From the local Fermi liquid to the heavy Fermi liquid

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Magnetic-ion concentration dependence of some physical quantities in heavy-fermion systems are investigated on the basis of the periodic Anderson model with randomly distributed sites without f electrons. A scheme consisting of the dynamical mean-field theory and the coherent-potential approximation is applied to calculate the density of states, the resistivity, and the specific heat. By the present scheme, both the heavy Fermi liquid in heavy-fermion systems and the local Fermi liquid in dilute Kondo impurity systems can be studied on the same footing.

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I. INTRODUCTION

Several types of the ground state in heavy-fermion compounds have been studied so far. Some of compounds do not have any magnetic ordering down to extremely low temperature. In these typical heavy-fermion compounds which have no magnetic ordering, spin degrees of freedom of localized f electrons disappear at low temperature and those f electrons construct the heavy Fermi-liquid state by the mixing with conduction electrons. The heavy Fermi liquid which became realized in heavy-fermion compounds originates from the strong many-body effect between f electrons. When the concentration of magnetic ions is low in those compounds, the Kondo effect is also expected to occur by the many-body effect. The relation between heavy-fermion systems and single Kondo impurity systems has been investigated in some experimental studies in which nonmagnetic ions are substituted for magnetic ions.[1] In Ref. 1, nonmagnetic La^{3+} ions were substituted for Ce^{3+} ions in $(Ce,La)Cu_6$, and the magnetic-ion concentration dependence of the resistivity was mainly studied. In magnetic-ion-dense compounds, the resistivity decreases with decreasing temperature and it has a T^2 dependence which is the Fermi-liquid behavior at lower temperatures. In compounds with dilute magnetic ions, the resistivity increases monotonically as temperature decreases, and at the lowest temperature it reaches the residual resistivity corresponding to the unitarity limit in the single Kondo impurity system.

The theoretical study of the magnetic-ion concentration dependence of the resistivity was first carried out by Yoshimori and Kasai (YK).[2] They proposed a theoretical model on the basis of the periodic Anderson model for the system with randomly distributed magnetic ions, and applied the coherent-potential approximation (CPA) to treat the randomness effect in the system. In their study, they considered the energy ranges divided into the higher-energy part and the lower-energy one, and applied different treatments to each energy range. Using the slave-boson mean-field approximation (SBMFA), another group later improved the insufficient point whereby the electronic state in the whole energy range was not treated by the single theoretical scheme in the study by YK.[3] However, the SBMFA cannot treat the many-body correlation effect sufficiently; it is insufficient to describe the high-energy excitation due to the strong correlation between f electrons.

In order to take account of the many-body effect beyond the Hartree-Fock approximation and to treat the electronic state in the whole energy range by the single scheme, we propose a scheme consisting of the dynamical mean-field theory (DMFT) and the CPA. Since a lattice problem can be reduced to an impurity problem embedded in an effective medium within the DMFT framework, one can treat the many-body correlation effect more correctly by solving the effective impurity problem appropriately.[4] The physical idea of the effective medium (the dynamical mean field) is the same as that of the coherent potential in the CPA.[5] Although the spatial correlation is not taken into account beyond the mean-field treatment in both the DMFT and the CPA, one can expect that the present scheme is effective to treat the system with randomly distributed magnetic ions since f orbitals in magnetic ions are rather localized. The purpose of the present study is to clarify magnetic-ion concentration dependencies of some physical quantities such as the resistivity and to study the change from the local Fermi-liquid state to the heavy Fermi-liquid state by the above scheme.

This paper is organized as follows. In Sec. II, we introduce the model we use and propose the framework consisting of the DMFT and the CPA. We show numerical results of the resistivity, the density of states, and the specific heat in Sec. III. At last, in Sec. IV, we summarize results and give some discussions.

