakultät für Physik, Marburg

In various studies on single-band Hubbard models, see, e.g., Ref. [1,2], the time-dependent Gutzwiller theory has been shown to be a valuable tool for the investigation of frequency and wave-vector dependent two-particle response functions. We have successfully generalised this approach for the study of arbitrary multi-band Hubbard models. With our new approach it is now possible to investigate such response functions, as e.g., the magnetic susceptibility for realistic three-dimensional multi-band models. This opens the way for a better understanding of various experimental results on systems with medium or strong Coulomb-interaction effects. In our presentation, we give a brief introduction to our theoretical approach and outline its prospects for future studies of real materials. As a first application, we show results for the magnetic susceptibility and the spin-wave properties of a two-band Hubbard model. We compare our findings with those of a Hartree-Fock based random-phase approximation, which is the standard textbook method for the calculation of two-particle response functions.

[1] G. Seibold, J. Lorenzana, PRL **94**, 107006 (2005)

[2] G. Seibold, F. Becca, J. Lorenzana, PRL **100**, 016405 (2008)

TT 8.14 Mon 17:30 H21

Lattice Density Functional Theory of the inhomogeneous Hubbard model. — •Matthieu Saubanère and G. M. Pastor — Institut für Theoretische Physik, Universität Kassel, Kassel, Germany

The inhomogeneous Hubbard Hamiltonian is investigated in the framework of lattice density functional theory (LDFT). The single-particle

density-matrix γ_{ij} with respect to the lattice sites is considered as the basic variable of the many-body problem. Two new approximations to the interaction-energy functional $W[\gamma_{ij}]$ are proposed. The first one is based on the scaling properties of $W[\gamma_{ij}]$. It allows to recover the exact limit of strong correlations for the homogeneous Hubbard Hamiltonian at half band-filling. The second one is obtained by projecting the many-body ground-state on the different states with defined occupations of the atomic sites. A system of equations is then derived, from which $W[\gamma_{ij}]$ is obtained. As examples of applications we present results for the kinetic, Coulomb and total ground-state energy, charge excitation gap, and charge susceptibility of the inhomogeneous Hubbard model in one, two and three dimensional periodic lattices, as well as in small clusters. The accuracy of the method is demonstrated by comparison with available analytical and numerical exact solutions.