Effect of antiferromagnetic correlation to single-particle excitations in strongly correlated electron systems

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Abstract. An effect of antiferromagnetic fluctuations on single-particle excitations is examined on the basis of an extended dynamical mean-field theory that takes account of long-range spin fluctuations onto the local self energy. We demonstrate that the single-particle spectral intensity in the two-dimensional Hubbard model at half-filling exhibits the pseudo-gap behavior near the Fermi energy due to the critical antiferromagnetic fluctuations. We also show that for the symmetric case in the Anderson lattice model, the hybridized-band gap is enlarged by the antiferromagnetic fluctuations. In both models the antiferromagnetic fluctuations suppress the double occupancy of the correlated electrons.

1. Introduction
A long-standing issue in strongly correlated electron systems is how to describe microscopically the dichotomy between localized and itinerant characters of correlated electrons. A particle-hole pair of high-energy incoherent states represents a local spin, and an interaction between the local spins yields low-energy spin dynamics with proper momentum dependences. On the other hand, a low-energy electronic state is often described by a coherent quasiparticle, which has close interplay between the low-energy spin fluctuations. A subtle connection among the quasiparticles and the spin fluctuations leads to rich phenomena such as anisotropic superconductivity, electronic long-range orders, heavy fermions and so on.

Dynamical mean-field theory (DMFT) has been proven successfully to describe the dual nature of the electronic states in energy, e.g., the opening of the Mott gap at half-filling for sufficiently strong Coulomb repulsion [1, 2]. It is also possible to describe proper momentum dependences in two-particle fluctuations via local but energy-dependent vertices [1]. However, DMFT lacks nonlocal correlations in self energy, and an effect of spatial spin fluctuations have no influences on nature of single-particle quantities. The drawback becomes serious especially in the vicinity of the boundary of second-order phase transitions.

In the light of these circumstances, a hybrid approach has emerged [3]. We assume the local but energy-dependent irreducible vertices to construct the nonlocal fluctuations within the DMFT framework. Then, the nonlocal corrections from the spatial fluctuations are taken into account to improve the DMFT self energy. A similar approach named as the dynamical vertex approximation (DΓA) has recently been developed [4, 5]. In comparison with the cluster DMFT [6], the present approach has some advantages: (i) long-range fluctuations are taken
into account, (ii) the translational invariance is preserved, and (iii) only a similar computational effort as DMFT is required.

The formulation of the hybrid approach is found elsewhere [3]. Here we demonstrate the effect of the antiferromagnetic (AF) spin fluctuations onto the single-particle spectrum using the Hubbard model

\[
H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{ci\uparrow} n_{ci\downarrow},
\]

and the Anderson lattice model

\[
H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_f \sum_{i\sigma} n_{fi\sigma} + U \sum_i n_{fi\uparrow} n_{fi\downarrow} + V \sum_{i\sigma} \left( f_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.} \right),
\]

on the square lattice with the nearest neighbor hopping, i.e., \( \varepsilon_k = -2t(\cos k_x a + \cos k_y a) \). We set \( t = a = 1 \) and consider the case \( \langle n_{ci\sigma} \rangle = \langle n_{fi\sigma} \rangle = 1/2 \), \( \epsilon_f = -U/2 \) and \( U = 8 \) throughout this paper. The effective impurity problem in the DMFT framework is solved by the iterated perturbation theory [1, 3].

2. The effect of the spatial fluctuations on Hubbard model

Figure 1 shows the intensity map of the spectral weight, \( A(k, \omega) = -(1/\pi) \text{Im} G(k, \omega) \), along the high-symmetry lines of the Brillouin zone for \( T = 0.245 \), which is slightly higher than the Neel temperature, \( T_N \sim 0.24 \). The overall structure of the spectral intensity is roughly the same as that obtained by DMFT (not shown). In contrast to DMFT, the pseudo-gap behaviors at \( \omega = 0 \) appears in the coherent quasiparticle state due to the strong AF spin fluctuation (see, the X-M’ Fermi line). The opening of the pseudogap is consistent with that obtained by the cluster DMFT [6, 7].