II. MODEL AND FORMULATION

In the present study, we use the periodic Anderson model (PAM) with randomly distributed sites which have no f electrons as a theoretical model for the magnetic-ion-diluted heavy-fermion system. The model is the same as that used in Ref. 2,

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_f,$$

$$\mathcal{H}_0\equiv\sum_{\boldsymbol{k},\sigma}(\varepsilon_{\boldsymbol{k}}c^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}+\varepsilon^{f}_{\boldsymbol{k}}f^{\dagger}_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma})+V\sum_{i,\sigma}(c^{\dagger}_{i\sigma}f_{i\sigma}+\text{H.c.}),$$

$$\mathcal{H}_f\equiv\sum_{i,\sigma}\left\{(1-\xi_i)\frac{U}{2}f^{\dagger}_{i\sigma}f_{i\sigma}[f^{\dagger}_{i-\sigma}f_{i-\sigma}-1]+\xi_i E_1 f^{\dagger}_{i\sigma}f_{i\sigma}\right\}.$$

We refer sites with and without f electrons as a host site (denoted by H) and an impurity site (denoted by I), respectively. Host and impurity sites correspond to magnetic and nonmagnetic ions in real systems. In the expression of $\mathcal{H}_f$, ξ_i denotes a random variable defined as $\xi_i=1$ $(i\in I)$ and $\xi_i=0$ $(i\in H)$. The impurity concentration x is expressed as $x=\Sigma_i\xi_i/N$; N denotes the number of lattice sites. The energy level of f electrons on impurity sites is denoted by E_{I} in the expression of $\mathcal{H}_f$. In the practical calculation, we take the limit $E_{\mathrm{I}}\to\infty$ to exclude f electrons on impurity sites.[2,3,6,7] The density of electrons is as $n^f+n^c=2-x$. In the present model, it is assumed that f electrons have a small energy dispersion and it is defined as $\varepsilon_{\boldsymbol{k}}^f\equiv\alpha\varepsilon_{\boldsymbol{k}}$ for simplicity.[2] The value of α should be determined so that the hybridization gap does not open;[8] the condition that the gap does not open is as $\alpha>(V/D)$.[2] The density of states $\rho_0(\nu)=\Sigma_{\boldsymbol{k}}\delta(\nu-\varepsilon_{\boldsymbol{k}})/N$ is assumed as the half-elliptic form of $\rho_0(\nu)$;[9] $\rho_0(\nu)=2\sqrt{1-(\nu/D)^2}/(\pi D)$ for $|\nu|\leqslant D$ and $\rho_0(\nu)=0$ for $|\nu|>D$. Hereafter we take D as the unit of energy; $D=1$. The present system has the particle-hole symmetry.

We use the infinite-dimensional approach[5] in the present study; namely, we assume that the wave-number dependence of the self-energy can be neglected (the local approximation). Under the assumption, we apply both the DMFT and the CPA to the present problem. First, the usual CPA procedure is applied to the present model according to YK. We start with the effective one-body Hamiltonian,

$$\mathcal{H}^{\mathrm{eff}}=\mathcal{H}_0+\sum_{i,\sigma}\{(1-\xi_i)\Sigma_\sigma(i\omega_n)+\xi_iE_{\mathrm{I}}\}f_{i\sigma}^\dagger f_{i\sigma},$$

where $\Sigma_\sigma(i\omega_n)$ denotes the self-energy (from which the Hartree term is subtracted) due to the electronic correlation between f electrons. The CPA Hamiltonian is defined as

$$\mathcal{H}^{\mathrm{CPA}}=\mathcal{H}_0+\sum_{i,\sigma}S_\sigma(i\omega_n)f_{i\sigma}^\dagger f_{i\sigma},$$

where $S_\sigma(i\omega_n)$ denotes the coherent potential. We define the site-dependent potential v_i as

$$\sum_i v_i\equiv\mathcal{H}^{\mathrm{eff}}-\mathcal{H}^{\mathrm{CPA}}.$$

Using the site-dependent potential v_i, we introduce the site-dependent Green's function (operator) $G_i(i\omega_n)$ defined as

$$G_i(i\omega_n)\equiv\{i\omega_n-(\mathcal{H}^{\mathrm{CPA}}+v_i)\}^{-1}.$$

On the other hand, the CPA Green's function $G^{\mathrm{CPA}}(i\omega_n)$ is introduced as follows:

$$G^{\mathrm{CPA}}(i\omega_n)\equiv(i\omega_n-\mathcal{H}^{\mathrm{CPA}})^{-1}.$$

