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Crossover from a Low-Temperature Heavy-Quasiparticle State to a High-Temperature Local-Moment State in the Heavy-Fermion System

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We investigate the crossover from a low-temperature state in which heavy quasiparticles are formed to the high-temperature state in which conduction electrons separated from the degrees of freedom of f electrons exist in the heavy-fermionic model with the hybridization between conduction electrons and f electrons. To study the temperature dependence of spectral functions, the dynamical mean-field approach is adopted to treat the electron correlation between f electrons. By considering the competition between the effective hybridization energy V^* and the characteristic energy Γ of quasiparticle excitation, it is found that there is a condition, that is, $\Gamma > V^*$, for a system to show this crossover, whereas for $\Gamma \lesssim V^*$, the quasiparticle states in the hybridization band become ambiguous with increasing temperature before the effective hybridization between f electrons and conduction electrons is lost.

1. Introduction

In heavy-fermion systems, it is established that characteristic electronic states such as the formation of the heavy-quasiparticle state and unconventional superconductivity originate from the strong correlation between almost localized f electrons that hybridize with conduction electrons in a wide band.[1)] In a simple picture of the origin of the heavy effective mass of a quasiparticle, that is, the large specific heat coefficient, it is considered that spin degrees of freedom of almost localized f electrons are not lost by any magnetic orders and that they persist until at low temperature, and the system releases the entropy of the spin degrees of freedom in a narrow temperature range at once by the occurrence of the Fermi condensation of quasiparticles that consist of hybridized f electrons and conduction electrons. At high temperature, the spin degree of freedom of the localized f electron does not couple with that of the conduction electron (here, we call this state the c-f separated state). With decreasing

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temperature, both degrees of freedom couple and they form a heavy Fermi liquid state with a similar mechanism to the Kondo effect. There is no phase transition but a crossover from the heavy Fermi liquid state at low temperature to the c-f separated state at high temperature.

In the above simple picture of the formation of the heavy Fermi liquid state with the large specific heat coefficient, it is assumed that the c-f separated state is well-defined at high temperature, that is, the almost localized f electrons with large spin degrees of freedom and the almost free conduction electrons separated from the f electrons exist at high temperature. In this situation, even at high temperature at which the hybridization between f electrons and conduction electrons effectively disappears, a kind of quasiparticle state that can be regarded as the almost free conduction electron should still exist.

Concerning the crossover from the localized to the itinerant state of heavy-fermion systems, the temperature dependence of the spectral function and the optical conductivity were reported in a theoretical study of the model with a realistic band structure obtained by the local density approximation for $CeIrIn_5$.[2)] In this study, it was shown that the electronic state in which f electrons are tightly bound and localized on the Ce atom exists at room temperature. This state corresponds to the c-f separated state mentioned above. Although it is natural to consider that a well-defined c-f separated state exists at high temperature, the condition of its existence is not trivial. In the theoretical point of view, it cannot be described by the one-body approximation such as the Hartree approximation that the hybridization between f electrons and conduction electrons effectively disappears at high temperature. In order to describe the temperature dependence of the effective hybridization, it is necessary to treat the correlation effect beyond the one-body approximation.

In this study, we address the crossover from the heavy Fermi liquid state at low temperature to the c-f separated state at high temperature in a simple model of the heavy-fermion system. Moreover, we investigate the condition of the existence of a well-defined c-f separated state with almost localized moments at high temperature to answer the question of whether the quasiparticle state that consists of hybridized conduction electrons and f electrons always becomes the c-f separated state at high temperature. We adopt the periodic Anderson model (PAM) as the simple model of the heavy-fermion system. It is necessary to consider the realistic band structure to discuss details of the characteristic properties of various compounds in the heavy-fermion systems. In this study, however, we use a simple tight-binding energy dispersion since we concentrate ourselves only on investigating the temperature dependence of the quasiparticle state. To visually show the effect of the effective hybridization on the formation of the Fermi surface, a two-dimensional system and not a

realistic three-dimensional system is adopted. As mentioned above, we need to treat the correlation effect beyond the one-body approximation to study the temperature dependence of the electronic state of the system. We treat the correlation effect in the PAM by the dynamical mean-field approach.[2–4] In Ref. 2, the authors used a vertex-corrected one-crossing approximation (VCOCA) or a continuous-time quantum Monte Carlo method (CTQMC) as an impurity solver of the dynamical mean-field theory (DMFT). In the present calculation, we adopt the iterated perturbation theory (IPT)[5] as the impurity solver of the DMFT framework, since the IPT is useful for obtaining a real-frequency spectrum such as a density of states and it is easy in the IPT to treat the system in a wide temperature range including absolute zero in contrast to the CTQMC. It is also expected that the IPT is complementary to the VCOCA because the former is based on the perturbation in the Coulomb interaction.

