Title

Spin susceptibility of magnetic-ion-diluted Kondo insulators

Author(s)

Yasuteru Sekiya, Hirofumi Hada, and Tetsuya Mutou

Journal

Journal of the Physical Society of Japan > Volume 80, Number 3

Published

February 25, 2011

URL

https://doi.org/10.1143/JPSJ.80.034703

Spin susceptibility of magnetic-ion-diluted Kondo insulators

Yasuteru Sekiya, Hirofumi Hada, and Tetsuya Mutou*

Interdisciplinary Faculty of Science and Engineering, Shimane University, Shimane 690-8504, Japan

The static spin susceptibility and spectral function of the system corresponding to the magnetic-ion-diluted Kondo insulator is calculated using the framework of dynamical mean-field theory with a coherent potential approximation. The system is described by a periodic Anderson model with randomly distributed impurity sites which have no f electron. The impurity concentration dependence of the static spin susceptibility in the present result is in qualitative agreement with the experimental magnetic susceptibility measurements of (Yb,Lu)B_{12}.

KEYWORDS: Kondo insulator, spin susceptibility, dynamical mean-field theory

1. Introduction

Heavy fermion systems have received considerable attention because of their various ground states, some of which can exhibit superconductivity. Certain heavy fermion compounds have an insulating (or semiconducting) ground state, and are referred to as Kondo insulators (or semiconductors). The origin of the tiny energy gap in these compounds has attracted interest, and it is currently believed that the tiny energy gap is essentially a hybridization gap, which is renormalized by a strong correlation effect.1,2) There have been experimental studies in which non-magnetic ions were substituted for magnetic ions in heavy fermion compounds to investigate the relationship between heavy fermion systems and single Kondo impurity systems.3)

For Kondo insulators, magnetic-ion dilution experiments are another important area of investigation, and play an essential role in the study of the properties of the tiny energy gap.4,5) In theoretical studies of heavy fermion systems, including Kondo insulators, several theoretical and numerical methods to treat the strong correlation effect have been developed. In these methods, dynamical mean-field theory (DMFT) has been effectively used to investigate strongly correlated electron systems.6) In order to study the above magnetic-ion-diluted system theoretically, however, one must also appropriately treat the randomness effect caused by non-magnetic ions distributed randomly at the same time.

---

*E-mail address: tmutou@riko.shimane-u.ac.jp

One of the authors developed a scheme by which one can treat the local electronic correlation effect and the randomness effect on the same footing by including a coherent potential approximation (CPA) in the DMFT using a perturbative approach.[7] The scheme was also applied to study a theoretical model corresponding to a magnetic-ion-diluted Kondo insulator, and the temperature dependence of the static resistivity and the impurity concentration dependence of the optical conductivity were investigated.[8] The transport properties of heavy-fermion systems were also investigated by the DMFT-CPA scheme using a numerical renormalization-group method.[9] For magnetic properties such as spin susceptibility in magnetic-ion-diluted heavy fermion systems, however, the theoretical investigation is still lacking since an appropriate treatment has yet to be developed. It is therefore necessary to theoretically understand the magnetic properties of these systems.

In the present work, we apply the DMFT-CPA scheme with a perturbative approach to calculate the static spin susceptibility of a theoretical model corresponding to a magnetic-ion-diluted Kondo insulator. The purpose of the present study is to investigate the temperature dependence of the spin susceptibility in the above magnetic-ion-diluted systems by extending the DMFT-CPA scheme to a system with spin degrees of freedom. In particular, we consider the spin susceptibility measurement of the Yb-based Kondo insulator $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$ by Iga *et. al.* in order to compare the present results to the previous experimental results.

2. Model and Formulation

In the present paper, we treat the periodic Anderson model (PAM), in which non-magnetic sites without f electrons are randomly distributed.[10] Sites with and without f electrons are referred as a host site (denoted by H) and an impurity site (denoted by I), respectively. The former corresponds to a magnetic ion site (Yb^{3+} in $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$), and the latter corresponds to a non-magnetic ion site (Lu^{3+} in $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$).

We define the model Hamiltonian as follows;

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_f \\
\mathcal{H}_0 &= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + V \sum_{i,\sigma} (c^\dagger_{i\sigma} f_{i\sigma} + \mathrm{H.c.}) \\
&- \sum_{i,\sigma} (\mu + h\sigma)(c^\dagger_{i\sigma} c_{i\sigma} + f^\dagger_{i\sigma} f_{i\sigma}) \\
\mathcal{H}_f &= \sum_{i,\sigma} \left\{ (1-\xi_i) \left(\frac{U}{2} f^\dagger_{i\sigma} f_{i\sigma} f^\dagger_{i-\sigma} f_{i-\sigma} + \epsilon_f f^\dagger_{i\sigma} f_{i\sigma} \right) + \xi_i E_{\mathrm{I}} f^\dagger_{i\sigma} f_{i\sigma} \right\},
\end{aligned}
$$

where $\varepsilon_{\boldsymbol{k}}$, V, and μ denote the kinetic energy of conduction electrons, the hybridization energy between f electrons and conduction electrons, and the chemical potential, respectively. In $\mathcal{H}_0$, there is also a term corresponding to the Zeeman energy; h corresponds to the magnetic field, and should be expressed as $h = \mu_{\mathrm{B}} H$ if the g factor values are the same for f electrons and conduction electrons.[11)]