The site-dependent Green's function $G_i(i\omega_n)$ is expressed in terms of $G^{\mathrm{CPA}}(i\omega_n)$ and the T matrix: $T_i(i\omega_n)\equiv v_i[1-G^{\mathrm{CPA}}(i\omega_n)v_i]^{-1}$ as follows:

$$G_i(i\omega_n)=G^{\mathrm{CPA}}(i\omega_n)+G^{\mathrm{CPA}}(i\omega_n)T_i(i\omega_n)G^{\mathrm{CPA}}(i\omega_n).$$

By equating the random average of the site-dependent Green's function $G_i(i\omega_n)$ with the CPA Green's function $G^{\mathrm{CPA}}(i\omega_n)$, we obtain the CPA condition. The condition that the random average of $G_i(i\omega_n)$ is equal to $G^{\mathrm{CPA}}(i\omega_n)$ is nothing but the condition that the random average of the T matrix is equal to zero,

$$(1-x)T_{i\in\mathrm{H}}+xT_{i\in\mathrm{I}}=0.$$

Taking the limit $E_{\mathrm{I}}\to\infty$, the above CPA condition leads to a simple form expressed by the following equation:[2]

$$\{\Sigma(i\omega_n)-S(i\omega_n)\}G^{ff}(i\omega_n)=x\quad(x\neq1),\tag{1}$$

where we have omitted the spin index because we deal with only the paramagnetic state. The f component of the CPA (or averaged) Green's function $G^{ff}(i\omega_n)$ is expressed as

$$G^{ff}(i\omega_n)=\int d\nu\rho_0(\nu)G^{ff}(i\omega_n;\nu)=\int d\nu\frac{\rho_0(\nu)}{i\omega_n-\alpha\nu-S(i\omega_n)-\dfrac{V^2}{i\omega_n-\nu}}.\tag{2}$$

The next step of the procedure is to determine the self-energy $\Sigma(i\omega_n)$. In the present study, we calculate $\Sigma(i\omega_n)$ by the iterated perturbation theory (IPT) in the DMFT framework. We introduce what is called the Weiss function $\mathcal{G}(i\omega_n)$ (Ref. 4) as follows:

$$\mathcal{G}(i\omega_n)\equiv\frac{1}{[G^{ff}(i\omega_n)]^{-1}+S(i\omega_n)}.\tag{3}$$

Using this Weiss function, the site-dependent Green's function $G_{i\in\mathrm{H}}^{ff}(i\omega_n)$ on the host site is expressed as $G_{i\in\mathrm{H}}^{ff}(i\omega_n)=\{[\mathcal{G}(i\omega_n)]^{-1}-\Sigma(i\omega_n)\}^{-1}$. Following the IPT procedure, we calculate $\Sigma(i\omega_n)$ in terms of $\mathcal{G}(i\omega_n)$ by the second-order perturbation. We symbolically express $\Sigma(i\omega_n)$ as the functional of $\mathcal{G}(i\omega_n)$,

$$\Sigma(i\omega_n)=\Sigma[\mathcal{G}(i\omega_n)].\tag{4}$$

Now we have four equations, Eqs. (1)–(4), for four functions $G^{ff}(i\omega_n)$, $\mathcal{G}(i\omega_n)$, $S(i\omega_n)$, and $\Sigma(i\omega_n)$. We determine these four functions self-consistently from the above equations.

From the averaged Green's function one can obtain the one-particle density of states (DOS) as

$$\rho_{f(c)}(\omega)=-\frac{1}{\pi}\mathrm{Im}G^{ff(cc)}(\omega+i\delta),$$

where $G^{cc}(i\omega_n)$ is defined similarly to $G^{ff}(i\omega_n)$:

$$G^{cc}(i\omega_n)=\int d\nu\rho_0(\nu)G^{cc}(i\omega_n;\nu)=\int d\nu\frac{\rho_0(\nu)}{i\omega_n-\nu-\dfrac{V^2}{i\omega_n-\alpha\nu-S(i\omega_n)}}.$$

