

TT 61: Correlated Electrons: (General) Theory 2

Time: Thursday 9:30–13:00

Location: HSZ 204

TT 61.1 Thu 9:30 HSZ 204

Magnetic response of spin-orbit coupled d-electrons in non-spherical potentials — ●DANIL TOLOUI-MANTADAKIS, MARC HOEPPNER, and PHILIPP HANSMANN — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Hubbard model and its multi-orbital extensions is one of the most prominent microscopic starting points to understand properties of ground state and low energy excitations. Its explicit formulation in terms of single particle operators and the effective Coulomb interaction crucially relies on approximations which are based on an assumed hierarchy of energy scales: while in 3d transition metal compounds crystal field effects dominate and yield good quantum numbers, in 4f rare-earth compounds (e.g. heavy fermion systems like CeX_2Si_2) strong spin-orbit coupling renders total angular momentum to be a much better single particle basis. However, a clear hierarchy is not always present and when we move towards the 4d and 5d compounds we can hardly define any good quantum numbers at all.

Here, we present a dynamical mean-field study of a generic three band model including both crystal field- and spin-orbit coupling operators on equal footing, using the fully $\text{SU}(2)$ symmetric Coulomb interaction. We show the results of the two-particle uniform magnetic response which is, other than single particle spectra quantities, much more sensitive to effects of electronic correlations, and we compare them with the exact atomic limit ones.

TT 61.2 Thu 9:45 HSZ 204

Dual Fermion Approach for the Honeycomb Lattice — ●DANIEL HIRSCHMEIER¹, HARTMUT HAUFERMANN², and ALEXANDER I. LICHTENSTEIN¹ — ¹I. Institut für Theoretische Physik, Universität Hamburg, Germany — ²Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., Paris

The study of strongly correlated electron systems remains a hot topic in modern condensed matter physics due to its rich phenomenology and its wide range of applications. Lately the material graphene has become one of the most frequently studied objects in this field, having a number of interesting properties arising due to its extraordinary crystal structure.

In this work we explore the consequences of correlation effects for electrons on a lattice with the very same structure, by applying the recently developed Dual Fermion approach to the Hubbard model on the honeycomb lattice. The Dual Fermion approach is a multiscale diagrammatic expansion around the Dynamical Mean Field Theory incorporating non-local correlations.

We show that the Dual Fermion approach describes the occurrence of non-trivial correlation effects like the formation of extended Van Hove singularities in the quasiparticle spectrum close to Van Hove filling. Furthermore we investigate the Hubbard model on the honeycomb lattice at half-filling. Our results show an exponential scaling of antiferromagnetic fluctuations with temperature, which is in good agreement with analytical results and provide a revision of the semimetal-insulator scenario in DMFT.

TT 61.3 Thu 10:00 HSZ 204

Site-selective Mott insulator-metal transition and charge disproportionation in Fe_2O_3 under pressure — ●IVAN LEONOV — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — Materials Modeling and Development Laboratory, National University of Science and Technology 'MISIS', 119049 Moscow, Russia

We present a theoretical study of the electronic structure and phase stability of hematite ($\alpha\text{-Fe}_2\text{O}_3$) near a pressure-induced Mott insulator-metal transition using the fully charge self-consistent DFT+DMFT approach. Our results reveal that upon compression above ~ 45 GPa, Fe_2O_3 undergoes a Mott insulator (MI) to site-selective MI phase transition. The latter is characterized by a collapse of local magnetic moments and emergence of a metallic state only on half of the Fe sites. Our results suggest that the phase transition is accompanied a charge disproportionation of the Fe ions, implying a complex interplay between electronic correlations and the lattice. We explain the high-pressure behavior of Fe_2O_3 and suggest that it is primary a localized to itinerant moment behavior transition that gives

rise to magnetic collapse of the Fe ions under pressure.

TT 61.4 Thu 10:15 HSZ 204

L-hole Pocket of the Palladium Fermi Surface Revealed by Positron Annihilation Spectroscopy — ●MICHAEL SEKANIA^{1,2}, WILHELM HANS APPELT^{3,4}, ANDREAS ÖSTLIN¹, LIVIU CHIONCEL^{1,4}, and DIETER VOLLHARDT¹ — ¹Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — ²Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia — ³Theoretical Physics II, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — ⁴Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

The existence of the L-hole pocket of the palladium Fermi surface was extensively discussed in the past decades. Although scalar-relativistic density functional theory calculations are not able to reproduce this feature, it is expected that relativistic corrections, among them spin-orbit coupling, are strong enough to create an L-hole pocket. So far, no clear experimental evidence is reported in the literature. In our study we find that relativistic corrections indeed create such a L-hole pocket. Furthermore we show that the computed two dimensional Angular Correlation of Electron Positron Annihilation Radiation (the so called 2D-ACAR) clearly demonstrates the features associated with the L-hole pocket. We also show that electronic correlations do not alter these features significantly. A 2D-ACAR experiment should be able to resolve the disputes concerning the existence of the L-hole pocket in the Palladium Fermi surface.