![Figure 1](image1.png)

**Figure 1.** The contour plot of the single-particle spectrum \( A(k, \omega) \) along the high-symmetry lines of the Brillouin zone for \( T = 0.245 \). The pseudo-gap behavior is observed at the X-M’ (Fermi) line.

![Figure 2](image2.png)

**Figure 2.** The temperature dependences of the specific heat. The inset shows the \( T \) dependence of the double occupancy. The result of DMFT is shown for comparison.

Next, we show the \( T \) dependence of the specific heat in Fig. 2, which is calculated by the numerical differentiation of the internal energy. The result by DMFT is also shown for comparison. Owing to the short-range AF order, the specific heat is strongly enhanced toward \( T_N \). As shown in the inset, the double occupancy rapidly decreases toward the AF instability in contrast to the increasing behavior in DMFT. It should be noted that the strong enhancement in the specific heat near \( T_N \) originates mainly from the reduction of \( d \) rather than that of the kinetic energy. This suggests that the AF correlation enhances the tendency of the Mott localization.
3. The effect of the spatial fluctuations on Anderson lattice model

Let us turn to the case of the Anderson lattice model. We first show the $V$ dependence of the Neel temperature in Fig. 3. For small $V$, $T_N$ gradually increases due to the increase of the RKKY interaction, which is roughly proportional to $J^2/t$ with $J = 4V^2/U$. For larger $V$, the RKKY interaction competes with the collective Kondo effect, whose characteristic energy scale is given by $T_K/t \sim \sqrt{ge^{-1}/g}$ with $g = J/t$. As a result, the upper phase boundary becomes very steep in change of $V$. The resultant phase diagram is known as the Doniach phase diagram [8].

Figure 3. The $V$-$T$ phase diagram of the Anderson lattice model. The Neel temperature in small $V$ region is roughly determined by the RKKY interaction. The upper boundary of $V$ is remarkably steep due to the competition between the RKKY interaction and the collective Kondo effect.

Figure 4. The density of states with or without contributions from AF fluctuations. The inset shows the temperature dependence of the double occupancy. The hybridized-band gap is enlarged and the double occupancy is suppressed by the AF fluctuations.

Figure 4 shows the density of states for $V = 2.0$ and $T = 0.1$. In the symmetric case at half filling, the lower hybridized band is completely filled and the system becomes the Kondo insulator. As shown in Fig. 4, the effect of AF fluctuations enlarges the Kondo insulating gap as compared with that of DMFT, and enhances the peaks at gap edges. The $T$ dependence of the double occupancy is shown in the inset of Fig. 4. The effect of AF fluctuations becomes prominent below $T = 0.25$ and it suppresses considerably the double occupancy of $f$ electrons. These tendency may remain for heavy-fermion states when the electron density differs from half filling.

4. Summary and Outlook

We have demonstrated that the single-particle spectral intensity of the 2D Hubbard model at half filling shows the pseudo-gap behavior at the Fermi energy due to the critical AF fluctuation. The specific heat is considerably enhanced by the AF short-range order, which is accompanied by the reduction of the double occupancy, indicating the enhanced tendency of the Mott localization. More detailed results may be found in the literature [3]. For the Anderson lattice model, the Kondo insulating gap is enlarged by the AF fluctuations with decrease of the double occupancy.

Now, we discuss the possible future applications using the extended DMFT. A straightforward application is to examine a particle-hole asymmetric case with the longer range hoppings and/or the electron/hole doping. For this purpose, the recently proposed continuous-time quantum monte carlo algorithm would be the most efficient [9, 10]. For the particle-hole symmetric case, the AF fluctuation always dominates over the superconducting one. Away from the symmetric case, the superconducting fluctuation may have a chance to play a dominant role.
This interesting issue can be managed by using the fluctuation-exchange type approach with the dynamical vertices used in the present work [3].

Throughout this work, we have updated the self energy only once. Therefore, the spatial fluctuation contains no feedback from the formation of the pseudo gap. If such a feedback is taken into account, the critical AF fluctuation as well as the pseudo-gap behavior would slightly be suppressed. A full self-consistent calculation may bring about further insight.

Since DMFT has a formal resemblance to the coherent-potential approximation (CPA) [11, 12], disordered systems have become under the scope of investigation.

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