TT 71: Correlated Electrons: Other Theoretical Topics

Time: Friday 9:30–12:00 Location: HSZ 304

TT 71.1 Fri 9:30 HSZ 304

GW calculations of electron momentum densities and Compton profiles — •Eddie Harris-Lee[1], Alyn James[1], John Kay Dewhurst[2], and Stephen Dugdale[1] — [1]H. H. Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom — [2]Max-Planck Institute of Microstructure Physics, Halle, Germany

Compton scattering gives direct access to the single-particle momentum density, which contains information about the ground state wave functions of the many-body system. Theoretical calculations of electron momentum densities and Compton profiles, using Kohn-Sham density functional theory, don't fully agree with experimental measurements [1]. This could be partly due to the approximate description of correlation and partly because the Kohn-Sham wave functions are chosen to reproduce the density in real space, not in momentum space [2]. There is therefore good motivation to try alternative first principles theories. GW methods are an obvious choice [3], since these employ quasiparticle wave functions and use a different, non-local, description of exchange and correlation [4]. A method for obtaining a set of wave functions and occupation numbers from the output of a GW calculation will be described. The resulting electron momentum densities will be compared to experimental measurements for various materials.

[1] W. Schülke et al., Phys. Rev. B **54** 14381 (1996)
[2] L. Lam and P.M. Platzman, Phys. Rev. B **9** 5122 (1974)
[3] V. Olevano et al., Phys. Rev. B **86** 195123 (2012)
[4] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61** 237 (1998)

TT 71.2 Fri 9:45 HSZ 304

Constrained Random Phase Approximation: Why and When it Works — •Erik van Loon[1], Malte Rösner[2], Mikhail Katsnelson[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Radboud University, Nijmegen, the Netherlands

The constrained Random Phase Approximation (cRPA) is an important part of the modern theory of correlated electron materials. In the downfolding from the full band structure to an effective low-energy (Hubbard) model, the cRPA provides a way to calculate the Hubbard parameter U for the low-energy model, taking into account screening by the other electronic states. Although it is a popular tool, a formal justification for the cRPA has been lacking. Here, we show when the cRPA is a good approximation.

TT 71.3 Fri 10:00 HSZ 304

Nonergodic Observables in the Hubbard Model at finite temperatures — •Clemens Watzenböck, Anna Kauch, Alessandro Toschi, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

We show the appearance of nonergodic observables in specific regions of the phase-diagram for the Hubbard-Model. The nonergodicity can be quantified by the difference between the static isolated susceptibility and the isothermal suszeptibility. This is equivalent to the infinite time limit of <A(t) B> - <A><B> [1,2]. We present various ways to extract the nonergodic term from numerical data (e.g. quantum Monte Carlo simulations performed in imaginary time [3,4]). Our results are relevant for numerical analytic continuation of susceptibilities, and also give insight into symmetry broken phases.

[1] Wilcox et al. (1968) Phys. Rev., 174, 624-629
[2] Suzuki (1971) Physica, 51(2), 277 - 291
[3] Georges et al. (1996) Rev. Mod. Phys., 68, 13-125
[4] Wallerberger et al. (2019) Comput. Phys. Commun., 235, 388 - 399

TT 71.4 Fri 10:15 HSZ 304

Ground-state properties and enhancement of pairing correlations in an asymmetric Hubbard ladder — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Germany

We investigate ground-state properties and correlation functions of an asymmetric two-leg Hubbard ladder using the density matrix renormalization group method. The ladder consists in a Hubbard chain (Hubbard leg) and a tight-binding chain (Fermi leg) connected by a single-particle hopping between the adjacent sites. This two-leg ladder system is a generalization of the asymmetric ladder investigated in [1,2] by allowing the hopping terms in the Hubbard leg and the Fermi leg to be unequal. We determine the excitation gaps and the corresponding charge and spin densities as well as several correlation functions. For strong on-site interactions at half filling, we observe finite pair-binding energies for range of intra-leg hopping terms in the Hubbard leg and rung hopping terms larger than the intra-leg hopping term in the Fermi leg. There is no enhancement of pairing correlations at half filling. For dopped ladders, the pair-binding energies reduce but persist and we observe strong enhancement of pairing correlations that decay in power-law. The exponent of the dcay is close to one for some parameter sets.

[1] A. Abdelwahab, E. Jeckelmann, M. Hohenadler, Phys. Rev. B 91, 155119 (2015)
[2] A. Abdelwahab, E. Jeckelmann, Eur. Phys. J. B 91, 207 (2018)

TT 71.5 Fri 10:30 HSZ 304

Influence of lattice geometry and dimensionality on the critical properties of magnetic transitions: A dynamical vertex approximation analysis — •Andreas Hausoel[1], Georg Rohringer[2], Thomas Schäfer[3], Giorgio Sangiovanni[1], and Alessandro Toschi[4] — [1]University of Würzburg, Germany — [2]University of Hamburg, Germany — [3]École Polytechnique and Collège de France, Paris, France — [4]Technical University of Vienna, Austria

We present a fundamental analysis of the effects of non-local spatial correlations on the magnetic transitions in different lattice types. To this aim, we have applied the dynamical vertex approximation (DΓA), a non-perturbative diagrammatic extension [1] of the dynamical mean-field theory (DMFT), to the simple, the body-centered and face-centered cubic lattices to the corresponding DMFT ones.

