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Magnetic properties of a Kondo insulator with RKKY interaction: extended dynamical mean field study

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Abstract
We study the Kondo lattice model with the Heisenberg-type RKKY exchange coupling among localized f spins in the presence of a magnetic field. By means of an extended dynamical mean field theory combined with the non-crossing approximation, we investigate the one-particle spectral function and the dynamical spin correlation function in the Kondo insulating phase. It is shown that the magnetic field and the RKKY exchange interaction both cause instability to the antiferromagnetic order with enhanced transverse spin fluctuations, which give rise to a strong renormalization of quasi-particles as the system approaches the quantum critical point. This leads to a tendency to retain the Kondo insulating gap up to rather large fields.

1. Introduction

Electron correlations caused by the interactions between conduction electrons and localized magnetic moments have provided a variety of important subjects in condensed matter physics. In dilute magnetic alloys, a local moment is screened by conduction electrons via the Kondo effect below its characteristic temperature, and the system is described as a local Fermi liquid [1]. In concentrated systems, such as heavy-fermion systems, the indirect exchange among the localized moments mediated by the RKKY interaction becomes important [2, 3]. The interplay between the Kondo effect and the RKKY interaction gives rise to competing phases in heavy-fermion systems.

Recent experimental observations of quantum critical behaviour in heavy-fermion materials have attracted renewed interest in this field. In $CeCu_{6-x}Au_x$ [4] and $YbRh_2Si_2$ [5], the system is driven to the antiferromagnetic phase by alloying, applying pressure, etc. In the vicinity of the quantum critical point, both Kondo and RKKY interactions become essential and physical properties observed in this region differ from those of ordinary Fermi liquids [6]. Experimental observations of such non-Fermi-liquid behaviour [7] stimulated detailed theoretical study beyond the standard framework [8–11] of the quantum critical point [12].

The interplay between Kondo and RKKY interactions has been investigated using various methods such as slave-particle mean field theory [13, 14], large-N expansion [15], quantum Monte Carlo (QMC) simulations [16], dynamical mean field theory (DMFT) [17–20], etc. Recently, an extension of the dynamical mean field theory has been developed [21–24], which allows us to incorporate spatially extended spin correlations. Si *et al* have addressed the problem of non-Fermi-liquid behaviour near the quantum critical point by the extended-DMFT (EDMFT) analysis of the Kondo lattice model (KLM) with the Ising-type RKKY exchange among localized moments [25, 26]. These investigations focused on magnetic properties around the quantum critical point in heavy-fermion systems. Also, Sun and Kotliar have addressed the same issues by exploiting the periodic Anderson model (PAM) [27, 28].

Magnetic fields should play a particularly important role if the system is in the proximity of magnetic instability, because the applied fields may possibly trigger a magnetic phase transition. Recent studies on the half-filled KLM in two dimensions based on mean field theory and QMC simulations have indeed found that the magnetic field induces a second-order phase transition from the paramagnetic to the transverse antiferromagnetic phase [29, 30]. Also, in our previous paper we have investigated the field-induced phase transition in the three-dimensional case [31]. We have studied the half-filled PAM by means of DMFT combined with QMC. However, DMFT cannot incorporate inter-site fluctuations due to the RKKY interaction. It is desirable to investigate the effects of the RKKY interaction on electronic properties by means of EDMFT.

In this paper, we study the KLM with the Heisenberg-type RKKY exchange among localized f spins. By means of EDMFT combined with the non-crossing approximation (NCA) [32–35], the one-particle spectral function and the dynamical spin susceptibility are calculated. We also investigate the field-induced antiferromagnetic instability and discuss the remarkable behaviour in spectral properties in the vicinity of the critical point.

The paper is organized as follows. In the next section we briefly summarize our model and method. In section 3, we present our numerical results, and discuss the effects of the RKKY interaction in a magnetic field. A brief summary is given in section 4.