2. Model and Formulation

The model Hamiltonian of the PAM that we consider in the present paper is defined as

$$\mathcal{H} = \sum_{\boldsymbol{k},\sigma}(\varepsilon_{\boldsymbol{k}}-\mu)c^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\sigma}(\varepsilon^{f}_{\boldsymbol{k}}-\mu)f^{\dagger}_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma} + V\sum_{\boldsymbol{k},\sigma}(c^{\dagger}_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma} + f^{\dagger}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}) + U\sum_{i} f^{\dagger}_{i\uparrow}f_{i\uparrow}f^{\dagger}_{i\downarrow}f_{i\downarrow}, \quad (1)$$

where $\varepsilon_{\boldsymbol{k}}$ and μ denote the kinetic energy of a conduction electron and chemical potential, respectively. We assume the nearest-neighbor hopping on the square lattice, and then the kinetic energy of the conduction electron is expressed as $\varepsilon_{\boldsymbol{k}} = -2t[\cos(k_x a)+\cos(k_y a)]$, where t and a denote the hopping energy and a lattice constant, respectively. Hereafter, t is taken as a unit of energy and a is set to 1. Note that dispersive f electrons are introduced in the present model and that the kinetic energy of an f electron is denoted by $\varepsilon^{f}_{\boldsymbol{k}}$.[6] We assume that the f electron has the same dispersion as that for the conduction electron: $\varepsilon^{f}_{\boldsymbol{k}} \equiv \varepsilon^{f} + \alpha\varepsilon_{\boldsymbol{k}} \quad (\alpha > 0)$, where ε^{f} denotes the f electron energy level.[7] The hybridization energy is assumed as $\boldsymbol{k}$-independent and real; it is denoted by V. The on-site Coulomb repulsion energy between f electrons is denoted by U. The case with an efficiently larger U than V and an efficiently deeper f-level ($U \sim |\varepsilon^{f}| \gg V$) corresponds to the almost localized f-electron system, and one can derive the low-energy effective model in this case, that is, the Kondo lattice model (KLM) from the PAM. The antiferromagnetic exchange energy J between the localized f-spin and the spin of the conduction electron in the KLM is obtained by the second-order perturbation of V, and J is estimated as $J \sim V^2/U$.

In this study, we apply the dynamical mean-field approach to model (1) with the local approximation of the self-energy. In order to investigate Green's function in a wide temperature range, we use the IPT as the impurity solver in the DMFT, as mentioned in Sect. 1. The

IPT is effective for the system with a particle-hole symmetry.[3] In model (1), the particle-hole symmetric condition is expressed as $\varepsilon^f + U/2 = \mu = 0$. Under this condition, the f-electron Green's function matrix is expressed as follows (we omit the spin index since we consider the paramagnetic state only):

$$\begin{pmatrix} G_{\boldsymbol{k}}^{cc}(z) & G_{\boldsymbol{k}}^{cf}(z) \\ G_{\boldsymbol{k}}^{fc}(z) & G_{\boldsymbol{k}}^{ff}(z) \end{pmatrix} = \begin{pmatrix} z - \varepsilon_{\boldsymbol{k}} & -V \\ -V & z - \alpha\varepsilon_{\boldsymbol{k}} - \tilde{\Sigma}(z) \end{pmatrix}^{-1}, \tag{2}$$

where $\tilde{\Sigma}(z)$ denotes the self-energy without the Hartree term under the local approximation. Note that the conventional PAM without the f-electron dispersion has the hybridization gap at the Fermi level under the particle-hole symmetric condition. In the present study, we introduce the dispersive f electron to model (1) since we are interested in the metallic ground state with the well-defined Fermi surface. In the system with parameters satisfying the condition $\alpha > (V/D)^2$, the hybridization gap vanishes (where D denotes the band width of the unperturbed conduction electron and $D = 4$ in the present model). The local f-electron Green's function $G^{ff}(z)$ is defined by $G^{ff}(z) \equiv \sum_{\boldsymbol{k}} G_{\boldsymbol{k}}^{ff}(z)/N$, where the number of $\boldsymbol{k}$-points in the first Brillouin zone is denoted by N.

