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Interplay between magnetic correlation and evolution of Fermi liquid in the periodic Anderson model

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Abstract. A simple effective scheme to improve the self energy obtained by the dynamical mean field theory is proposed, in which a feedback of magnetic fluctuations is taken into account. We demonstrate effectiveness of the scheme for the two-dimensional periodic Anderson model by investigating the effect of the magnetic fluctuation in the formation of heavy quasiparticles. It is found that the spectral intensity near the Fermi level is strongly suppressed by the antiferromagnetic fluctuation slightly above the magnetic instability.

1. Introduction

In the heavy-fermion systems, the Kondo effect leading to a coherent Fermi-liquid state and the inter-site interaction for a magnetic order often compete with each other. The heavy quasiparticle emerges as a consequence of the strong local fluctuations, and simultaneously the evolution is affected by developing magnetic fluctuations. As a result, the interplay between nonlocal magnetic fluctuations and the evolution of the Fermi liquid has attracted considerable interest to elucidate the origin of the characteristic phenomena observed in the heavy fermion systems, especially so-called the quantum critical behaviors. However, a useful scheme to treat effects of the magnetic fluctuations and the strong local correlations on the same footing is still under development. In the present study, we propose a simple effective scheme to treat the strong local correlations and the nonlocal magnetic fluctuations based on the dynamical mean field theory (DMFT). We demonstrate effectiveness of the scheme for the periodic Anderson model by showing the effect of the antiferromagnetic spin fluctuations on the formation of the heavy quasiparticles.

2. Model and Method

In order to demonstrate our scheme, let us consider the periodic Anderson model on a two-dimensional square lattice,

$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma}\{(\varepsilon_{\boldsymbol{k}}-\mu)c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + (\varepsilon^f_{\boldsymbol{k}}-\mu)f^\dagger_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma} + V(c^\dagger_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma} + f^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma})\} + U\sum_i f^\dagger_{i\uparrow}f_{i\uparrow}f^\dagger_{i\downarrow}f_{i\downarrow},$$

$$\varepsilon_{\boldsymbol{k}} = -2(\cos k_x + \cos k_y), \qquad \varepsilon^f_{\boldsymbol{k}} = \varepsilon^f + \alpha\varepsilon_{\boldsymbol{k}},$$

where ε^f denotes the f level and α is a dispersiveness coefficient of the f electron, and the nearest-neighbor hopping on the square lattice is assumed (the hopping energy of the conduction

electron and a lattice constant is set to be unity). In the present model, we introduce the energy dispersion of the f electron so that the metallic ground state can be realized in the model under the particle-hole symmetric condition between the f level ε^f, the on-site Coulomb energy U, and the chemical potential μ: $\varepsilon^f + U/2 = \mu = 0$.

To treat the strong local correlation between f electrons, we employ the DMFT, i.e., the local approximation for the self energy [1]. As an impurity solver in the DMFT framework, we adopt the iterative perturbation theory (IPT) [1, 2]. It is well known that the IPT is accurate to calculate the Green's function at wide temperature range in the presence of the particle-hole symmetry [3]. We calculate the local Green's function of f electrons $G_{ff}(z)$ by the DMFT with the IPT,

$$G_{ff}(z) = \frac{1}{N}\sum_{\boldsymbol{k}} G_{ff}(\boldsymbol{k}, z), \quad G_{ff}(\boldsymbol{k}, z) = \left(z - \varepsilon^f_{\boldsymbol{k}} - \Sigma(z) - \frac{V^2}{z - \varepsilon_{\boldsymbol{k}}} \right)^{-1},$$

where z denotes either the Matsubara frequency or the real frequency, and N represents a total number of the lattice points (hereafter a paramagnetic phase is considered and spin indices are omitted). In the IPT, the self energy is approximated by the second-order contribution in terms of the Weiss function $\mathcal{G}(z)$,

$$\begin{aligned} \Sigma(i\varepsilon_n) &\simeq U^2 T \sum_m \bar{\chi}_0(i\omega_m)\mathcal{G}(i\varepsilon_n + i\omega_m), \quad \bar{\chi}_0(i\omega_m) \equiv -T\sum_n \mathcal{G}(i\varepsilon_n)\mathcal{G}(i\varepsilon_n + i\omega_m), \\ \mathcal{G}(z)^{-1} &= G_{ff}(z)^{-1} + \Sigma(z). \end{aligned}$$

After the self-consistent solution of the Green's function is obtained in the IPT-DMFT framework, we take account of the magnetic fluctuations as follows. First, we construct the (longitudinal) spin susceptibility $\chi^{ff}_{\rm S}(\boldsymbol{q}, z)$ by the RPA-like procedure with use of the renormalized repulsion U^*,

$$\chi^{ff}_{\rm S}(\boldsymbol{q}, z) = \frac{\chi^{ff}_0(\boldsymbol{q}, z)}{1 - U^*\chi^{ff}_0(\boldsymbol{q}, z)}, \quad \chi^{ff}_0(\boldsymbol{q}, i\omega_m) = -\frac{1}{N}\sum_{\boldsymbol{k}} T\sum_n G_{ff}(\boldsymbol{k}, i\varepsilon_n) G_{ff}(\boldsymbol{k}+\boldsymbol{q}, i\varepsilon_n + i\omega_m).$$