We can also calculate the total energy of the system by using the averaged Green's function. According to the approach

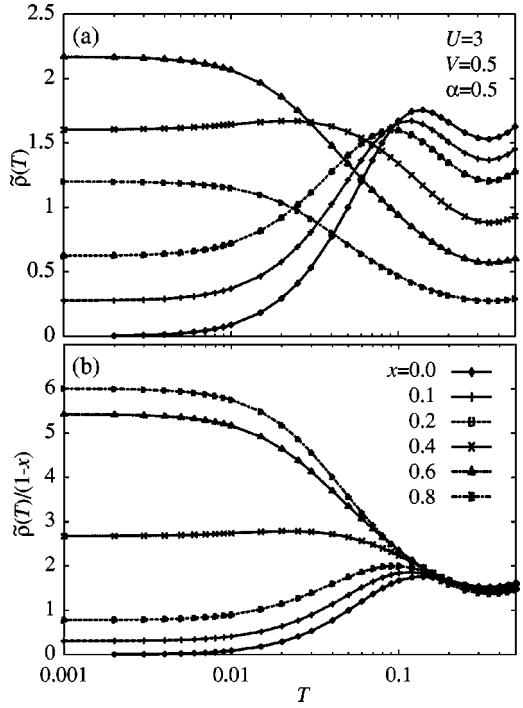

FIG. 1. (a) Temperature dependence of the resistivity for several values of x: $x=0.0$, 0.1, 0.2, 0.4, 0.6, and 0.8 ($U=3$, $V=0.5$, and $\alpha=0.5$). (b) Data divided by $1-x$ for same parameters.

from the infinite-dimensional limit, we can calculate the conductivity in terms of the averaged Green's function without vertex parts, since the contribution to the conductivity due to vertex corrections vanishes in the limit.[10] We obtain the following expression of the conductivity by assuming that the expression of the conductivity formulated on the hypercubic lattice in $d=\infty$ can be also applied to the system on the general lattice. By omitting some constant factors, we define the reduced conductivity,[11,12]

$$\tilde{\sigma}(T) \equiv \int d\nu \rho_0(\nu) \int d\epsilon \{[\rho^{cc}(\epsilon;\nu)]^2 + 2\alpha[\rho^{cf}(\epsilon;\nu)]^2 + \alpha^2[\rho^{ff}(\epsilon;\nu)]^2\} \left(-\frac{\partial f(\epsilon)}{\partial \epsilon}\right),$$

where $\rho^{cc(cf,ff)}(\epsilon;\nu) = -\mathrm{Im}G^{cc(cc,ff)}(\epsilon+i\delta;\nu)/\pi$ and $f(\epsilon)$ denotes the Fermi distribution function. The resistivity $\tilde{\rho}(T)$ is defined as $\tilde{\rho}(T)=1/\tilde{\sigma}(T)$.

III. RESULTS

Figure 1 shows the temperature dependence of the resistivity for several values of impurity concentrations (x). Note that data in the lower panel [Fig. 1(b)] show the resistivity divided by the concentration of host sites $1-x$, which corresponds to the magnetic-ion concentration. In Fig. 1, one can see that the resistivity for $x=0$ increases as temperature decreases down to $T\simeq 0.1$, below which it decreases rapidly and goes to zero at the lowest temperature. The resistivity at lower temperatures has a T^2 dependence as expected in the Fermi liquid. For finite but low impurity concentrations, the resistivity has a residual resistivity at the lowest temperature. With increasing impurity concentration, the residual resistivity increases. The temperature dependence of the resistivity changes for higher impurity concentrations above $x\simeq 0.5$. For higher impurity concentrations, the resistivity curve does not have any peak, it increases monotonically with decreasing temperature, and it reaches the residual resistivity which is the maximum value of the resistivity at the lowest temperature. This behavior of the resistivity for higher concentrations is similar to that for the single Kondo impurity system. In the impurity-concentration dependence of the residual resistivity shown in Fig. 2, one can see that the residual resistivity at the limit of $x\rightarrow 1$ has a finite value. This finite value should correspond to the unitarity limit in the single Kondo impurity system.