In the DMFT scheme, the local f-electron Green's function is also expressed with the cavity Green's function (or the Weiss function) $\mathcal{G}(z)$ and the usual self-energy $\Sigma(z)$ including the Hartree term under the local approximation as follows:

$$(G^{ff}(z))^{-1} = (\mathcal{G}(z))^{-1} - \Sigma(z) = (\tilde{\mathcal{G}}(z))^{-1} - \tilde{\Sigma}(z), \tag{3}$$

where $[\tilde{\mathcal{G}}(z)]^{-1}$ is defined without the Hartree term similarly to $\tilde{\Sigma}(z)$. In the IPT, the self-energy is approximated by the second-order perturbative contribution, which consists of the cavity Green's function:[5]

$$\tilde{\Sigma}(i\varepsilon_n) \simeq -U^2T^2 \sum_{l,m} \tilde{\mathcal{G}}(i\varepsilon_l)\tilde{\mathcal{G}}(i\varepsilon_m)\tilde{\mathcal{G}}(i\varepsilon_n + i\varepsilon_l - i\varepsilon_m), \tag{4}$$

where ε_n is the fermionic Matsubara frequency defined by $\varepsilon_n = (2n+1)\pi T$ with the integer n and the temperature T.

By solving Eqs. (2), (3), and (4) self-consistently, we obtain the f-electron spectral function $\rho^f(\boldsymbol{k}, \varepsilon)$ and the conduction-electron spectral function $\rho^c(\boldsymbol{k}, \varepsilon)$ defined as

$$\rho^f(\boldsymbol{k}, \varepsilon) \equiv -\frac{1}{\pi}\mathrm{Im}G_{\boldsymbol{k}}^{ff}(\varepsilon + i\eta), \tag{5}$$

$$\rho^c(\boldsymbol{k}, \varepsilon) \equiv -\frac{1}{\pi}\mathrm{Im}G_{\boldsymbol{k}}^{cc}(\varepsilon + i\eta), \tag{6}$$

where η is a positive infinitesimal. The local density of states $\rho^{f(c)}(\varepsilon)$ is obtained by the

summation of the spectral function over the first Brillouin zone: $\rho^{f(c)}(\varepsilon) = \sum_{\boldsymbol{k}} \rho^{f(c)}(\boldsymbol{k}, \varepsilon)/N$. In the efficiently low-temperature and low-energy region, we can express Green's function by renormalized quantities as

$$G^{ff}_{\boldsymbol{k}}(\varepsilon + i\eta) \simeq \frac{Z}{\varepsilon + i\eta - \varepsilon^{f*}_{\boldsymbol{k}} - \dfrac{(V^*)^2}{\varepsilon + i\eta - \varepsilon_{\boldsymbol{k}}}}, \tag{7}$$

$$\varepsilon^{f*}_{\boldsymbol{k}} \equiv Z(\varepsilon^{f}_{\boldsymbol{k}} + \mathrm{Re}\tilde{\Sigma}(0 + i\eta)), \tag{8}$$

$$V^* \equiv \sqrt{Z}V, \tag{9}$$

$$Z \equiv \left(1 - \left.\frac{d\mathrm{Re}\tilde{\Sigma}(\varepsilon + i\eta)}{d\varepsilon}\right|_{\varepsilon=0}\right)^{-1}, \tag{10}$$

where Z is the renormalization factor and we refer to V^* as the (renormalized) effective hybridization energy hereafter.

Once Green's function and the self-energy are obtained, we can calculate the expectation value d^f of the f-electron double occupancy for $U > 0$ as

$$\begin{aligned} d^f \equiv& \frac{1}{N}\sum_i \langle f^\dagger_{i\uparrow} f_{i\uparrow} f^\dagger_{i\downarrow} f_{i\downarrow}\rangle \\ =& \frac{1}{U}\int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\left\{-\frac{1}{\pi}\mathrm{Im}\left(\Sigma(\varepsilon + i\eta)G^{ff}(\varepsilon + i\eta)\right)\right\}, \end{aligned} \tag{11}$$

where the Fermi distribution function is denoted by $f(\varepsilon)$. Equation (11) also holds in the general case without the particle-hole symmetry, and $\Sigma(z)$ in Eq. (11) includes the Hartree term. Then, the effective spin s^f of the f-electron is estimated from d^f as

$$s^f(s^f + 1) \equiv \frac{1}{N}\sum_i \langle \boldsymbol{S}^f_i \cdot \boldsymbol{S}^f_i\rangle = \frac{3}{4}\frac{1}{N}\sum_{i\sigma}\langle f^\dagger_{i\sigma} f_{i\sigma}\rangle - \frac{3}{2}d^f, \tag{12}$$

where $\boldsymbol{S}^f_i$ denotes the f-electron spin operator on the site i and is defined as $\boldsymbol{S}^f_i \equiv \sum_{\tau\tau'} f^\dagger_{i\tau}(\boldsymbol{\sigma})_{\tau\tau'} f_{i\tau'}/2$ with the Pauli matrix $\boldsymbol{\sigma}$.