Next, we improve the DMFT self energy by taking account of the spin fluctuations as

$$\Sigma(\boldsymbol{k}, i\varepsilon_n) = \Sigma(i\varepsilon_n) + \frac{UU^*}{2}\frac{1}{N}\sum_{\boldsymbol{q}} T\sum_m \left(\chi^{ff}_{\rm S}(\boldsymbol{q}, i\omega_m) - \chi^{ff}_{\rm S}(i\omega_m) \right) G_{ff}(\boldsymbol{k}+\boldsymbol{q}, i\varepsilon_n + i\omega_m), \quad (1)$$

where we have subtracted the local contributions in the second term, since it is already taken into account in the DMFT self energy, $\Sigma(i\epsilon_n)$. $\chi^{ff}_{\rm S}(z)$ is the local counterpart of the susceptibility defined by

$$\chi^{ff}_{\rm S}(z) \equiv \frac{\chi^{ff}_0(z)}{1 - U^*\chi^{ff}_0(z)}, \quad \chi^{ff}_0(i\omega_m) = -T\sum_n G_{ff}(i\varepsilon_n) G_{ff}(i\varepsilon_n + i\omega_m).$$

In fact, the $\boldsymbol{k}$-summation of $\Sigma(\boldsymbol{k}, i\varepsilon_n)$ in the above expression (1) gives the local self energy though the present framework is phenomenologically constructed. In the present framework, U^* is the phenomenological parameter, corresponding to the local and instantaneous approximation of the four-point vertex function in the longitudinal particle-hole channel [4]. Here, we have neglected the charge fluctuations because the charge fluctuations are strongly suppressed in our parameter range in question. Finally, we obtain the final expression of the spectral function $\rho_f(\boldsymbol{k}, \varepsilon)$ with including the spin fluctuations,

$$\rho_f(\boldsymbol{k}, \varepsilon) = -\frac{1}{\pi}{\rm Im}\left(z - \varepsilon^f_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, z) - \frac{V^2}{z - \varepsilon_{\boldsymbol{k}}} \right)^{-1}\Bigg|_{z=\varepsilon+i\eta}.$$

We have used $U = 8$, $V^2 = 3$, and $\alpha = 0.3$ in the present work. In the computation, we have solved the self-consistent equation in the DMFT scheme and the dynamical spin susceptibilities in the first Brillouin zone with equally spaced mesh of 256 × 256 and 2048 in the real frequency range, [-15,15]. Note that since all the above equations can be analytically continued explicitly, we have performed the computations in the real-frequency domain with the damping factor, $\eta = 0.01$.

3. Results

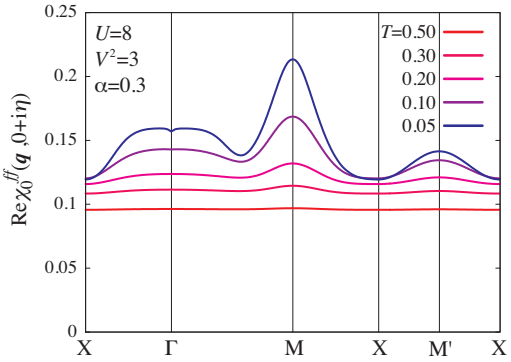

Figure 1. The f-electron static spin susceptibility (proper part) along the high symmetry line at $T = 0.50$, 0.30, 0.20, 0.10, and 0.05.

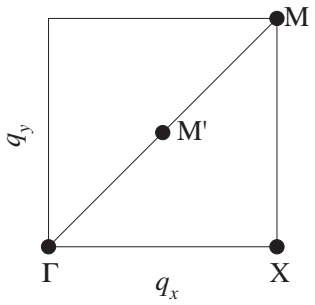

Figure 2. The high symmetry points of the first Brillouin zone.

At first, we show the T dependence of a proper part of the f-electron static spin susceptibility, $\mathrm{Re}\chi_0^{ff}(\boldsymbol{q}, 0+i\eta)$, along the high symmetry line of the first Brillouin zone in Fig. 1 (The definition of the high symmetry points is shown in Fig. 2). The peak of $\mathrm{Re}\chi_0^{ff}(\boldsymbol{q}, 0+i\eta)$ is always located at $\boldsymbol{q} = (\pi, \pi) \equiv \boldsymbol{Q}$ (M point) at all temperatures due to the perfect nesting across the hybridized bands, indicating that the antiferromagnetic fluctuation is dominant in the present system. In order to demonstrate the effect of the critical spin fluctuations, we choose the phenomenological parameter U^* so that the magnetic instability occurs at slightly below the lowest temperature in the present computation, i.e., $T = 0.05$. By the instability condition, $1 - U^* \mathrm{Re}\chi_0^{ff}(\boldsymbol{Q}, 0+i\eta) = 0$, we have chosen $U^* = 4.68$. In principle, the renormalized vertex U^* does depend on the temperature, however, we have neglected it for simplicity.