2. Model and method

2.1. Kondo lattice model

We study the following Kondo lattice model including the Heisenberg-type RKKY interaction:

$$H = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - \mu \sum_{i} c_{i\sigma}^{\dagger} c_{i\sigma} + J_{\mathrm{K}} \sum_{i} \mathbf{S}_i^{\mathrm{c}} \cdot \mathbf{S}_i^{\mathrm{f}} + \frac{J}{2} \sum_{\langle i,j\rangle} \mathbf{S}_i^{\mathrm{f}} \cdot \mathbf{S}_j^{\mathrm{f}} - g\mu_{\mathrm{B}} B \sum_{i} [S_{iz}^{\mathrm{c}} + S_{iz}^{\mathrm{f}}], \tag{1}$$

where $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) annihilates (creates) a conduction electron on the ith site with spin σ and $\mathbf{S}_i^{\mathrm{c}}$ ($\mathbf{S}_i^{\mathrm{f}}$) is the spin operator for a conduction electron (spin-$\frac{1}{2}$ localized f electron). Here, t is the nearest-neighbour hopping matrix in the conduction band (referred to as the c band in the following), J_{K} describes the on-site Kondo coupling, and J denotes the RKKY exchange among the nearest-neighbour f spins. We consider the three-dimensional simple cubic lattice with dispersion $\varepsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z)$ and the RKKY interaction $J_q = J(\cos q_x + \cos q_y + \cos q_z)$. We focus on the Kondo insulating phase at half-filling, and take half the band width as the energy unit. The magnetic field B applied along the z direction is coupled to both of the c and f electrons. We assume that the g factors of the c and f electrons are the same, and set $g\mu_{\mathrm{B}} = 1$. We use the Kondo coupling $J_{\mathrm{K}} = 0.5$ in the following discussions.

2.2. Extended DMFT for the Kondo lattice model

DMFT is a powerful framework to study strongly correlated electron systems. Since its power was proved by providing the first unified scenario for the longstanding problem of the Mott transition in the Hubbard model [36], various correlated electron models have been studied by using DMFT [17–20, 34, 36–45]. EDMFT is an extension of DMFT so as to allow dynamical treatment of inter-site interactions, which can be dealt with only at the mean field level within the standard DMFT framework. EDMFT has been successfully applied to the Kondo lattice model [26, 46, 47], the periodic Anderson model [27], the extended Hubbard model [48], the t–J model [35], etc.

In EDMFT the original lattice model is mapped onto an effective impurity model with a bosonic bath in addition to a fermionic bath that is included in the standard DMFT. The bosonic effective bath describes a fluctuating magnetic field and allows dynamical treatment of inter-site spin correlations. This approximation becomes exact in the limit of infinite dimensions, $d \to \infty$, provided that t and J are scaled as $t/\sqrt{d}$ and $J/\sqrt{d}$ respectively. It may give a good approximation even in three dimensions. We assume the paramagnetic Kondo insulating phase without long-range order. In this case, the Kondo lattice model (1) can be mapped onto the following Bose–Fermi Kondo Hamiltonian [23] as an effective impurity model:

$$H_{\mathrm{EDMFT}} = H_{\mathrm{loc}} + H_{\mathrm{bath}} + H_{\mathrm{mix}}, \tag{2}$$

$$H_{\mathrm{loc}} = -\mu \sum_{\sigma} c_{\sigma}^{\dagger} c_{\sigma} + J_{\mathrm{K}} \mathbf{S}^{\mathrm{c}} \cdot \mathbf{S}^{\mathrm{f}} - B S_z^{\mathrm{c}} - \tilde{B} S_z^{\mathrm{f}}, \tag{3}$$

$$H_{\mathrm{bath}} = \sum_{k,\sigma} E_{k\sigma} a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{q,\alpha} \omega_{q\alpha} h_{q\alpha}^{\dagger} h_{q\alpha}, \tag{4}$$

$$H_{\mathrm{mix}} = V \sum_{k,\sigma} [c_{\sigma}^{\dagger} a_{k\sigma} + a_{k\sigma}^{\dagger} c_{\sigma}] + I \sum_{q,\alpha} S_{\alpha}^{\mathrm{f}} [h_{q\alpha} + h_{-q\alpha}^{\dagger}]. \tag{5}$$