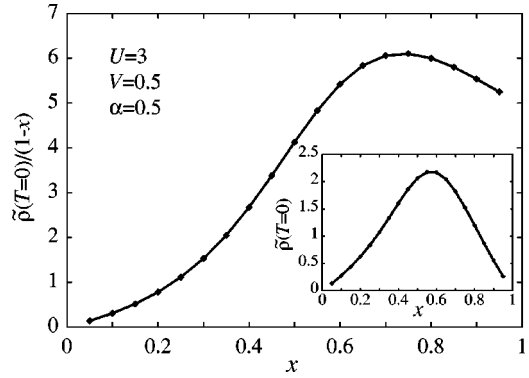

FIG. 2. Impurity-concentration dependence of the residual resistivity divided by $1-x$. Inset shows the dependence of the residual resistivity itself.

At higher temperature, on the contrary, resistivity curves for all impurity concentrations have a common temperature dependence; the resistivity increases with decreasing temperature in the region $0.1\lesssim T\lesssim 0.3$. This temperature dependence in the result is expected to correspond to the logarithmic increase observed in the Kondo effect. Since the spin degree of freedom of each f electron is active at higher temperature and it becomes a center of the Kondo resonating scattering, the resistivity increases with decreasing tempera-

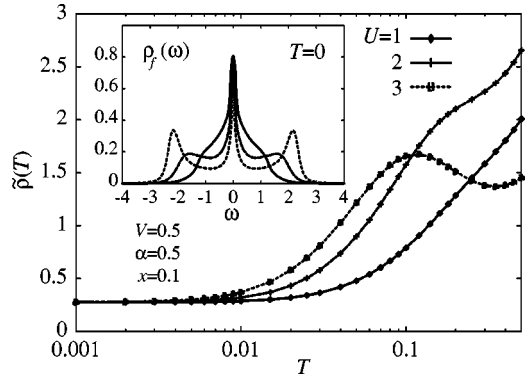

FIG. 3. Temperature dependence of the resistivity for different values of the Coulomb interaction U: $U=1$, 2, and 3 ($V=0.5$, $\alpha=0.5$, and $x=0.1$). Inset shows the f component $\rho_f(\omega)$ of the density of states (divided by $1-x$) for corresponding parameters.

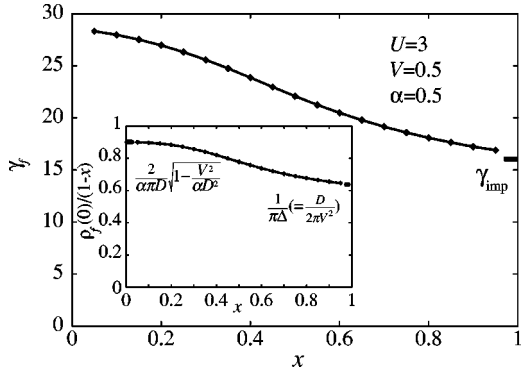

FIG. 4. Impurity-concentration dependence of γ_f. The short thick line at the end of $x=1$ indicates the value of $\gamma_{\rm imp}$ (see text). Inset shows the impurity concentration of the density of states $\rho_f(0)$ (divided by $1-x$) at the Fermi level. Short thick lines at both ends of $x=1$ and $x=0$ indicate the value for the SIAM with corresponding parameters and the analytical value of $\rho_f(0)$ for $x=0$, respectively.

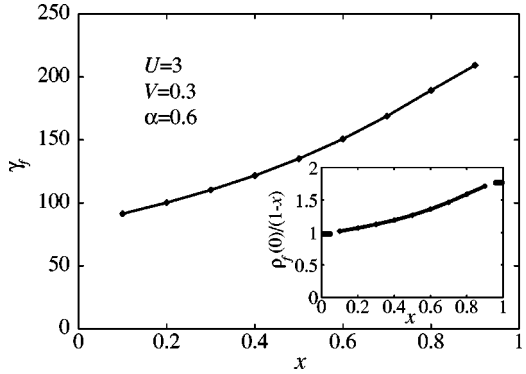

FIG. 5. Impurity-concentration dependence of same quantities as shown in Fig. 4 for the different parameter set referred as set B: $U=3$, $V=0.3$, and $\alpha=0.6$ (see text).

