TT 94: Correlated Electrons: Other Theoretical Topics

Time: Thursday 15:00–18:30 Location: H 3010

TT 94.1 Thu 15:00 H 3010

Charge disproportionation, mixed valence, and Janus effect in multi-orbital systems: A tale of two insulators — •Aldo Isidori, Maja Berovic, Laura Fanfarillo, Michele Fabrizio, and Massimo Capone — International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

We propose an interpretation for the Janus effect in multi-orbital electron systems, suggested by the duality between Jahn-Teller and Hund's metals at commensurate fillings. The effect emerges from the competition between two distinct insulating states, namely a Mott and a charge disproportionation insulator, favored either by the Coulomb interaction or the exchange coupling, respectively, and characterized by a different ionic valence. This competition results in an asymptotic mixed-valence metallic state, at arbitrarily large interaction strength, along the line where the two parent insulators are degenerate. In this state, charge fluctuations arise from the presence of hopping processes that connect the two degenerate insulators. Experimental evidence for the mixed-valence state and the charge disproportionation insulator-to-metal transition can be found in the chromium perovskite system.

TT 94.2 Thu 15:15 H 3010

Lattice coordination vs. space dimension in 2nd order phase transitions: a dynamical vertex approximation study — •Andreas Hausoel[1], Georg Rohringer[2], Thomas Schäfer[3], Giorgio Sangiovanni[1], and Alessandro Toschi[4] — [1]University of Wuerzburg, Germany — [2]Russian Quantum Center, Moscow, Russia — [3]École Polytechnique and Collège de France, Paris, France — [4]Technical University of Vienna, Austria

The dynamical vertex approximation (DΓA) includes spatial correlations of all length scales beyond the dynamical mean-field theory (DMFT) description. The most relevant changes due to nonlocal fluctuations are a deviation from the mean-field critical behaviour and a sizeable reduction of magnetic ordering temperatures [1].

Here we extend the analysis to different lattice types; in particular, we compare DΓA calculations for the simple, the body-centered and face-centered cubic lattices to the corresponding DMFT ones.

On general grounds, one expects a overall reduction of the differences w.r.t. DMFT, the larger the coordination number of the lattice considered is. Our analysis will clarify the underlying aspects of this trend, investigating the difference between (i) an increase of the coordination number by changing the lattice type (i.e. keeping space dimension fixed), and (ii) an increase of coordination number by keeping the lattice type fixed and increasing the space dimension.

[1] G. Rohringer, A. Toschi, A. Katanin, K. Held, PRL **107**, 256402.

TT 94.3 Thu 15:30 H 3010

Breakdown of Traditional Many-Body Theories for Correlated Electrons — •Thomas Schäfer[1,2,3], Olle Gunnarsson[4], Georg Rohringer[5], Giorgio Sangiovanni[6], and Alessandro Toschi[1] — [1]TU Wien, Austria — [2]Collège de France, Paris, France — [3]CPHT École Polytechnique, Palaiseau, France — [4]MPI Stuttgart, Germany — [5]Russian Quantum Center, Moscow, Russia — [6]Uni Würzburg, Germany

Starting from the (Hubbard) model of an atom, we demonstrate that the uniqueness of the mapping from the interacting to the noninteracting Green function, $G \to G_0$, is strongly violated, by providing numerous explicit examples of different G_0 leading to the same physical G. We argue that there are indeed infinitely many such G_0, with numerous crossings with the physical solution. We show that this rich functional structure is directly related to the divergence of certain classes of (irreducible vertex) diagrams, with important consequences for traditional many-body physics based on diagrammatic expansions. Physically, we ascribe the onset of these highly nonperturbative manifestations to the progressive suppression of the charge susceptibility induced by the formation of local magnetic moments and/or resonating valence bond (RVB) states in strongly correlated electron systems.

TT 94.4 Thu 15:45 H 3010

Divergences of the irreducible vertex functions in correlated metallic systems: Insights from the Anderson Impurity Model — •Patrick Chalupa[1], Patrik Gunacker[1], Thomas Schäfer[1,2,3], Karsten Held[1], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Technische Universität Wien, 1040 Vienna, Austria — [2]Collége de France, 75005 Paris, France — [3]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France

We analyze in detail the occurrence of divergences in the irreducible vertex functions of the Anderson impurity model (AIM). These divergences — a surprising hallmark of the breakdown of many-electron perturbation theory — have been recently observed in several contexts, including the dynamical mean-field solution of the Hubbard model. Hitherto, however, a clarification of their origin could be obtained only in the limit of high temperatures and large interactions, where the underlying physics is greatly simplified by the absence of low-energy quasiparticle excitations. In this respect, our numerical calculations for the AIM, as well as their comparison with the corresponding results for the Hubbard model, allow us to clarify several open questions about the origin and the properties of vertex divergences occurring in a more interesting context, the correlated metallic regime at low- temperatures. In particular, our analysis (i) rules out a direct correspondence between the vertex divergences and the presence of a Mott metal-insulator transition, (ii) clarifies their relation with the underlying Kondo physics, and, eventually, (iii) individuates which divergences might also appear on the real frequency axis in the limit of zero temperature.