Here, H_{loc} is the local part of the effective Hamiltonian at the site chosen as an 'impurity', which includes the Hartree contribution of the RKKY interaction among the f spins, $\tilde{B} = B - 2J_{q=[0,0,0]} \langle S_z^{\mathrm{f}} \rangle S_z^{\mathrm{f}}$. The effective baths are described as H_{bath}, where $a_{k\sigma}^{\dagger}$ creates a fermionic bath with the dispersion $E_{k\sigma}$, and $h_{q\alpha} (\alpha = x, y, z)$ creates a bosonic bath with the dispersion $\omega_{q\alpha}$. The latter incorporates the effect of a fluctuating magnetic field. The 'impurity' part and the effective baths are mixed by H_{mix}, where the electron (spin) of the 'impurity' couples to a fermionic (bosonic) bath via V (I). The parameters for the effective baths, $E_{k\sigma}$, $\omega_{q\alpha}$, V and I, are determined self-consistently by equating the Green function and the spin susceptibility obtained in the effective impurity model with those in the original lattice model. The local Green function for c electrons and the susceptibility for f moments are defined as $G_{\mathrm{c}\sigma}(\tau) = -\langle T_{\tau} c_{i\sigma}(\tau) c_{i\sigma}^{\dagger}(0) \rangle$ and $\chi_{\mathrm{f}\alpha}(\tau) = \langle T_{\tau} S_{i\alpha}^{\mathrm{f}}(\tau) S_{i\alpha}^{\mathrm{f}}(0) \rangle$, which are calculated by solving the impurity model. We solve the effective Hamiltonian H_{EDMFT} by means of NCA [32–34] and calculate $G_{\mathrm{c}\sigma}^{\mathrm{imp}}$ and $\chi_{\mathrm{f}\alpha}^{\mathrm{imp}}$ [35]. The Green function and the susceptibility satisfy the following equations:

$$G_{\mathrm{c}\sigma}^{\mathrm{imp}}(\omega) = [\omega + \mu + \tfrac{1}{2}\sigma B - G_{a\sigma}(\omega) - \Sigma_{\sigma}(\omega)]^{-1}, \tag{6}$$

$$\chi_{\mathrm{f}\alpha}^{\mathrm{imp}}(\omega) = [G_{h\alpha}(\omega) + M_{\alpha}(\omega)]^{-1}, \tag{7}$$

where $G_{a\sigma}(\omega)$ and $G_{h\alpha}(\omega)$ describe the effective fermionic and bosonic baths,

$$G_{a\sigma}(\omega) = \sum_{k} \frac{V^2}{\omega - E_{k\sigma}}, \tag{8}$$

$$G_{h\alpha}(\omega) = \sum_{q} \left[\frac{I^2}{\omega - \omega_{q\alpha}} - \frac{I^2}{\omega + \omega_{q\alpha}} \right]. \tag{9}$$

We can obtain the momentum-independent self-energy Σ_σ and M_α with these equations.

The local Green function and susceptibility in the lattice system are obtained in terms of the self-energy Σ_σ and M_α by using the relations

$$G_{c\sigma}^{\mathrm{loc}}(\omega) = \int \mathrm{d}\varepsilon \, \frac{\rho_t(\varepsilon)}{\omega + \mu + \frac{1}{2}\sigma B - \varepsilon - \Sigma_\sigma(\omega)}, \tag{10}$$

$$\chi_{f\alpha}^{\mathrm{loc}}(\omega) = \int \mathrm{d}\varepsilon \, \frac{\rho_J(\varepsilon)}{M_\alpha(\omega) + \varepsilon}, \tag{11}$$

where $\rho_t(\varepsilon)$ and $\rho_J(\varepsilon)$ are the density of states for the free c electrons and bosons representing spin fluctuations, which are defined as $\rho_t(\varepsilon) = \frac{1}{N}\sum_k \delta(\varepsilon - \varepsilon_k)$ and $\rho_J(\varepsilon) = \frac{1}{N}\sum_q \delta(\varepsilon - J_q)$. Equations (6)–(11) complete the self-consistent loop.