In the f-electron Hamiltonian $\mathcal{H}_f$, a random variable ξ_i is defined as

$$\xi_i = \begin{cases} 1 & (i \in \mathrm{I}) \\ 0 & (i \in \mathrm{H}). \end{cases}$$

The impurity concentration x is expressed as $x = \sum_i \xi_i / N$; N denotes the number of lattice sites. On impurity sites corresponding to non-magnetic ions, f electrons are excluded by taking the limit $E_{\mathrm{I}} \to \infty$ in the calculation.[12–15)]

Hereafter, we set $\epsilon_f = -U/2$ and $\mu = 0$. By setting these conditions, a system without a magnetic field has particle-hole symmetry, and a hybridization gap opens at the Fermi level in the homogeneous case ($\xi_i = 0$ for all sites). A simple PAM, which neglects orbital degeneracy in the particle-hole symmetric case, had often been used as a theoretical model of Kondo insulators.[16–19)] Since substituting impurity sites for host sites should break the coherence of the insulating ground state, the Hamiltonian can be a model of $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$.

In order to treat the above system with the DMFT-CPA scheme, we apply the local approximation to the self energy of the Green's function; the DMFT-CPA scheme is based on the assumption that the self energy has no wavenumber dependence.[6,7)] Under this assumption, the local f-electron Green's function on a host site can be expressed as

$$G^{\mathrm{host}}_{ff\,\sigma}(z) = \int \mathrm{d}\nu \frac{\rho(\nu)}{z + h\sigma - \varepsilon_f - \Sigma_\sigma(z) - \dfrac{V^2}{z + h\sigma - \nu}}, \tag{1}$$

where $\Sigma_\sigma(z)$ denotes the self energy. Eq.(1) introduces the density of states $\rho(\nu)$. For simplicity, we assume a semi-elliptical density of states in the present calculations:

$$\rho(\nu) = \frac{2}{\pi D}\sqrt{1 - \left(\frac{\nu}{D}\right)^2},$$

where half of the total band width is denoted by D, and we hereafter take $D = 1$ as the energy unit.

In the DMFT framework, there are several methods of solving the impurity problem in the effective medium, and of constructing the self energy. We use the modified iterated perturbation theory (MIPT)[20)] as the impurity solver, because it is easily applicable over a wide temperature range. The self energy in the MIPT is approximated by the second-order contribution constructed from the so-called Weiss function in the DMFT framework. With the Weiss function, the local f-electron Green's function on a host site can be expressed as

$$G^{\mathrm{host}}_{ff\,\sigma}(z) = \frac{1}{\mathcal{G}^{-1}_{\sigma}(z) + h\sigma - \tilde{\mu}_{\sigma} - \Sigma_{\sigma}(z)}, \tag{2}$$

where another parameter, $\tilde{\mu}_{\sigma}$, is defined. The self energy is approximated by $\tilde{\mu}_{\sigma}$ as follows:[21)]

$$\Sigma_{\sigma}(z) \simeq U n^{f}_{\bar{\sigma}} + \frac{U^2 n^{f}_{\bar{\sigma}}(1-n^{f}_{\bar{\sigma}})\tilde{\Sigma}^{(2)}_{\sigma}(z)}{U^2 \tilde{n}_{\bar{\sigma}}(1-\tilde{n}_{\bar{\sigma}}) - \{(1-n^{f}_{\bar{\sigma}})U - h\sigma + \tilde{\mu}_{\sigma}\}\tilde{\Sigma}^{(2)}_{\sigma}(z)}, \tag{3}$$

where n^{f}_{σ} and $\tilde{n}_{\sigma}$ are calculated using the Fermi distribution function $f(\varepsilon)$, as

$$\begin{aligned} n^{f}_{\sigma} &= \int \mathrm{d}\varepsilon \left(-\frac{1}{\pi}\mathrm{Im}G^{\mathrm{host}}_{ff\,\sigma}(\varepsilon + \mathrm{i}\eta)\right) f(\varepsilon), \\ \tilde{n}_{\sigma} &= \int \mathrm{d}\varepsilon \left(-\frac{1}{\pi}\mathrm{Im}\mathcal{G}_{\sigma}(\varepsilon + \mathrm{i}\eta)\right) f(\varepsilon), \end{aligned}$$