In the results with the spin fluctuation (denoted as DMFT+SF), the self energy is improved according to the expression (1). As shown in Fig. 3, the spectra of the f-electron density of states with or without the spin fluctuations exhibit considerable differences in approaching to the magnetic instability in spite of no essential differences at high temperatures. At temperatures below the characteristic temperature of the renormalized Fermi energy, the quasiparticle peak develops at the Fermi level in the spectrum without the spin fluctuation (Fig. 3(b)). On the other hand, in the spectrum with the spin fluctuation (Fig. 3(a)), the dip structure appears at the center of the quasiparticle peak, yielding the development of the pseudogap due to the critical spin fluctuations.

Next, we show the quasiparticle dispersion in the intensity map of the f-electron spectral function in Fig. 4. The f-electron spectral function without the spin fluctuation exhibits strong intensities corresponding to the dispersion of the heavy quasiparticle band near the Fermi level. The critical antiferromagnetic fluctuations strongly influence the electronic states near the Fermi

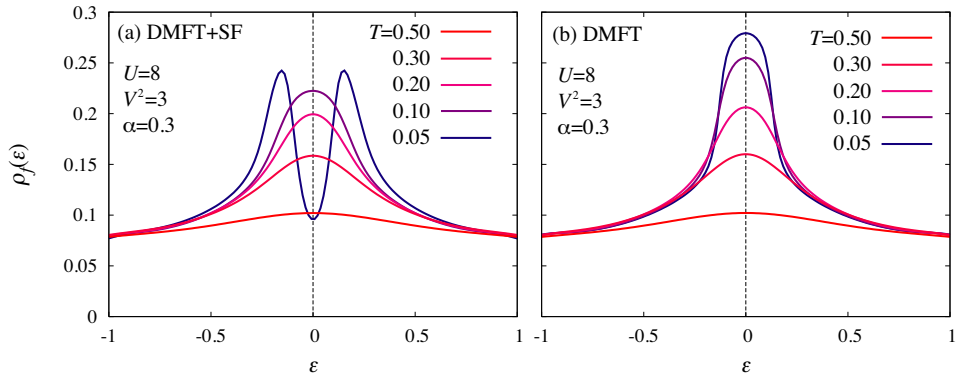

Figure 3. The density of states of f electron with the spin fluctuation (a), and without it (b) at $T = 0.50$, 0.30, 0.20, 0.10, and 0.05.

level, leading to considerable suppression of the spectral intensity near the Fermi level as shown in Fig. 4(a).

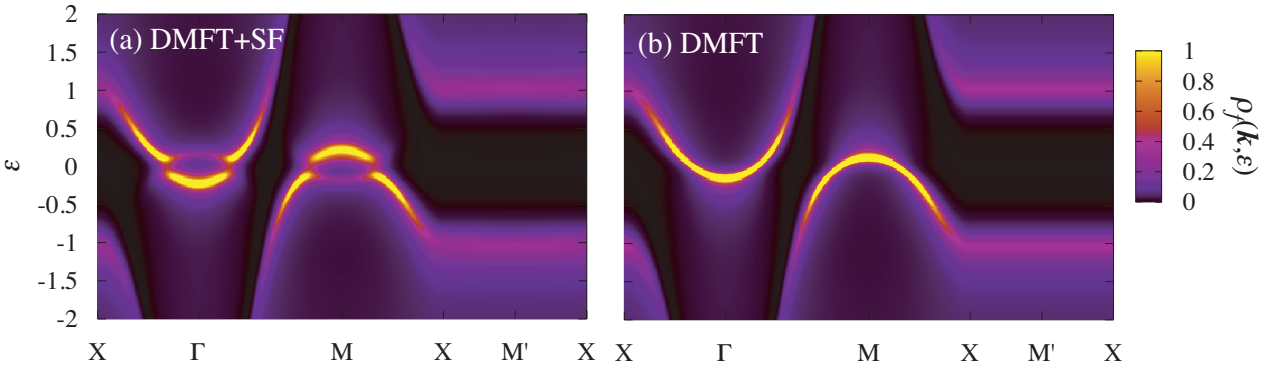

Figure 4. The intensity map of the spectral function of f electron with the spin fluctuation (a), and without it (b) at $T = 0.05$ in the vicinity of the antiferromagnetic instability.

4. Summary

We have proposed the simple scheme to treat the nonlocal magnetic fluctuations beyond the DMFT. The application to the periodic Anderson model on a square lattice clearly demonstrates that the evolution of the heavy quasiparticle is strongly suppressed by the critical antiferromagnetic spin fluctuations, yielding the pesudogap behavior in the f-electron spectrum near the Fermi level. The application to more realistic systems is left for future investigations.

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