3. Results

We first discuss how the RKKY exchange among f spins renormalizes the one-particle spectrum and the spin dynamics at $B = 0$. The one-particle Green function $G_{c\sigma}(k, \omega)$ for conduction electrons is calculated with the self-energy $\Sigma_\sigma(\omega)$,

$$G_{c\sigma}(k, \omega) = \frac{1}{\omega + \mu + \frac{1}{2}\sigma B - \varepsilon_k - \Sigma_\sigma(\omega)}. \tag{12}$$

In figure 1, we plot the one-particle spectral function $A_c(k, \omega) = -\mathrm{Im}\, G_{c\sigma}(k, \omega)/\pi$ for different values of the RKKY interaction J at a given temperature $T = 0.05$. In the absence of J, the spectrum acquires an insulating gap resulting from the Kondo coupling J_K, since we deal with the half-filled band here. The size of the gap Δ can be defined as the energy difference between two peaks with the lowest excitation energy, which are located at $k = [0, 0, 0]$ and $k = [\pi, \pi, \pi]$. The gap is almost unchanged upon introducing the RKKY interaction. This result partly comes from the NCA approximation, which has a tendency to overestimate the strength of Kondo singlets. We see, however, that the sharp peaks located around $k = [\pi/2, \pi/2, \pi/2]$ are suppressed and shifted to lower frequencies as the RKKY interaction increases, signalling that the local singlet state gradually becomes unstable in the presence of the RKKY interaction.

The effects of the RKKY interaction are observed more clearly in spin excitations. We calculate the dynamical spin susceptibility $\chi_{f\alpha}(q, \omega)$ with two-particle self-energy $M_\alpha(\omega)$,

$$\chi_{f\alpha}(q, \omega) = \frac{1}{M_\alpha(\omega) + J_q}. \tag{13}$$

In figure 2 we plot the imaginary part of the dynamical susceptibility $\mathrm{Im}\, \chi_f(q, \omega)$ for different values of J. The dominant structure in $\mathrm{Im}\, \chi_f(q, \omega)$ is the low-frequency peak featuring spin-triplet excitations. As the RKKY interaction increases, the spin-triplet peak at $q = [\pi, \pi, \pi]$ is strongly enhanced and the position of the peak shifts to lower frequencies, indicating that the system gradually approaches the antiferromagnetic instability.

We now discuss how the effects of the RKKY interaction are modified in the presence of a magnetic field. In figure 3 the one-particle spectra for up-spin electrons, $A_{c\uparrow}(k, \omega)$, are shown at $B = 0.3$. We recall that the Zeeman splitting due to the magnetic field pushes $A_{c\uparrow}(k, \omega)$ down to the negative-frequency side, so that the peak position at $k = [0, 0, 0]$ is shifted below the Fermi level, and thus the insulating gap is closed. This is indeed observed in the results for $J = 0$ in figure 3. Upon introduction of J, there appear two notable features. First, the effective Zeeman shift is increased in the presence of J, which is seen in the high frequency region of figure 3. This is caused by the competition between the Kondo and RKKY couplings.

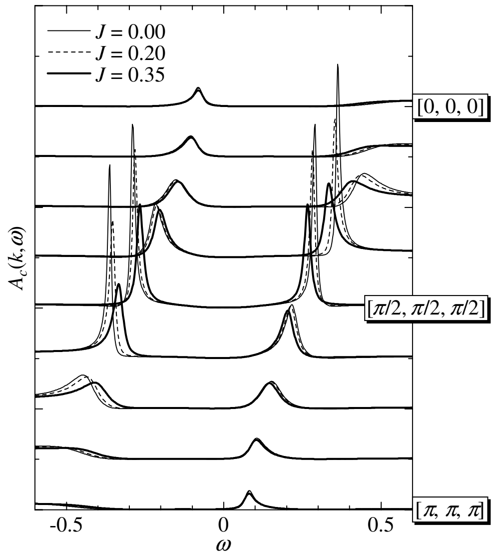

Figure 1. The momentum resolved one-particle spectra $A_c(k,\omega)$ at $J_K = 0.5$, $T = 0.05$ for different values of the RKKY interaction J. The data are plotted along the [1, 1, 1] direction in the k-space.