respectively, ($\bar{\sigma}$ denotes an opposite spin to σ). In Eq.(3), the second-order contribution $\tilde{\Sigma}^{(2)}_{\sigma}(z)$ is constructed from the Weiss function as follows:

$$\begin{aligned} &\tilde{\Sigma}^{(2)}_{\sigma}(z) \\ &= U^2 \int \mathrm{d}\varepsilon_1 \mathrm{d}\varepsilon_3 \mathrm{d}\varepsilon_3 \tilde{\rho}_{\bar{\sigma}}(\varepsilon_1)\tilde{\rho}_{\sigma}(\varepsilon_2)\tilde{\rho}_{\bar{\sigma}}(\varepsilon_3) \\ &\times \frac{\{1-f(\varepsilon_1)\}f(\varepsilon_2)f(\varepsilon_3) + f(\varepsilon_1)\{1-f(\varepsilon_2)\}\{1-f(\varepsilon_3)\}}{z + \varepsilon_1 - \varepsilon_2 - \varepsilon_3}, \\ &\quad \tilde{\rho}_{\sigma}(\varepsilon) = -\frac{1}{\pi}\mathrm{Im}\mathcal{G}_{\sigma}(\varepsilon + \mathrm{i}\eta). \end{aligned}$$

In the DMFT-CPA scheme, we introduce the extended coherent potential, which is the homogeneous potential obtained in the sense of the CPA, by averaging the local self energy at a host site and the impurity energy level E_{I} at an impurity site in the lattice system on which host and impurity sites are distributed randomly. By introducing the extended coherent potential, the (averaged) CPA Green's function matrix can be expressed as follows;

$$\begin{aligned} &\hat{G}^{\mathrm{CPA}}_{\sigma}(z;\nu) \\ &= \begin{pmatrix} G^{\mathrm{CPA}}_{cc\,\sigma}(z;\nu) & G^{\mathrm{CPA}}_{cf\,\sigma}(z;\nu) \\ G^{\mathrm{CPA}}_{fc\,\sigma}(z;\nu) & G^{\mathrm{CPA}}_{ff\,\sigma}(z;\nu) \end{pmatrix}, \\ &= \begin{pmatrix} z + h\sigma - \nu & -V \\ -V & z + h\sigma - \varepsilon_f - S_{\sigma}(z) \end{pmatrix}^{-1}, \end{aligned} \tag{4}$$

where the extended coherent potential is denoted by $S_{\sigma}(z)$. The local CPA f-electron Green's function is obtained as

$$G^{\mathrm{CPA}}_{ff\,\sigma}(z) = \int \mathrm{d}\nu \rho(\nu) G^{\mathrm{CPA}}_{ff\,\sigma}(z;\nu),$$

and can also be expressed using the Weiss function, as

$$G^{\mathrm{CPA}}_{ff\,\sigma}(z) = \frac{1}{\mathcal{G}^{-1}_{\sigma}(z) + h\sigma - \tilde{\mu}_{\sigma} - S_{\sigma}(z)}. \tag{5}$$

The CPA condition in the limit $E_{\mathrm{I}} \to \infty$ can be expressed by the following equation;[12)]

$$\{\Sigma_{\sigma}(z) - S_{\sigma}(z)\} G^{\mathrm{CPA}}_{ff\,\sigma}(z) = x \quad (x \neq 1). \tag{6}$$

If $x = 0$, then the extended coherent potential is equal to the self energy, as expected. Eliminating the Weiss function $\mathcal{G}_{\sigma}(z)$ from eqs. (2) and (5), and using eq. (6), we obtain the relation $G^{\mathrm{CPA}}_{ff\,\sigma}(z) = (1-x)G^{\mathrm{host}}_{ff\,\sigma}(z)$ $(x \neq 1)$ in the present case. We determine these functions $G^{\mathrm{CPA}}_{ff\,\sigma}(z)$, $\mathcal{G}_{\sigma}(z)$, $\Sigma_{\sigma}(z)$, and $S_{\sigma}(z)$ self-consistently. In the practical calculation, we start with $\mathcal{G}_{\sigma}(z)$ and $G^{\mathrm{CPA}}_{ff\,\sigma}(z)$. Using $\mathcal{G}_{\sigma}(z)$, we construct $\Sigma_{\sigma}(z)$ by eq. (3). From $G^{\mathrm{CPA}}_{ff\,\sigma}(z)$ and $\Sigma_{\sigma}(z)$, we obtain $S_{\sigma}(z)$ through eq. (6). Using $S_{\sigma}(z)$ itself and new $G^{\mathrm{CPA}}_{ff\,\sigma}(z)$ calculated with $S_{\sigma}(z)$, we obtain new $\mathcal{G}_{\sigma}(z)$ by eq. (5). Finally, we confirm the self-consistency of the calculation by checking the convergence of $\mathcal{G}_{\sigma}(z)$.