TT 94.5 Thu 16:00 H 3010

Signatures of non-Abelian anyons in the thermodynamics of a perturbed $\mathbf{SU(3)_{N_f}}$ WZNW model — •Daniel Borcherding and Holger Frahm — Institute for Theoretical Physics, Leibniz University Hannover

The contribution of anyonic degrees of freedom emerging in the non-Abelian spin sector of a one-dimensional system of interacting fermions carrying both $SU(3)$ and $SU(N_f)$ degrees of freedom to the thermodynamic properties of the latter is studied based on the exact solution of the model. For sufficiently small temperatures and fields the anyons appear as zero energy modes localized at the massive kink excitations. From their quantum dimension they are identified as $SU(3)_{N_f}$ anyons. The density of kinks (and anyons) can be controlled by external fields leading to the formation of collective states of these anyons described by various conformal embeddings of the $SU(3)_{N_f}$ WZNW model for large fields. Based on the numerical analysis of the thermodynamic Bethe ansatz equations we propose a phase diagram for the anyonic modes.

15 min. break.

Invited Talk TT 94.6 Thu 16:30 H 3010

Discrete Time Crystals — •Roderich Moessner — MPI-PKS, Dresden, Germany

Periodically driven ("Floquet") systems provide perhaps the simplest setting for studying quantum systems out of equilibrium. Their properties have turned out to be remarkably rich. In particular, the interplay of disorder and driving has given rise to an entirely new form of spatio-temporal ordering which has been given the name discrete time crystal.

This talk presents an introduction to the physics of Floquet systems and explains how non-equilibrium phases and their concomitant ordering arise.

This work was done in collaboration with Achilleas Lazarides, Arnab Das, Vedika Khemani, and Shivaji Sondhi. For an introductory review, see Nature Physics 13, 424-428 (2017).

TT 94.7 Thu 17:00 H 3010

Excitations of the square lattice Heisenberg model using tensor-network methods — •Ruben Verresen[1,2], Frank Pollmann[1], and Roderich Moessner[2] — [1]Technical University of Munich — [2]Max-Planck-Institute for the Physics of Complex Systems

The square lattice Heisenberg model is a paradigmatic example of spontaneous symmetry breaking. Despite the apparent simplicity of the model, spin wave theory fails to describe its excitations at certain momenta. Opposing descriptions —strongly-interacting magnons and emergent spinons— have been proposed. We use a time-dependent density matrix renormalization group (DMRG) method to obtain the dynamical structure factor. In particular, we investigate its features

by continuously tracking the spectral function as a function of a tuning parameter around a simple soluble limit. This leads us to a simple picture which already at low order in perturbation theory accounts for the features beyond SWT in a semi-quantitative way.

TT 94.8 Thu 17:15 H 3010

Heisenberg-like model for correlated electrons and quantum spin fluctuations near magnetic instabilities — •Evgeny Stepanov — Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Theory of magnetism and magnetic interactions is the one of the most attractive areas of physics nowadays. Nevertheless, a quantum nature of the exchange interaction that occurs between spins is not clear yet. Up to now, studies of magnetic interactions have been mostly limited to a classical description, which makes their generalization on the case of strongly correlated systems rather difficult.

Here we consider an extended Hubbard model for correlated electrons and derive a corresponding Heisenberg-like problem. Our approach is based on the Dual Boson theory, which allows to introduce quantum collective variables associated to bosonic excitations and separate charge and spin degrees of freedom. The obtained result for the exchange interaction accounts for important quantum fluctuations and improves Anderson's idea of the superexchange, which makes possible description of collective excitations in the most interesting physical regimes. Thus, the study of quantum spin fluctuations in paramagnetic (PM) phase near the PM to AFM phase transition allows to detect the antiferromagnetic "soft" mode and manifest the tendency of the system to the spin ordering before the actual transition to the ordered state happens. Importantly, the derived exchange interaction is expressed in terms of single-particle quantities, which can be efficiently used in realistic calculations of multiband systems.

