The mystery of correlations

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

***J. Stobbe, G. Rohringer**, I. Institut für Theoretische Physk, Universität Hamburg*

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.
- In our project, we will overcome such difficulties by means of an effective renormalization of physical response functions.

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.

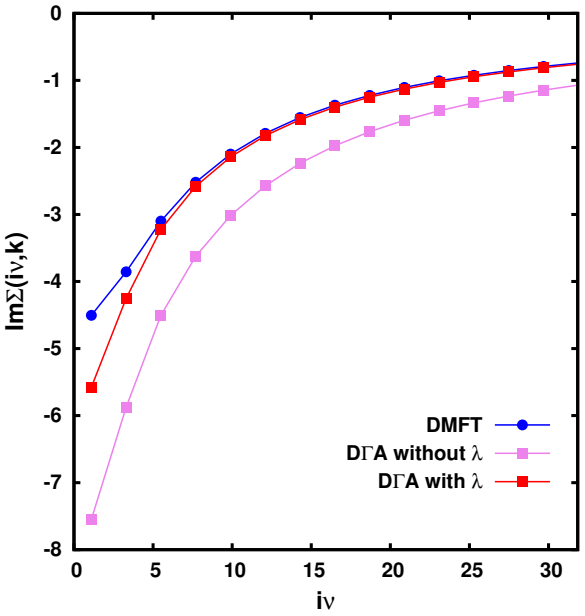

***Figure 1:** Self-energy $\Sigma(i\nu, \mathbf{k})$ of DMFT (blue circles) and the dynamical vertex approximatoin (DΓA), a diagrammatic extension of DMFT (red and pink squares), as a function of the fermionic Matsubara frequency ν. While the uncorrected DΓA result features an unphysical enhancement of the asymptotic high frequency behavior with respect to DMFT (pink squares), the introduction of a so called λ-correction mitigates this problem and restores the correct high-frequency tail (red squares).*

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 spectral function or from the 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]. Another good example is the dynamical vertex approximation (DΓA)[7] where the sum rule, which controls the asymptotic high frequency tail of the electronic self-energy, is violated (pink squares in Fig.1). One route to overcome this problem is the parquet formalism. Within

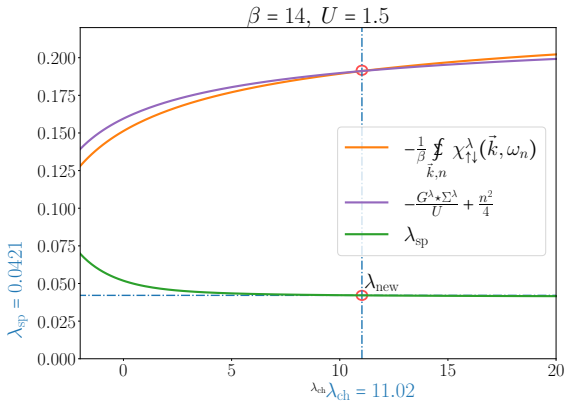

Figure 2: *Potential energies calculated form one-particle (pink) and two-particle (orange) correlation functions for the three-dimensional Hubbard model within DΓA as a function of the renormalization parameters λ_c and λ_s in the charge and spin channels, respectively.*

this approach a self-consistent renormalization of fluctuations in all scattering channels is performed which guarantees the fulfillment of certain sum rules and the asymptotic behavior of the self-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-band Hubbard model[8]. 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 inconsistencies. This consists in introducing an effective renormalization of the spin and charge susceptibilities. A preliminary version of this ideas 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 (see red squares in Fig. 1)[7]. We extend this idea by introducing additional renormalization parameters to obtain consistent results also for the potential and the kinetic energies of a correlated many-particle system. A first success has been already achieved by renormalizing both the charge and the spin susceptibility in such a way that the potential energies from one- and two-particle correlation functions coincide which corresponds to the crossing of the pink and orange lines for specific values of the renoramlization parameters λ_c and λ_s in Fig. 2. In the further course of the project we will extend 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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Project Partners

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