In the above scheme, the parameter $\tilde{\mu}_{\sigma}$ in the MIPT has not yet been determined. In the homogeneous case, the corresponding parameter is determined by a condition corresponding to a relation[22, 23)] from which the Luttinger sum rule is derived at absolute zero.[24)] In the inhomogeneous case, however, the relation corresponding to the Luttinger sum rule does not hold between the CPA Green's function and the extended coherent potential. In the present calculation, we employed the condition $n^{f}_{\sigma} = \tilde{n}_{\sigma}$ to determine the parameter $\tilde{\mu}_{\sigma}$ for simplicity,[21)] although we could have used the condition based on the corresponding relation between the local host-site Green's function and the local self energy on a host site.[25)]

3. Results

In the present study, we calculate the spectral functions $\rho_{f\,\sigma}(\varepsilon,\nu)$ and $\rho_{c\,\sigma}(\varepsilon,\nu)$, defined as

$$\begin{aligned} \rho_{f\,\sigma}(\varepsilon,\nu) &= -\frac{1}{\pi}\mathrm{Im}G^{\mathrm{CPA}}_{ff\,\sigma}(\varepsilon + \mathrm{i}\eta;\nu), \\ \rho_{c\,\sigma}(\varepsilon,\nu) &= -\frac{1}{\pi}\mathrm{Im}G^{\mathrm{CPA}}_{cc\,\sigma}(\varepsilon + \mathrm{i}\eta;\nu), \end{aligned} \tag{7}$$

respectively, and the static spin susceptibilities χ_f and χ_c, which are numerically approximated as magnetizations m_f and m_c divided by h (we take $h = 0.005$ in these calculations). Here, the magnetization is defined using (7) as follows:

$$\begin{aligned} m_f &= \frac{1}{2}\sum_{\sigma}\sigma\int \mathrm{d}\nu\rho(\nu)\int \mathrm{d}\varepsilon\rho_{f\,\sigma}(\varepsilon,\nu)f(\varepsilon), \\ m_c &= \frac{1}{2}\sum_{\sigma}\sigma\int \mathrm{d}\nu\rho(\nu)\int \mathrm{d}\varepsilon\rho_{c\,\sigma}(\varepsilon,\nu)f(\varepsilon). \end{aligned}$$

We first show the impurity-concentration dependence of contour graphs of the spectral functions $\rho_c(\varepsilon, \nu)$ and $\rho_f(\varepsilon, \nu)$ in the paramagnetic case with zero field (the spin indices are omitted here) in Figs. 1 and 2. The horizontal axis represents ν, and corresponds to the wave vector through the relation $\nu = \varepsilon_{\boldsymbol{k}}$. Near the Fermi level ($\varepsilon \simeq 0$), the strong-intensity component (the highlighted part) of the contour graph shows the energy dispersion of quasiparticles.

For $x = 0.1$, the system is almost homogeneous, and the energy dispersion is similar to that of the renormalized hybridization band expressed as $\left(\nu \pm \sqrt{\nu^2 + 4(V^*)^2}\right)/2$, in which V^* denotes a renormalized hybridization energy. The renormalized hybridization gap, which is an indirect gap given by $\sqrt{D^2 + 4(V^*)^2} - D$ (D has been set to $D = 1$), almost opens. In the renormalized hybridization gap, there is a non-dispersive impurity band. As the impurity concentration x increases, the impurity band grows and the renormalized hybridization gap disappears. Then, the energy dispersion in the conduction-electron part $\rho_c(\varepsilon, \nu)$ of the spectral function approaches that of a simple conduction band, without the hybridization shown in Fig. 1.

As shown in Fig. 2, at higher impurity concentration ($x \simeq 1$), the strong-intensity component of the f-electron spectral function loses its dispersion and approaches the renormalized f level (note that the intensity of the spectral function $\rho_f(\varepsilon, \nu)$ is divided by $1 - x$ since the f-electron spectral function decreases proportionally to the host-site concentration $(1 - x)$ as the value of x increases). In higher energy regions ($|\varepsilon| \sim 2$), there are side bands (the so-called Hubbard bands), and these are not dispersive. This behavior reflects local (non-dispersive) charge excitations in the present model at large values of U.

Figure 3 shows the temperature dependence of the total static spin susceptibility $\chi_{\text{total}} = \chi_f + \chi_c$. At higher temperatures, χ_{total} increases following Curie-Weiss law as temperature decreases, with a peak that falls off at lower temperatures. The decrease in χ_{total} at lower temperatures reflects an opening of the energy gap. For a homogeneous system with $x = 0$, the hybridization gap opens completely, and the susceptibility reaches zero at absolute zero. For systems with finite impurity concentrations, however, a residual susceptibility exists at absolute zero, since the hybridization gap disappears because of the impurity band. As the impurity concentration increases, the decrease in susceptibility at lower temperatures becomes weaker, and the peak disappears. The higher the impurity concentration, the smaller the total static susceptibility, because the f-component of the susceptibility becomes smaller as the impurity concentration increases.