ture as observed in the Kondo impurity system. In fact, we can see in Fig. 3 that the logarithmic increase of the resistivity with decreasing temperature is clearer for larger values of U.[13] As the strength of the Coulomb repulsion between f electrons increases, the spin fluctuation is enhanced and the charge fluctuation is suppressed. In the DOS spectrum, one can also see the example of the influence by the many-body effect; the satellite peak, which is not obtained by the SBMFA, grows and the width of the center peak is narrower with increasing value of U as shown in the inset of Fig. 3.

In order to see that the present system in the limit of $x\rightarrow 1$ corresponds to the single Kondo impurity system described by the single-impurity Anderson model (SIAM), we show the impurity-concentration dependence of the linear T specific-heat coefficient in Fig. 4. The f component γ_f of the linear T specific-heat coefficient is defined as

$$\gamma_f \equiv \frac{2\pi}{3}\frac{z_f^{-1}\rho_f(0)}{1-x},$$

where z_f denotes the renormalization factor for the f part; it is defined as

$$z_f \equiv \left(1-\left.\frac{\partial {\rm Re}\Sigma(\omega+i\delta)}{\partial\omega}\right|_{\omega=0}\right)^{-1},$$

and $\rho_f(0)\equiv -{\rm Im}G^{ff}(+i\delta)/\pi$. For the usual homogeneous PAM ($x=0$), $S(i\omega_n)$ is equal to $\Sigma(i\omega_n)$ and the linear T specific-heat coefficient is as $(2\pi/3)\{z_f^{-1}\rho_f(0)+\rho_c(0)\}$.[14] As shown in Fig. 4, with increasing impurity concentration, γ_f decreases monotonically, and finally reaches a finite value in the limit of $x\rightarrow 1$. The value in the limit $x\rightarrow 1$ is consistent with the rigorous value of the (symmetric) SIAM with corresponding parameters. Setting $\Delta=\pi\rho_0(0)V^2$, the linear T specific-heat coefficient $\gamma_{\rm imp}$ for the SIAM is expressed as

$$\gamma_{\rm imp}=\frac{2\pi}{3\Delta}\sum_{n=0}^{\infty} C_{2n}\left(\frac{U}{\pi\Delta}\right)^{2n},$$

where $C_n=(2n-1)C_{n-1}-(\pi/2)^2C_{n-2}$ with $C_0=C_1=1$.[15] For present parameters ($U=3$ and $V=0.5$), the value of $\gamma_{\rm imp}$ is equal to $16.04\ldots$, and one can expect that the present scheme is applicable to describe the strong-coupling regime such as $U/(\pi\Delta)\gg 1$. We also show the impurity-concentration dependence of the f component $\rho_f(0)$ of the density of states at the Fermi level in the inset of Fig. 4. For the homogeneous model ($x=0$), we can express the value of $\rho_f(0)$ analytically as

$$\rho_f(0)=\frac{2}{\alpha\pi D}\sqrt{1-\frac{V^2}{\alpha D^2}}.$$

At the other end ($x=1$), one can see that $\rho_f(0)/(1-x)$ approaches $1/(\pi\Delta)$ which is the density of states of the magnetic impurity in the SIAM at the Fermi level, as expected.

Here it is necessary to comment on the impurity-concentration dependence of γ_f shown in Fig. 4. In the system with the parameter set (referred to as set A), $U=3$, $V=0.5$, and $\alpha=0.5$, the value of γ_f for $x=1$ is smaller than that for $x=0$. However, this impurity-concentration dependence of γ_f shown in Fig. 4 is not general. In the system with another parameter set (referred as B), $U=3$, $V=0.3$, and $\alpha=0.6$, for example, the value of γ_f for $x=1$ is larger than that for $x=0$ (Fig. 5). Comparing with the parameter set A, one can see in Fig. 6 that the width of the center peak of the

