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

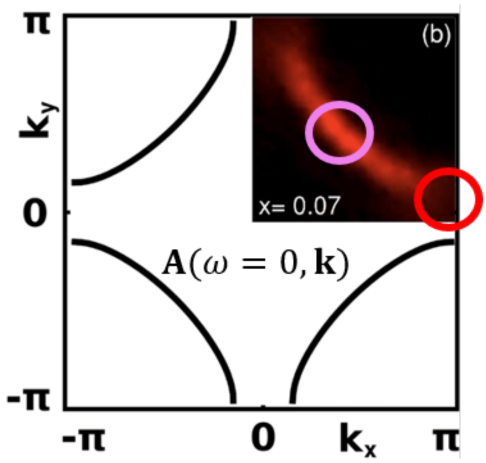

***Figure 1:** Angular resolved photo emission spectroscopy (ARPES) data for $La_{2-x}Sr_xCuO_4$ at $\omega = 0$ as a function of k_x and k_y. On can clearly observe a suppression of spectral weight at the antinodal point $\mathbf{k} = (0, \pi)$ (red circle) while at the nodal point $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$ the system is more metallic (pink circle). The figure has been readapted from Ref. [5].*

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 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]. A good example of the success of the diagrammatic extensions of DMFT for describing systems with strong local and nonlocal electronic correlations is the so-called pseudogap in the high-temperature superconducting cuprates. This feature consists in a suppression of spectral weight at the so-called antinodal momentum $\mathbf{k} = (0, \pi)$ and a metallic behavior (i.e., a high spectral weight) at the nodal point $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$. A corresponding experimental result for $La_{2-x}Sr_xCuO_4$ is depicted in Fig. [1] where the ARPES data for the cuprate compound $La_{2-x}Sr_xCuO_4$ clearly show the above described pseudogap feature. The corresponding theoretical results, which have been obtained through a simulation of the single band Hubbard model by means of a diagrammatic extension of DMFT, clearly reproduce the experimental findings as it can be seen in Fig. [2].

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 unfor-

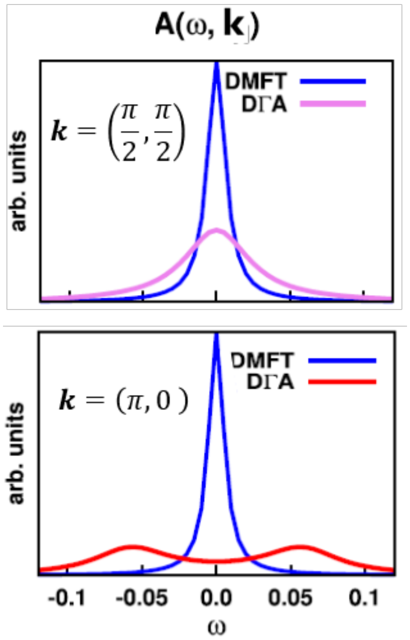

Figure 2: Spectral function $A(\omega, \mathbf{k})$ of the two-dimensional half-filled Hubbad model as obtained from the dynamical vertex approximation (DΓA), a diagrammatic extension of DMFT. While the spectral function of DMFT (blue) yields the same results for both $\mathbf{k}$*-points, the DΓA reproduces well the pseudogap feature indicated by ARPES measurements. The figure has been readapted from Ref. [6].*

tunately not the case for virtually all diagrammatic extensions of DMFT[6].

In our project, we will overcome this problem by introducing an effective renormalization of the spin- and charge-susceptibilities and apply this new approach to a specific diagrammatic extension of DMFT, the diagrammatic vertex approximation (DΓA). A simpler version of this idea has been already adopted within the DΓA where only the spin susceptibility has been renormalized in order to obtain the correct asymptotic behavior for the electronic self-energy self-energy[7]. We will apply our new and more complete technique to the the single band Hubbard model in order to test our new method for this probably most basic model for correlated electron systems. The actual calculations are numerical expensive and require the use of large high-performance computing system. Upon successful completion of our project, we expect to obtain a consistent description of the energetics (i.e., kinetic and potential energy) of correlated lattice electrons.

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More Information

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Project Partners

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