The temperature dependence of the f-component χ_f of the static spin susceptibility for several values of x is shown in Fig. 4. χ_f becomes small as the impurity concentration increases,

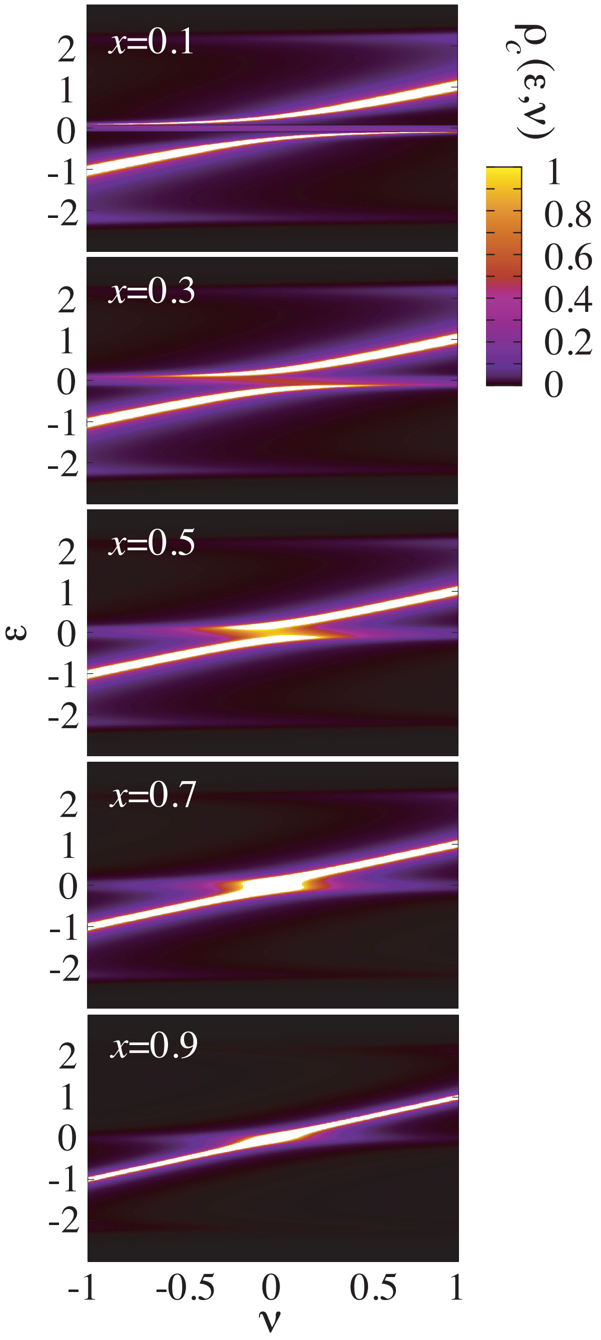

Fig. 1. (Color online) Impurity concentration dependence ($x = 0.1, 0.3, 0.5, 0.7$, and 0.9) of contour graphs of the spectral function $\rho_c(\varepsilon, \nu)$ for a conduction electron with $U = 3$ and $V = 0.5$ at $T = 0$.

except in the lower temperature region. At lower temperatures, χ_f increases as the impurity concentration increases because of the growth of the in-gap state. Fig. 5 (a) shows the impurity concentration dependence of χ_f at low and high temperatures. At the highest temperature investigated ($T = 1.0$), χ_f monotonically decreases as the impurity concentration increases.