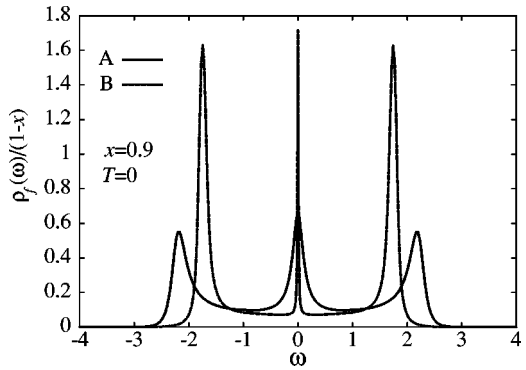

FIG. 6. Comparison of $\rho_f(\omega)$ for the parameter set A ($U=3$, $V=0.5$, and $\alpha=0.5$) and that for B ($U=3$, $V=0.3$, and $\alpha=0.6$).

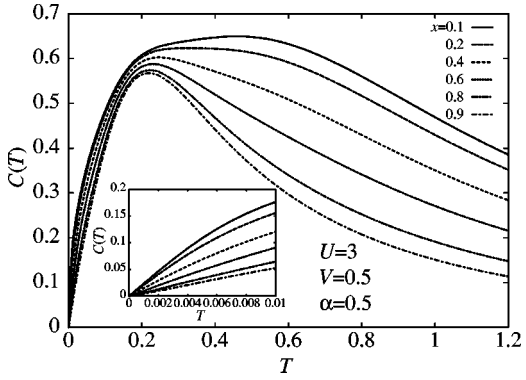

FIG. 7. Temperature dependence of the specific heat for several values of x: $x=0.1$, 0.2, 0.4, 0.6, 0.8, and 0.9. Inset shows an enlargement for lower temperature.

DOS spectrum is narrower and two satellite peaks are clearer. Namely, the quasiparticle band is strongly renormalized and the correlation effect in the system with the parameter set B is relatively stronger than that in the system with set A, since the mixing between f electrons and conduction electrons is smaller while the energy dispersion of f electrons themselves is slightly larger. The value of γ_f for $x=1$ which corresponds to the single-impurity limit tends to be larger than that for $x=0$ when the correlation effect is strong.

We can also see the impurity-concentration dependence of the total specific-heat coefficient itself in the temperature dependence of the specific heat shown in Fig. 7. These data are obtained by the numerical differential of the total energy. From the viewpoint of the Fermi-liquid theory, one can see that the effective mass of the quasiparticle decreases as the impurity concentration increases. It can be simply interpreted that the correlation effect itself becomes weak since the density of host sites on which the Coulomb repulsion exists decreases. The specific-heat curve for the highest concentration of impurity sites has a single peak. This temperature dependence is similar to that observed in the single Kondo impurity system, in which the specific-heat curve has a single peak around the Kondo temperature.

IV. SUMMARY

In the present study, we have treated the inhomogeneous PAM with randomly distributed sites without f electrons by the scheme consisting of the DMFT and the CPA, and investigated impurity-concentration dependence of the resistivity, the density of states, and the specific heat. Impurity sites in the present system have no f electrons and they correspond to nonmagnetic ions in real systems. For lower concentrations of impurities, the resistivity at lower temperature has a T^2 dependence and it decreases as temperature decreases. This temperature dependence corresponds to that observed in typical heavey-fermion compounds which have no magnetic ordering. The residual resistivity increases with increasing impurity concentration. When the impurity concentration increases much more, the temperature dependence of the resistivity changes; the resistivity increases monotonically with decreasing temperature. At the lowest temperature the resistivity reaches the residual resistivity. This residual resistivity in systems for dense-impurity sites corresponds to the unitarity limit of the single Kondo impurity system. In fact, by the calculation of the linear T specific-heat coefficient and the density of states at the Fermi level, we have obtained continuous impurity-concentration dependencies of the above quantities, and have found that the dense-impurity limit of the system approaches the single Kondo impurity system described by the SIAM in the strong-coupling regime. By using the scheme proposed in the present study, we can describe the electronic state in the whole region from the local Fermi liquid to the heavy Fermi liquid on the same theoretical footing.

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