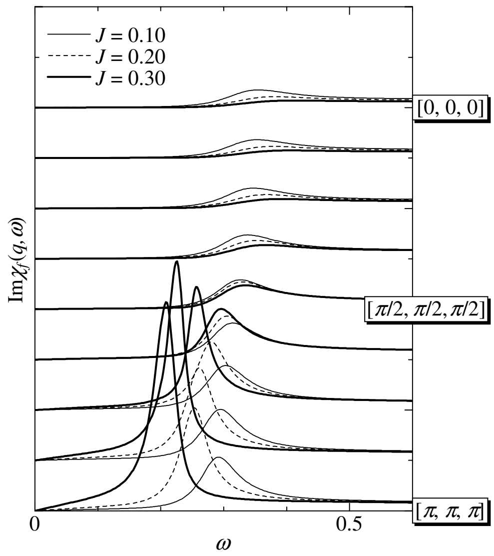

Figure 2. The dynamical spin susceptibility, Im $\chi_f(q,\omega)$, at $J_K = 0.5$ and $T = 0.05$ for different values of the RKKY interaction J.

For $J = 0$, the Kondo-singlet formation suppresses the effect of the Zeeman shift. Since the RKKY interaction enhances spin fluctuations of f electrons, it makes the Kondo effect weaker, thus reviving the large Zeeman shift.

Another important feature is the characteristic low-energy behaviour. For example, in the low-energy region for $J = 0.3$, the dispersion is highly renormalized to form a flat band around

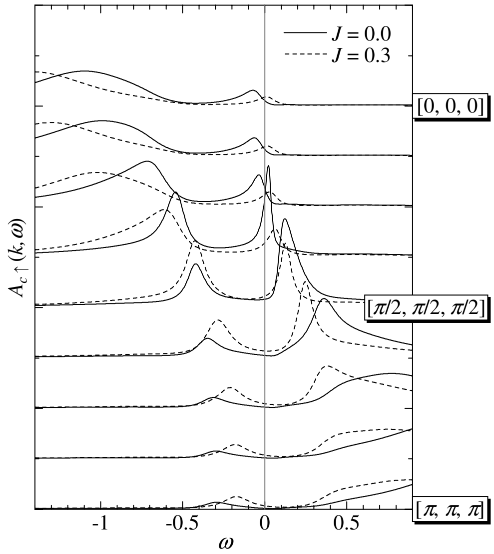

Figure 3. The one-particle spectral function for up-spin (majority-spin) electrons, $A_{c\uparrow}(k, \omega)$, at the magnetic field $B = 0.3$: $J_K = 0.5$, $T = 0.05$.

$\omega \sim 0$, which cannot be explained in terms of the effective Zeeman shift mentioned above. Such behaviour is seen more clearly in the quasi-particle dispersion of c electrons, $\omega_{c\sigma}(k)$, plotted in figure 4. This remarkable effect is regarded as the mass enhancement caused by critical f-spin fluctuations. In fact, the system at $J = 0.3$ is very close to the quantum phase transition, as discussed momentarily below. Conduction electrons scattered by such critical f-spin fluctuations get heavier, resulting in the flat dispersion. The corresponding gap is shown in figure 5 as a function of the field. In the absence of the RKKY interaction, the gap is reduced linearly and closed at the field corresponding to the gap size $B \sim 0.16$. As the RKKY interaction is increased, the gap can persist up to larger fields, reflecting the renormalization effect mentioned above.

In order to see how f-spin fluctuations behave in magnetic fields, we plot the field dependence of the imaginary part of the dynamical susceptibility $\mathrm{Im}\,\chi_{f\alpha}(q = [\pi, \pi, \pi], \omega)(\alpha = x, z)$ in figures 6 and 7. Comparing the susceptibility for $J = 0.1$ and 0.3 at $B = 0$, one can see that $[\pi, \pi, \pi]$ triplet modes are softened in the presence of the RKKY interaction. As the magnetic field is introduced, the longitudinal (z-component) and the transverse (x-component) susceptibilities exhibit different properties. Since $\mathrm{Im}\,\chi_{fz}(q = [\pi, \pi, \pi], \omega)$ excites an $S_z = 0$ triplet mode, its peak position is mostly unchanged even at finite fields, as is seen both for the $J = 0.1$ and 0.3 cases. On the other hand, the transverse susceptibility $\mathrm{Im}\,\chi_{fx}(q = [\pi, \pi, \pi], \omega)$ shows a splitting in the spectrum, corresponding to $S_z = \pm 1$ triplet modes. The peak on the higher-energy side is smeared considerably by the lifetime effect. It should be noticed here that the peak structure, which is shifted to lower frequencies, gets sharper as B increases, and this tendency becomes more significant as J becomes large. For example, for the $J = 0.3$ case, although weak magnetic fields ($B = 0.1$) merely suppress spin fluctuations and thus reduce the spin-triplet peak, larger magnetic fields ($B = 0.2$) increase the peak intensity again, signalling that the system approaches the antiferromagnetic instability. To see the antiferromagnetic instability directly, we show the transverse static susceptibility of localized f spins, $\chi_{fx}(q = [\pi, \pi, \pi])$, in figure 8. For smaller