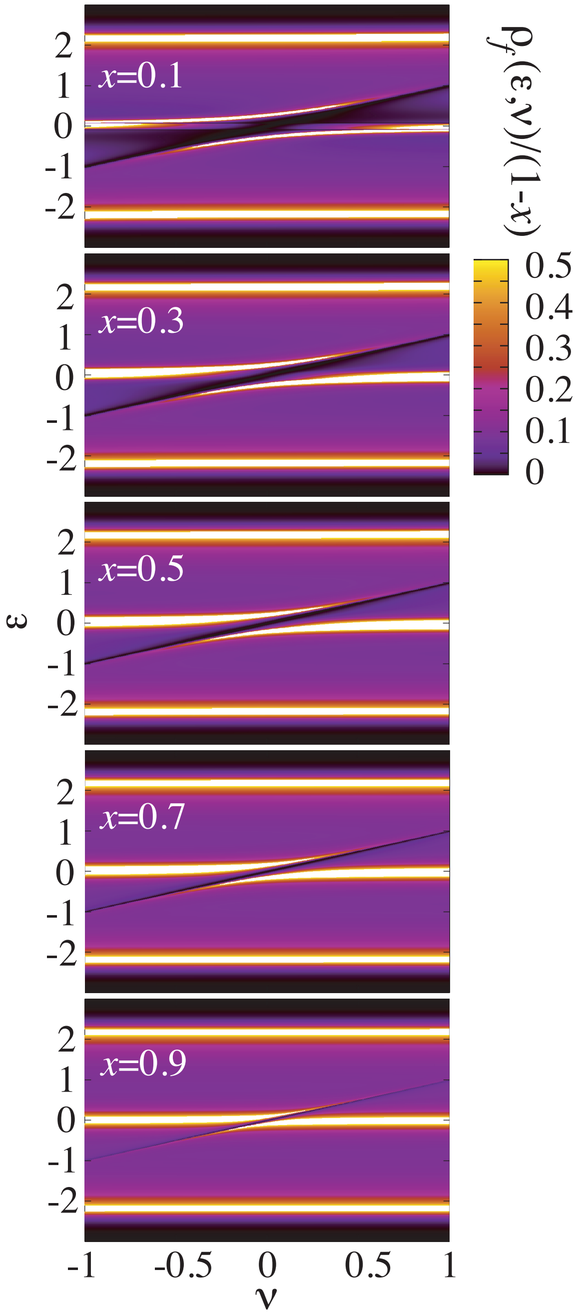

Fig. 2. (Color online) Impurity concentration dependence ($x = 0.1, 0.3, 0.5, 0.7$, and 0.9) of contour graphs of the spectral function $\rho_f(\varepsilon, \nu)$ for an f electron with $U = 3$ and $V = 0.5$ at $T = 0$.

$\chi_f(T = 1.0)$ decreases proportionally to $1-x$, as shown in Fig. 5 (b). On the other hand, χ_f at absolute zero does not change monotonically in Fig. 5 (a). We will discuss the non-monotonic behavior of $\chi_f(T = 0)$ in a later section.

Regarding the correlation effect, the variation of the temperature dependence of χ_{total} with U for $x = 0.1$ is plotted, as shown in Fig. 6, to examine the enhancement of the static

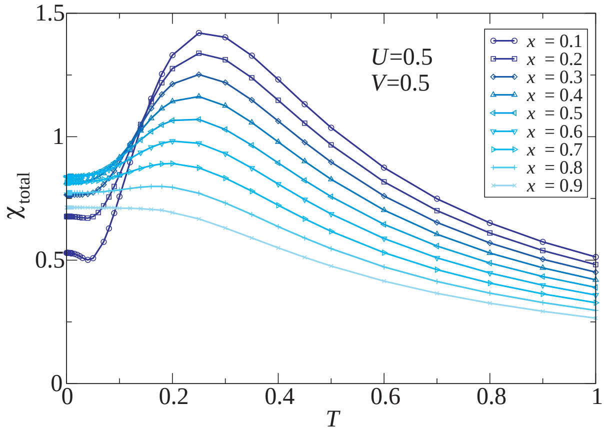

Fig. 3. (Color online) Impurity concentration dependence of the variation of the total static spin susceptibility with temperature ($U = 0.5$ and $V = 0.5$).

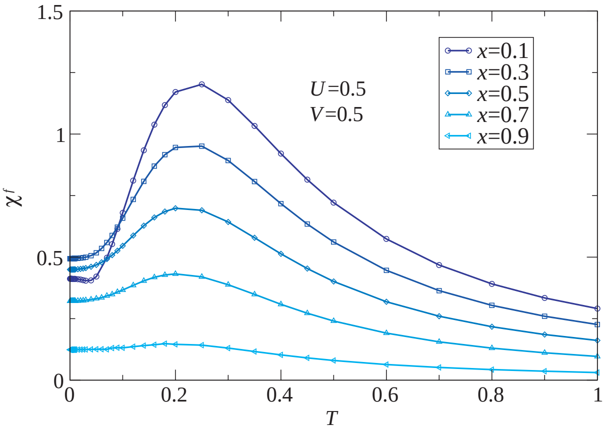

Fig. 4. (Color online) Temperature dependences of the f component of the static spin susceptibility for several values of x ($U = 0.5$ and $V = 0.5$).

spin susceptibility. It is generally expected that the spin susceptibility is enhanced by electron correlation, since the on-site Coulomb repulsion suppresses charge fluctuation and enhances the spin fluctuation. In the present result, the static spin susceptibility is strongly enhanced by the correlation effect.

4. Summary and Discussion

We have calculated the spectral function and static spin susceptibility of a periodic Anderson model with randomly distributed on-site Coulomb interactions between f electrons by the DMFT-CPA scheme, which corresponds to a theoretical model of a magnetic-ion-diluted Kondo insulator.