TT 61.5 Thu 10:30 HSZ 204

Electronic Correlations in Vanadium Revealed by Electron-Positron Annihilation Measurements — JOSEF ANDREAS WEBER¹, DIANA BENE², WILHELM HANS APPELT^{3,4}, HUBERT CEEH¹, WOLFGANG KREUZPAINTNER¹, MICHAEL LEITNER^{1,5}, DIETER VOLLHARDT⁶, CHRISTOPH HUGENSCHMIDT^{1,5}, and ●LIVIU CHIONCEL^{4,6} — ¹Physik-Department, Technische Universität München, James-Frank-Strasse, 85748 Garching, Germany — ²Faculty of Physics, Babes-Bolyai University, Kogalniceanu str. 1, 400084 Cluj-Napoca, Romania — ³Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ⁴Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany — ⁵Heinz Maier-Leibnitz Zentrum, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — ⁶Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The electronic structure of vanadium measured by Angular Correlation of electron-positron Annihilation Radiation (ACAR) is compared with the predictions of the combined Density Functional and Dynamical Mean-Field Theory (DMFT). Reconstructing the momentum density from five 2D projections we were able to determine the full Fermi surface and found excellent agreement with the DMFT calculations. In particular, we show that the local, dynamic self-energy corrections contribute to the anisotropy of the momentum density and need to be included to explain the experimental results.

TT 61.6 Thu 10:45 HSZ 204

Influence of non-local interactions on the Mott metal-insulator transition. — ●MALTE SCHÜLER^{1,2}, ERIK G. C. P. VAN LOON³, MIKHAIL I. KATSNELSON³, and TIM O. WEHLING^{1,2} — ¹University of Bremen, Institute for Theoretical Physics — ²University of Bremen, Bremen Center for Computational Materials Science — ³Radboud University, Institute for Molecules and Materials

We investigate how short- and long-ranged non-local Coulomb interactions influence the metal-insulator phase boundary of the half-filled Hubbard model on square lattices and honeycomb lattices. We find that generally, non-local interactions stabilize the Fermi-liquid regime and that the phase boundary behaves linearly with infinitesimal non-local interactions. We present an upper bound for the boundary's slope. Our findings help to elucidate if the Hubbard model can describe the Mott transition in real materials. For our investigations, we use a variational principle which maps extended Hubbard models to effective purely local Hubbard models. The mapping relies on Quantum

Monte Carlo solutions of the the local Hubbard model.

15 min. break.

TT 61.7 Thu 11:15 HSZ 204

Lattice effects on the superfluid stiffness — ●MATTHIAS HECKER and JÖRG SCHMALIAN — TKM, KIT, Karlsruhe, Germany

The underdoped regime of the copper oxide superconductors with its rich set of physical features has been intensely debated over years, while the overdoped side, perceived as simple and said to follow a BCS behavior, has been mostly disregarded. In a recent experiment on the overdoped side of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [1], yet, a stark contrast between the BCS prediction on the superfluid stiffness and the measurement outcome has been observed. We investigate whether the discrepancy in the superfluid stiffness can be rooted in the underlying lattice and the concomitant electronic dispersion relation. In particular, we work out the impact of fluctuation corrections to the superfluid stiffness in a Galilei-non-invariant system.

[1] Božović, I., He, X., Wu, J. & Bollinger, A.T., *Nature* **536**, 309 (2016).

TT 61.8 Thu 11:30 HSZ 204

The role of fluctuations for density-wave instabilities — ●MAREIKE HOYER^{1,2}, SONJA FISCHER^{3,1}, and JÖRG SCHMALIAN^{1,2} — ¹Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Deutschland — ²Institut für Festkörperphysik, Karlsruher Institut für Technologie, Deutschland — ³Institute for Theoretical Physics, Universiteit Utrecht, Nederlande

Density-wave instabilities have been observed and studied in a multitude of materials. In particular, in the context of unconventional superconductors like the iron-based superconductors, they have excited considerable interest, since they compete with the superconducting state in these materials. We analyze the fluctuation corrections to the equation of state of the density-wave order parameter for commensurate charge and spin-density waves due to perfect nesting. For XY magnets, we find that contributions due to longitudinal and transverse fluctuations cancel each other, making the mean-field analysis of the problem controlled. This is consistent with the observation by Kos, Millis, and Larkin [1], who analyzed fluctuation corrections to the BCS theory of superconductivity. However, in case of charge-density waves and spin-density waves with Heisenberg symmetry, we find that fluctuation corrections are not negligible, and hence mean-field theories are not justified. These singular fluctuations originate from the intermediate length-scale regime, with wavelengths between the lattice constant and the $T = 0$ correlation length. We comment on strategies to resolve this challenge in the description of density-wave instabilities.