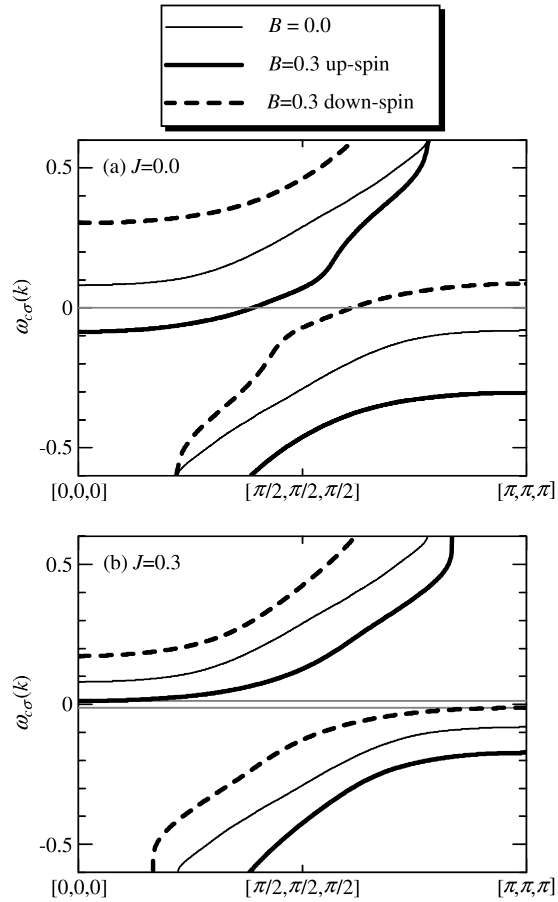

Figure 4. The quasi-particle dispersion $\omega_{c\sigma}(k)$ for (a) $J = 0.0$ and (b) $J = 0.3$. The dispersion is obtained by tracing the peak position of the one-particle spectra $A_c(k, \omega)$.

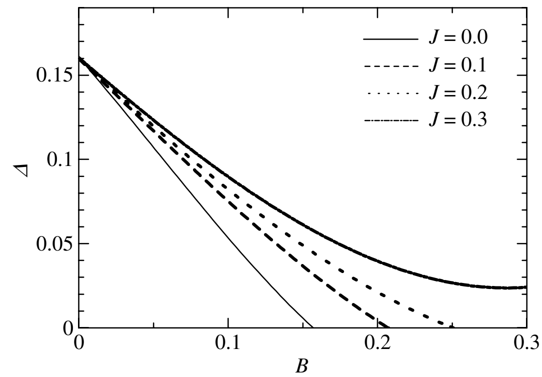

Figure 5. The magnetic field dependence of the gap for different values of J.

RKKY couplings ($J = 0.1, 0.2$) there is no indication of the instability as the magnetic field increases. We can see the rapid increase of $\chi_{fx}(q = [\pi, \pi, \pi])$ for $J = 0.3$ reflecting the

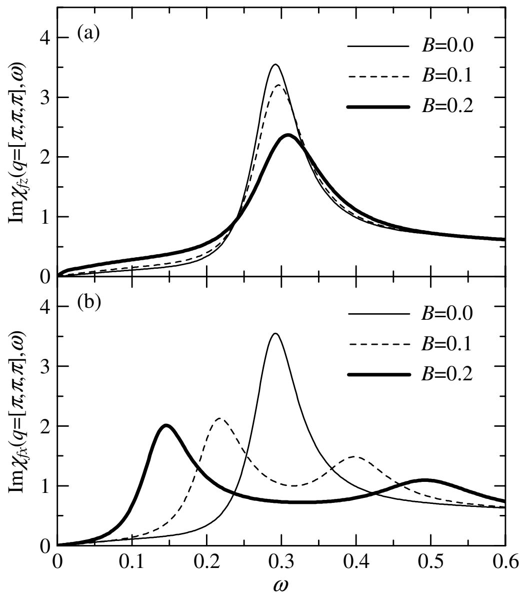

Figure 6. The imaginary part of the dynamical susceptibility $\mathrm{Im}\,\chi_{\mathrm{f}\alpha}(q = [\pi, \pi, \pi], \omega)$: (a) z direction and (b) x direction for different magnetic fields at $J = 0.1$.