While an overall reduction of the differences in the transition temperatures and critical properties w.r.t. DMFT for lattices with increasing coordination number is expected, our analysis will elucidate the underlying aspects of this trend. In particular, we investigate the difference between an increase of the coordination number by changing the lattice type (i.e., keeping space dimension fixed) and by increasing the space dimensions (for a selected lattice type).

[1] Rohringer, Toschi, et al., Rev. Mod. Phys. 90, 025003 (2018)

15 min. break.

TT 71.6 Fri 11:00 HSZ 304

Nonlocal Exchange Interactions in Strongly Correlated Electron Systems — •Edin Kapetanović[1,2], Malte Schüler[1,2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen — [2]Bremen Center for Computational Materials Science, Universität Bremen

We study the influence of ferromagnetic nonlocal exchange on correlated electrons in terms of a SU(2)-Hubbard-Heisenberg model and address the interplay of on-site interaction induced local moment formation and the competition of ferromagnetic direct and antiferromagnetic kinetic exchange interactions. In order to simulate thermodynamic properties of the system in a way that largely accounts for the on-site interaction driven correlations, we advance the correlated variational scheme introduced in [M. Schüler et al., Phys. Rev. Lett. 111, 036601 (2013)] to account for explicitly symmetry broken electronic phases by introducing an auxiliary magnetic field. After benchmarking the method against exact solutions of a finite system, we study the SU(2)-Hubbard-Heisenberg model on a square lattice. We obtain the U-J finite temperature phase diagram of a SU(2)-Hubbard-Heisenberg model within the correlated variational approach and compare to static mean field theory (MFT). While the generalized variational principle and MFT yield similar transitions, we find that the nature of the associated phase transitions differs between the two approaches. The fluctuations accounted for in the variational approach render the transitions continuous, while MFT predicts discontinuous transitions between ferro- and antiferromagnetically ordered states.

TT 71.7 Fri 11:15 HSZ 304

How to recognize confinement of a hole in a string-

like potential in doped antiferromagnets? — Krzysztof Bieniasz[1,2], •Piotr Wrzosek[3], Andrzej M. Oleś[2,4], and Krzysztof Wohlfeld[3] — [1]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4 — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland — [3]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [4]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

We study the problem of a single hole doped to the antiferromagnet and using analytical methods and state of the art numerics we establish (model independent) signature of the hole confinement in an antiferromagnetic spin background [1]. We show that once the hole is subject to a string-like potential its wave function coefficients need to decay faster than exponentially ('super-exponentially'). As the latter coefficients can be observed in recent cold atoms simulations of the Fermi-Hubbard model [2], we verify whether the hole confinement is realized in doped antiferromagnets.

[1] K. Bieniasz et al., SciPost Phys. 7, 066 (2019)
[2] C. S. Chiu et al., Science 365, 251-256 (2019)

TT 71.8 Fri 11:30 HSZ 304

Dynamical DMFT susceptibility at second orderphase transitions — •Abuduaini Niyazi, Dominique Geffroy, and Jan Kuneš — Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

We present a dynamical mean-field study (DMFT) of dynamical susceptibility in two-band Hubbard model. By varying model parameters(band asymmetry, crystal field, temperature) we realize transitions between various phases such as triplet excitonic condensate, spin-state order(solid), supersolid or antiferromagnetic solid. We analyze the behavior of relevant dynamical susceptibilities across these transitions, which break either continuous or discrete symmetries. Besides revealing the rich physics of the studied model, our results show how DMFT susceptibilities can be used to identify approximate (weakly broken) symmetries and incipient instabilities.

TT 71.9 Fri 11:45 HSZ 304

Plasmons In Doped Mott Insulators — •Andrej Lehmann, Evgeny Stepanov, and Alexander Lichtenstein — I. Institut für Theoretische Physik, Hamburg, Deutschland

Plasmons play an important role in nanophotonics and different metamaterials applications exhibiting interesting phenomena like negative refraction, superlensing and more. Plasmons are usually studied in the metallic regime, where the mobility of charge carrier density is large. Recently, correlated plasmons attracted a lot of attention in Mott-like insulating oxides showing a low loss in the visible optical range. In order to study plasmons in insulators, one has to apply doping to induce fluctuations of a charge density. Theoretically, plasmons can be described by the Lindhardt dielectric function using the random phase approximation (RPA). However, the RPA is applicable only in the weakly interacting regime, which corresponds to small-gap or metallic systems. For description of plasmons in Mott insulating regime one have to use more elaborated methods, such as the Dual Boson (DB) theory. In this work we study correlated plasmons in a single band Mott insulator with a prototype of C2F and C2H materials. For this aim we apply a ladder DB approach that considers the polarization operator in the two-particle ladder form written in terms of local three- and four-point vertex functions. Recently, it has been shown that two-particle vertex functions can be drastically simplified in the regime of strong collective fluctuations in the system. In this case the DB theory can be reduced to a much simpler RPA+EDMFT approach. Thus, we finally compare our results with results of the RPA method.