TT 94.9 Thu 17:30 H 3010

Single-particle properties of the 2D Hubbard model within a four-pole approximation — •Andrea Di Ciolo and Adolfo Avella — Dipartimento di Fisica "E. R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy

We present a solution of the 2D Hubbard model in the framework of the Composite Operator Method (COM) [1-3] within a four-pole approximation (4p). First, we characterize the 2-site exact solution and identify the crucial role played by spin fluctuations. Then, we adopt a basis of fields given by the two Hubbard operators plus two fields describing the electronic transitions dressed by the nearest-neighbor spin fluctuations. As well as this approximate solution is in remarkable agreement with the 2-site exact one, the corresponding 2D solution performs very well once compared to advanced (semi-)numerical methods, being by far less computational-resource demanding. Moreover, this solution, featuring a well-developed momentum selectivity of the spectral properties, opens up the possibility to directly address the underdoped-cuprate puzzle. Therefore, we adopt this 4p approximation to study the single-particle properties of the 2D model in the strong coupling regime (intermediate-large interaction and small-intermediate doping), where the effects of spin-fluctuations, accurately treated in our approach, are more relevant and induce anomalous features in all analyzed properties.

[1] F. Mancini, and A. Avella, *Adv. Phys.* **53**, 537 (2004).
[2] A. Avella, *Eur. Phys. J. B*, **87**, 45 (2014).
[3] A. Avella, *Adv. Cond. Matt. Phys.* **2014**, 515698 (2014).

TT 94.10 Thu 17:45 H 3010

Sharp entanglement thresholds in the logarithmic negativity of disjoint blocks — •Younes Javanmard[1], Daniele Trapin[1], Soumya Bera[1,2], Jens. H Bardarson[1,3], and Markus Heyl[1] — [1]MPIpks, Dresden, Germany — [2]Indian Institute of Technology Bombay, Mumbai, India — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Entanglement has developed into an essential concept for the characterization of quantum many-body phases and phase transition in the ground state. However, the conventional approach using the entanglement entropy faces a challenge for thermal states where it loses its status as an entanglement measure. In this work, we study the entanglement properties of the transverse-field Ising chain using the logarithm negativity, which remains a valid entanglement measure also for mixed states. Specifically, we investigate the logarithm negativity for two disjoint blocks as a function of their separation. In this way, we obtain information on the spatial structure of entanglement. In particular, we find a sharp entanglement threshold as a function of the distance of the two blocks beyond which the logarithm negativity exactly vanishes, indicating that beyond this critical distance the two blocks become unentangled as measured by the logarithm negativity. We explore this feature as a function of temperature and size of the two blocks and thereby map out the spatial structure of entanglement in the transverse-field Ising chain.

TT 94.11 Thu 18:00 H 3010

Error estimates for extrapolations with matrix-product states — •Claudius Hubig[1,2], Jutho Haegeman[3], and Ulrich Schollwöck[1] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Department of Physics and Astronomy, Ghent University, Ghent, Belgium

We introduce a new error measure for matrix-product states (MPS) based on an approximation of the full variance $\langle\psi|(\hat{H}-E)^2|\psi\rangle$. When applied to a series of MPS at different bond dimensions obtained from a single-site density matrix renormalization group (1DMRG) calculation, it allows for the extrapolation of observables towards the zero-error case representing the exact ground state of the system.

The calculation of the error measure is split into a sequential part of cost equivalent to two calculations of $\langle\psi|\hat{H}|\psi\rangle$ and a trivially parallelized part scaling like a single operator application in two-site DMRG (2DMRG). The reliability of the new error measure is demonstrated at four examples and extrapolation in the new error measure is shown to be on-par with extrapolation in the 2DMRG truncation error or the full variance $\langle\psi|(\hat{H}-E)^2|\psi\rangle$ at a fraction of the computational effort.
[1] arxiv.org/abs/1711.01104

TT 94.12 Thu 18:15 H 3010

Conditions where RPA becomes exact in the high-density limit — •Klaus Morawetz[1,2,3], Vinod Ashokan[4], Renu Bala[5], and Kare Narain Pathak[4] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum if the relation between Fermi energy and Fermi momentum is $\epsilon_{\rm f} \sim p_{\rm f}^{\beta}$ and the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d<\beta+\alpha$ specifies systems where RPA is exact in the high-density limit. The one-dimensional structure factor is found to be the interaction-free one in the high-density limit. A cancellation of RPA and vertex corrections render this result alternatively valid up to second-order contact interaction. For finite-range potentials of cylindrical wires a large-scale cancellation appears and found to be independent of the width parameter. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.