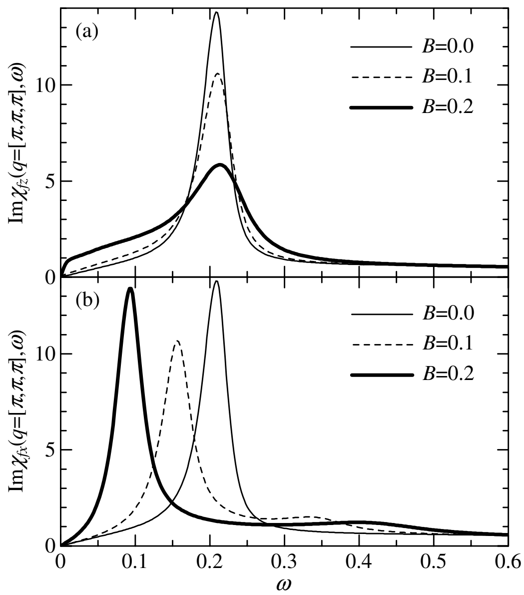

Figure 7. The same plots of the dynamical susceptibility as in figure 6. The RKKY interaction is chosen as $J = 0.3$.

antiferromagnetic instability: the system is driven to the transverse antiferromagnetic phase (x–y plane) with finite values of z-components (canted order).

The above characteristic properties also affect the static quantities in magnetic fields. For instance, we plot the magnetization curve in figure 9. At $J = 0$, M_{f} (M_{c}) has a relatively

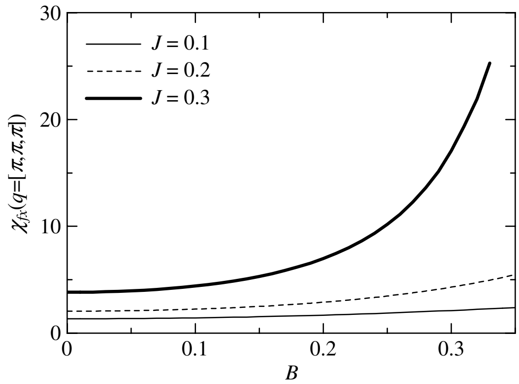

Figure 8. The transverse spin susceptibility in the x direction $\chi_{fx}(q = [\pi, \pi, \pi])$ as a function of the magnetic field B for different strengths of the RKKY interaction J.

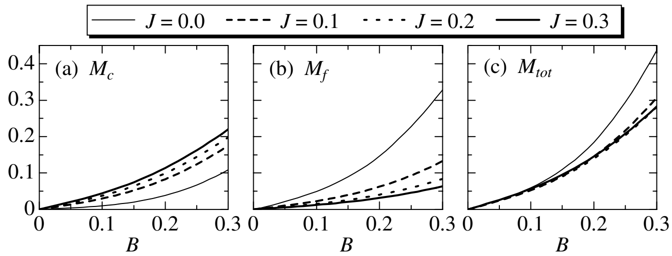

Figure 9. The magnetization process: (a) c electrons, (b) f electrons and (c) the total contribution. M_c, M_f and M_{tot} are defined by $M_c = \langle S_z^c \rangle$, $M_f = \langle S_z^f \rangle$ and $M_{tot} = M_c + M_f$.

