The mystery of correlations

Two-particle self-consistency in diagrammatic theories for strongly correlated electron systems

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In Short

- The theoretical description of correlated electron system is one of the main challenges for the cutting-edge research in condensed matter theory.
- Feynman diagrammatic extensions of the dynamical means field theory can capture long-range correlations which lead to magnetism or superconductivity in correlated materials.
- These theories suffer from intrinsic inconsistencies for the description of physical observables such as the kinetic and the potential energy.
- An extension of these approaches to realistic multi-orbital systems is still missing.
- In our project, we will overcome such difficulties by means of an effective renormalization of physical response functions which is feasible also in the multi-orbital case.

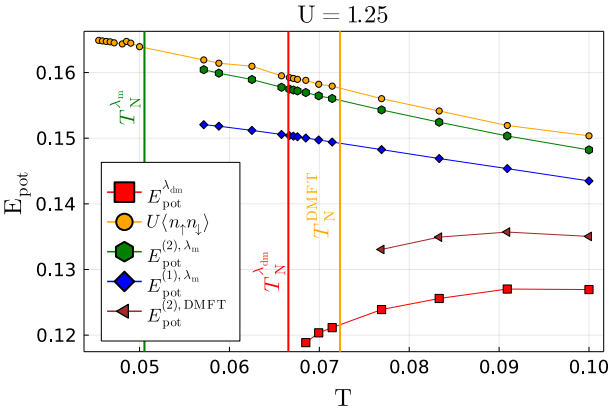

***Figure 1:** Potential energy as a function of temperature T. Data is shown for DMFT and non-selfconsistent ladder DΓA obtained from one-particle (orange circles and blue diamonds) and two-particle (brown triangles and green hexagons) correlations functions, respectively. For our new two-particle selfconsistent ladder DΓA we obtain a unique result for the potential energies (red squares) which features the expected decreasing behavior upon lowering the temperature. Figure is reproduced from Ref. [8].*

Materials with strongly correlated electrons feature a wide variety of fascinating physical properties such as correlation-driven metal-to-insulator transitions, magnetism or high-temperature superconductivity. Unfortunately, the same physical mechanism which is responsible for these interesting phenomena, namely the strong Coulomb repulsion between the electrons, hamper the theoretical description of such systems. In particular, no independent particle approach or static mean field technique can provide an at least qualitatively correct understanding of such compounds. In this respect, the advent of dynamical means field theory (DMFT) has represented a huge step forward in the field. This method is able to describe a substantial part of the correlations, i.e., the purely local ones between two electrons at the same lattice site, exactly. This has allowed to analyze the celebrated Mott metal-to-insulator transition, which occurs in a number of transition metal oxides[1], even quantitatively. However, properties such as magnetism or supercdoncuctivity originate from—or are at least strongly influenced by— long-range correlation effects. To adequately include this nonlocal physics into the theoretical considerations, several so-called diagrammatic extensions of DMFT have been proposed in the last decade[2]. They perform a perturbation theory around DMFT by constructing diagrammatic corrections from DMFT building blocks, i.e., the spectral function and the local two-particle scattering amplitude (=vertex) of DMFT. These approaches have been able to successfully describe several aspects of correlated electron systems such as antiferromagnetism[3] or superconductivity[4].

In spite of their impressive successes for the description of correlation effects on all length scales, almost all diagrammatic extensions suffer from certain limitations which restrict their predictive power. In fact, within these approaches a number of physical observables such as the kinetic and the potential energies can be calculated in two ways, either from the one-particle spectral function or from the two-particle scattering amplitude. While for an exact treatment both results should be obviously the same, this is unfortunately not the case for virtually all diagrammatic extensions of DMFT[5].

Such inconsistencies occur already in DMFT where the potential energies calculated from one- and two-particle correlation functions differ[5,6]. One route to overcome this problem is the parquet formalism. Within this approach a self-consistent renormalization of fluctuations in all scattering channels is performed which guarantees the fulfillment of certain sum rules and the consistency of the potential energy. This method has been already successfully applied within this project for the analysis of the pseudogap phase in the half-filled two-dimensional single-

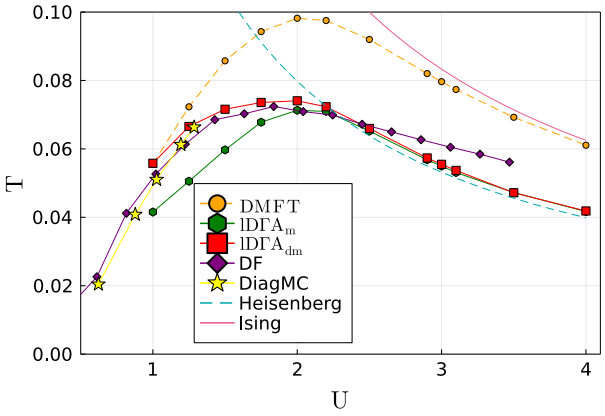

Figure 2: *Antiferromagnetic phase diagram in the three-dimensional Hubbard model as a function of the interaction strength U. The lines indicate the transition temperature to the low-temperature antiferromagnetic state calculated with the methods indicated in the plot legend. Figure is reproduced from Ref. [8].*

band Hubbard model[7]. However, this approach is numerically highly demanding which prevents the investigation of more realistic multi-band systems even when high-performance computing systems such as the HLRN are used for the numerical calculations.

In this project, we follow a simpler path to overcome the above-mentioned limitations. This consists in introducing an effective renormalization of the spin and charge susceptibilities. A preliminary version of this idea has already been adopted within the DΓA where only the spin susceptibility has been renormalized in order to restore the correct asymptotic behavior of the electronic self-energy. We extend this idea by introducing additional renormalization parameters to obtain consistent results also for the potential energies of a correlated many-particle system. The results are shown in Fig. 1, where the potential energies for DMFT, the old non-selfconsistent DΓA as well as our new consistent approach are depicted. While for the first two methods we obtain different results from one-particle (orange circles and blue diamonds) and two-particle (brown triangles and green hexagons) correlation functions an unambiguous result is obtained from our new consistent approach (red squares). In addition, our new technique provides also more reliable results for the transition line to the antiferromagnetic state as it is demonstrated in Fig. 2. There we can see that our new data (red squares) perfectly coincide with exact benchmark result from diagrammatic Monte Carlo calculations (yellow stars) while the old DΓA approach (green hexagons) predicts a much lower transition temperature. These successes are very encouraging to further develop these ideas to more complex multi-band systems which will allow us to consistently describe the physics of realistic correlated many-electron systems and materials.

WWW

https://www.physik.uni-hamburg.de/en/th1/ag-rohringer-georg.html

More Information

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Funding

DFG Emmy Noether project, 407372336

DFG Subject Area

307-02