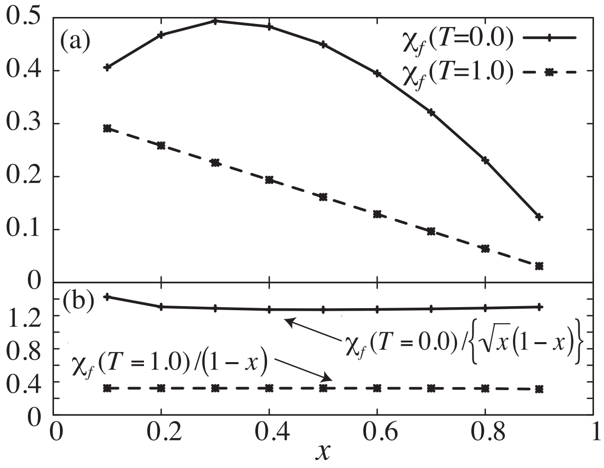

Fig. 5. (a) Impurity concentration dependence of the f component of the static spin susceptibility at $T = 0$ and $T = 1.0$ ($U = 0.5$ and $V = 0.5$). (b) $\chi_f(T = 0)$ and $\chi_f(T = 1.0)$ divided by $\sqrt{x}(1 - x)$ and $1 - x$, respectively (see text).

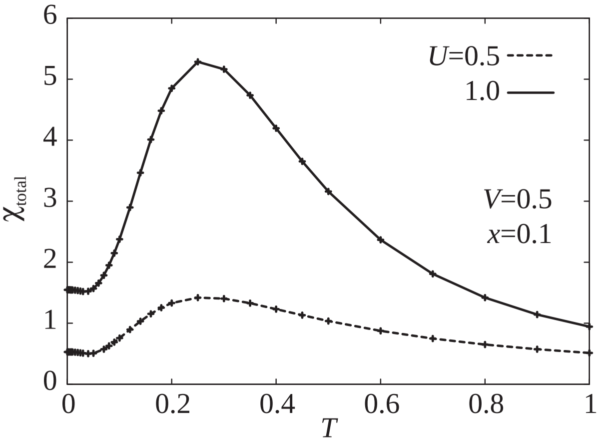

Fig. 6. Temperature dependence of the total static spin susceptibility for $U = 0.5$ and $U = 1.0$ ($V = 0.5$ and $x = 0.1$).

In the impurity concentration dependence of the spectral functions, the hybridization gap disappears because of the growth of the impurity band, and the renormalized hybridization band is continuously separated into a conduction electron component and an f electron component as the impurity concentration increases. The former becomes the original conduction band dispersion ($\varepsilon = \nu = \varepsilon_{\boldsymbol{k}}$), and the latter becomes the renormalized f level without dispersion ($\varepsilon = 0$). The upper and lower satellite bands in the f component of the spectral function have no energy dispersion. Since these bands correspond to local charge excitations, they are not affected by diluting the host sites on which on-site Coulomb interactions exist (although the total intensity of the f component of the spectral function becomes small as the host sites are diluted).

The impurity concentration dependence of the variation of static susceptibility with temperature in the experimental results obtained for $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$[5)] is in qualitative agreement with that for the f-component χ_f of the susceptibility (Fig. 4) . If the theory is applicable to treat the system with a sufficiently large value of U, the susceptibility obtained experimentally should be compared with the total susceptibility χ_{total}. In the present study, however, it is difficult to calculate the Green's function for much larger values of U than the band width since the scheme is based on the perturbative construction of the self energy, and we cannot obtain the spin susceptibility for a system with such a large value of U. In such a case, it is appropriate to compare the magnetic susceptibility in the experimental result with χ_f rather than χ_{total} because it is expected that the spin fluctuation of f electrons in real heavy fermion compounds is strongly enhanced by the correlation effect and the f component is a major component of the magnetic susceptibility. Actually, the experimental result obtained for $\mathrm{Yb}_{1-x}\mathrm{Lu}_x\mathrm{B}_{12}$ is comparable with the f component of the susceptibility in the present results. We believe that the above qualitative agreement between χ_f in the present results and the magnetic susceptibility in the experimental result indicates that the treatment of the present model with the DMFT-CPA scheme is a valid description of a magnetic-ion-diluted Kondo insulator.

Finally, let us discuss the non-monotonic impurity concentration dependence of the static spin susceptibility at absolute zero. The Pauli susceptibility at low temperatures is proportional to the density of states at the Fermi level, and the f component $\chi_f(T = 0)$ of the static spin susceptibility at absolute zero should also be proportional to $\rho_f(0) = \int \mathrm{d}\nu \rho(\nu)\rho_f(0, \nu)$. In the present system with particle-hole symmetry, the f component of the density of states at the Fermi level can be expressed as $\rho_f(0) = D/(2\pi V^2)\sqrt{x}(1 - x)$.[8,15)] Fig. 5 (b) shows a plot of $\chi_f(T = 0)$ divided by $\sqrt{x}(1 - x)$ versus x. The proportional relationship holds, although $\chi_f(T = 0)$ at the lowest impurity concentration deviates from proportionality. This deviation may be due to the numerical approximation of the spin susceptibility, which is obtained by dividing the magnetization by the finite magnetic field. The plot indicates that the non-monotonic behavior of $\chi_f(T = 0)$ can be explained by the proportional relationship between $\chi_f(T = 0)$ and $\rho_f(0)$.