[1] Š. Kos, A. J. Millis, and A. I. Larkin, *PRB* **70**, 214531 (2004)

TT 61.9 Thu 11:45 HSZ 204

Numerical investigation of the reduction in the topological classification due to interactions in 2D — ●JOHANNES S. HOFMANN¹, RAQUEL QUEIROZ^{2,3}, ESLAM KHALAF², and FAKHER F. ASSAAD¹ — ¹Institut für Theoretische Physik und Astrophysik, Würzburg, Deutschland — ²Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland — ³Weizmann Institute of Science, Rehovot, Israel

Symmetry protected topological phases have been classified for non-interacting models by A. P. Schnyder et. al.[1]. As first shown by Kitaev and Fidkowski[2] for class BDI in 1D and later extended to all symmetry classes [3], interactions lead to a reduction of topologically distinct phases. R. Queiroz et. al. present explicit rules for the construction of such interactions [4].

Here we consider the symmetry class A' in 2 dimensions, i.e. models with time-reversal, particle-hole and a unitary $\mathbb{Z}_2$ symmetry R , where interactions reduce the topological classification from $\mathbb{Z}$ to $\mathbb{Z}_4$. We realize this class by a lattice Dirac Hamiltonian and the goal of this project is to first confirm the arguments provided in the previous studies numerically by explicitly connecting a topological phase with winding $n = 4$ adiabatically to the trivial insulator ($n = 0$). We then study the mechanism, how both the gap closing and the symmetry breaking, required in the non-interacting model, is avoided.

[1] Schnyder et. al., *PRB* **78**, 195125

[2] Fidkowski and Kitaev, *PRB* **81**, 134509

[3] Morimoto et. al., *PRB* **92**, 125104

[4] Queiroz et. al., *PRL* **117**, 206405

TT 61.10 Thu 12:00 HSZ 204

Gridless Stochastic Sampling: Analytic Continuation of Quantum Monte Carlo Data — ●KHALDOON GHANEM and ERIK KOCH — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real axis. Although StochS does not have explicit parameters, the results depend on the discretization grid which acts as a default model.

To reduce the effect of the grid, we extend StochS into a gridless method (gStochS) by sampling the grid points from a default model instead of having them fixed. The effect of the default model is much reduced in gStochS compared to StochS and depends mainly on its width rather than its shape. The proper width can be then chosen using a simple recipe.

To avoid fixing the width, we go one step further and extend gStochS to sample over a class of default models with different widths. The method is then able to automatically relocate the grid points and concentrate them into the important region. Results show that gStochS gives good results and resolves sharp features in the spectrum without the need for fine tuning a default model.

TT 61.11 Thu 12:15 HSZ 204

Continuous-time quantum Monte Carlo for fermion-boson lattice models: Improved bosonic estimators and application to the Holstein model — ●MANUEL WEBER, FAKHER F. ASSAAD, and MARTIN HOHENADLER — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We extend the continuous-time interaction-expansion quantum Monte Carlo method with respect to measuring observables for fermion-boson lattice models. Using generating functionals, we express expectation values involving boson operators, which are not directly accessible because simulations are done in terms of a purely fermionic action, as integrals over fermionic correlation functions. We also demonstrate that certain observables can be inferred directly from the vertex distribution, and present efficient estimators for the total energy and the phonon propagator of the Holstein model. Furthermore, we generalize the covariance estimator of the fidelity susceptibility to retarded interactions. The new estimators are applied to half-filled spinless and spinful Holstein models in one dimension. The observed renormalization of the phonon mode across the Peierls transition in the spinless model suggests a soft-mode transition in the adiabatic regime. The critical point is associated with a minimum in the phonon kinetic energy and a maximum in the fidelity susceptibility.

TT 61.12 Thu 12:30 HSZ 204

Relating correlation measures: the importance of the energy gap — ●CARLOS L. BENAVIDES-RIVEROS¹, NEKTARIOS LATHIOTAKIS², CHRISTIAN SCHILLING³, and MIGUEL A. L. MARQUES¹ — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany — ²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635 Athens, Greece — ³Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom

The concept of correlation is at the core of all approaches to describe many-body quantum systems. In general, multipartite correlation is a property that can be assigned to quantum states independent of the underlying physics (Hamiltonian). This is in contrast to quantum chemistry where the correlation energy (the energy not seized by the Hartree-Fock ansatz) plays a more prominent role. By concise means, we show that these two different viewpoints on the concept of correlation are closely related. By studying few site Hubbard models and the hydrogen dimer H_2 we relate popular fermionic correlation measures to the correlation energy and emphasize the role of the energy gap.

TT 61.13 Thu 12:45 HSZ 204

The Quantum-Statistical Condensate of One-Dimensional Anyons — ●THORE POSSKE¹, BJÖRN TRAUZETTEL², and MICHAEL THORWART¹ — ¹I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — ²Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg

We develop an exact many-body formalism for one-dimensional anyons, the hybrid particles between bosons and fermions. Besides providing characteristic observables, we reveal the quantum-statistical condensate. This genuine many-body condensate is created purely by

quantum-statistical attraction. It is potentially more stable than a Bose-Einstein condensate and carries a rich structure of degenerate in-

ternal excitations. Parallels to the Lieb-Liniger model of interacting bosons are discussed.