large (small) response to the field. As the strength of the RKKY interaction increases, M_f is suppressed whereas M_c is enhanced. The magnetic-field dependence indeed comes from the competition between the Kondo coupling and the RKKY interaction, as explained below. The increase of J has a tendency to suppress the Kondo singlet formation, so that the conduction electrons start to polarize rather freely for finite J, increasing the magnetization. On the other hand, M_f is generally suppressed with the increase of J. Such behaviour is consistent with the change of the density of states (DOS) shown in figure 10. Comparing the DOS between the cases of $J = 0$ and 0.3, we see that the effective Zeeman shift in conduction electrons is somewhat enhanced for $J = 0.3$, which is clearly observed around $|\omega| \sim 1$. This shift gives rise to the increment of M_c as seen in figure 9. Note that the clear spin-gap behaviour expected at zero temperature in the magnetization process is obscured at finite temperature ($T = 0.05$) in figure 9, although it shows a sign of the spin-gap formation: the curvature of the magnetization is upturned around the field roughly corresponding to the spin-gap energy deduced from the one-particle spectra and the dynamical spin susceptibilities. For instance, at $J = 0$ the magnetization curves show a rather clear upturn around $B \sim 0.2$, which indeed signals the spin-gap formation. On the other hand, as the RKKY interaction J increases, it gets more difficult to see the spin-gap formation in the magnetization process, since the introduction of J suppresses the Kondo-singlet formation, making the size of the spin gap smaller.

Finally, we make a comment on the low-energy behaviour of the DOS in figure 10. If we look at the DOS around $\omega \sim 0$, the shift of the peak structure is smaller for $J = 0.3$ than $J = 0$, contrary to the effective Zeeman shift. This is what we have claimed as the

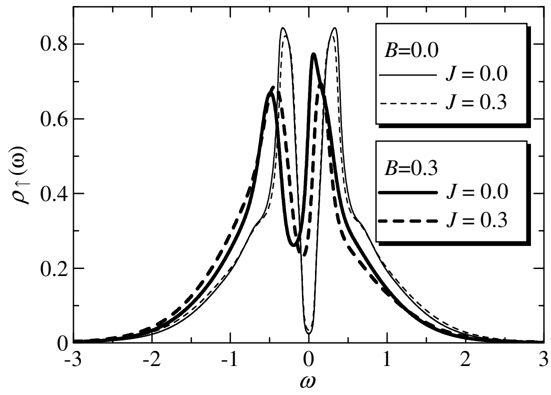

Figure 10. The density of states for up-spin conduction electrons for some different choices of the magnetic field B and the RKKY interaction J.

mass renormalization effect due to critical transverse f-spin fluctuations in figure 3; it is a typical correlation effect between conduction electrons and f spins, which is beyond the naive mean-field picture.

4. Summary

We have studied the KLM with the RKKY exchange interaction among local f spins in the presence of a magnetic field. For this purpose we have exploited an extended version of DMFT combined with NCA. This approach enables us to treat inter-site spin correlations dropped in the DMFT framework. By investigating the one-particle spectral function and the dynamical spin susceptibility, we have confirmed that the RKKY interaction has a tendency to enhance field-induced magnetic instability to the transverse magnetic order of f spins, as should be expected. We have clarified two characteristic features caused by the competition of the Kondo and RKKY interactions in magnetic fields. One is a simple mean-field type effect: the RKKY interaction enhances the Zeeman shift for conduction electrons, which modifies the profile of the one-particle spectrum at high frequencies as well as the magnetization curve. Another important feature is a renormalization effect observed in the low-energy region: the quasi-particle spectrum gets renormalized to form heavy quasi-particles when the system is close to the phase transition point. This effect appears as if the RKKY interaction protects the Kondo insulating gap in magnetic fields. Anyway, this remarkable feature at low energies is a typical correlation effect beyond the mean field picture, which characterizes the critical region of the field-induced phase transition in the Kondo insulator.

Field-induced transitions to the transverse antiferromagnetic order should be observed in heavy-fermion Kondo insulators. Unfortunately, there have been few examples of such transitions reported so far. Recently, it has been experimentally found [49, 50] that a typical filled skutterudite, $CeOs_4Sb_{12}$, which may be classified as an Kondo insulator, exhibits a field-induced magnetic phase transition. This transition could be a transition to the transverse antiferromagnetic phase discussed here, although more detailed study should be done since the above skutterudite has rather complicated electronic structure including orbital degrees of freedom. We think that a variety of compounds exhibiting such field-induced transitions may be found in the class of heavy-fermion Kondo insulators.

Acknowledgments

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