The present study demonstrates that the DMFT-CPA scheme with an MIPT impurity solver is applicable to the calculation of magnetic properties. Moreover, the present scheme can effectively treat the general system without particle-hole symmetry, and we will discuss the application of the present scheme to the generalized system in a future report.

Acknowledgments

We would like to thank H. Kusunose for informative discussions on the framework of the DMFT-CPA scheme. This work was supported by a Grant-in-Aid for Scientific Research (No. 19740209) from the Ministry of Education, Culture, Sports, Science and Technology. A main part of the numerical calculations was performed on the facilities of Shimane University General Information Processing Center.

References

1) For a few review of experimental studies, see G. Aeppli and Z. Fisk, Comments Cond. Mat. Phys. **16** (1992) 155; L. Degiorgi, Rev. Mod. Phys. **71** (1999) 687.

2) For a few review of theoretical studies, see P. Schlottmann, in *Current Problem in Condensed Matter : Theory and Experiment*, edited by J. L. Moran-Lopez (Plenum, New York, 1998); P. Riseborough, Adv. Phys. **49** (2000) 257.

3) For example, A. Sumiyama, Y. Oda, H. Nagano, Y. Ōnuki, K. Shibutani and T. Komatsubara, J. Phys. Soc. Jpn. **55** (1986) 1294.

4) M. F. Hundley, P. C. Canfield, J. D. Thompson and Z. Fisk, Phys. Rev. B**50** (1994) 18142.

5) F. Iga, S. Hiura, J. Klijn, N. Shimizu, T. Takabatake, M. Ito, Y. Matsumoto, F. Masaki, T. Suzuki and T. Fujita, Physica B **259-261** (1999) 312.

6) A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, Rev. Mod. Phys. **68** (1996) 13.

7) T. Mutou, Phys. Rev. B**64** (2001) 245102.

8) T. Mutou, Phys. Rev. B**64** (2001) 165103.

9) C. Grenzebach, F. B. Anders, G. Czycholl and T. Pruschke, Phys. Rev. B**77** (2008) 115125.

10) Magnetic ions Yb^{3+} have an f *hole* in Yb-based compounds. Here, however, we refer them as f *electrons* in the present theoretical model.

11) The g factor for f electrons generally differs from that for conduction electrons. With considering the fact, it is often assumed that the magnetic filed is applied only to f electrons in the theoretical model of the Kondo insulator.18) In the present study, however, we assume that the magnetic field is applied to both, for simplicity.

12) A. Yoshimori and H. Kasai, Solid State Commun. **58** (1986) 259.

13) Z. Li and Y. Qiu, Phys. Rev. B**43** (1991) 12906.

14) P. Schlottmann, Phys. Rev. B**46** (1992) 998.

15) R. Shiina, J. Phys. Soc. Jpn. **64** (1995) 702.

16) M. Jarrell, H. Akhlaghpour and Th. Pruschke, Phys. Rev. Lett. **70** (1993) 1670; M. Jarrell, Phys. Rev. B **51** (1995) 7429.

17) D. S. Hirashima and T. Mutou, Physica B **199**&**200** (1994) 206; T. Mutou and D. S. Hirashima, J. Phys. Soc. Jpn. **63** (1994) 4475.

18) T. Saso and M. Itoh, Phys .Rev. B**53** (1996) 6877.

19) It was pointed out that the careful consideration of the orbital degeneracy and/or the wave vector dependence of the kinetic energy and the hybridization energy themselves is needed to discuss the condition that the hybridization gap opens; see H. Kuroiwa, Y. Imai, and T. Saso, J. Phys. Soc. Jpn. **76** (2007) 124704.

20) H. Kajueter and G. Kotliar, Phys. Rev. Lett. **77** (1996) 131; H. Kajueter, G. Kotliar, and G. Moeller, Phys. Rev. B**53** (1996) 16214.

21) M. Potthoff, T. Wegner, and W. Nolting, Phys. Rev. B**55** (1997) 16132.

22) J. M. Luttinger and J. C. Ward, Phys. Rev. **118** (1960) 1417.

23) T. Mutou and H. Kontani, Phys. Rev. B**74** (2006) 115107.

24) J. M. Luttinger, Phys. Rev. **119** (1960) 1153.

25) We have confirmed that there is no serious difference between results obtained by both conditions as long as we restrict ourselves to treat the system near the particle-hole symmetric case and/or

for not so large values of U (not shown here).