3. Results

First, we show the temperature dependence of the local f-electron density of states (DOS) $\rho^f(\varepsilon)$ for the system with $U = 8$, $V^2 = 0.25$, and $\alpha = 0.5$ in Fig. 1. At absolute zero, a sharp peak indicating the formation of well-defined quasiparticles exists at the Fermi level ($\varepsilon = 0$). With increasing temperature, the sharp peak becomes broad and it disappears at high temperature. Large peaks exist in the high-energy region at approximately $\varepsilon \sim \pm 5$ and those correspond to high-energy local excitations (the upper and lower Hubbard bands). One can see that those high-energy peaks persist even at high temperature in contrast to the central

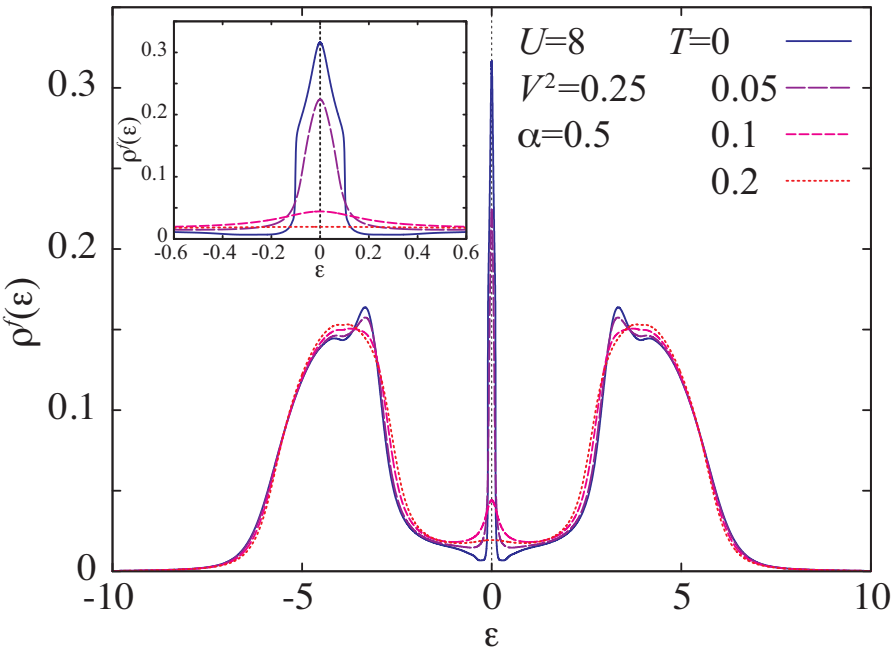

Fig. 1. (Color online) Spectra of the local f-electron DOS $\rho^f(\varepsilon)$ at $T = 0$, 0.05, 0.1, and 0.2 for $U = 8$, $V^2 = 0.25$, and $\alpha = 0.5$. The inset shows the DOS near the Fermi level ($\varepsilon = 0$).

sharp peak.

The existence of high-energy local excitation peaks reflects the enhancement of the local spin fluctuation. In the system with $V^2 = 0.25$ and $U = 8$, actually, one can see that the f-electron double occupancy is strongly suppressed and the value of the effective spin becomes almost $1/2$ with increasing U for any α (Fig. 2). The spin fluctuation is more suppressed for a larger V. Nevertheless, the effective spin even for $V^2 = 2.0$ approaches $1/2$ in the system with $U = 8$ (Fig. 3). Thus, concerning the present system with $U = 8$, we adopt V^2/U corresponding to the antiferromagnetic exchange energy J of the KLM mentioned in Sect. 1 as a parameter that reflects the correlation effect hereafter.

In Fig. 1, the disappearance of the central sharp peak corresponds to the fact that quasiparticles cannot be well-defined at high temperature. To estimate the temperature below which the quasiparticle is well-defined, we adopt the FWHM denoted by Γ of the central peak as the quantity corresponding to the inverse of the lifetime of the quasiparticle. Since the half-width Γ indicates the energy scale or the temperature below which the quasiparticle is well-defined, it is considered as the characteristic energy corresponding to the renormalized Fermi temperature $T_{\rm F}^*$ of the quasiparticle. On the other hand, one can consider another characteristic energy that reflects the frequency of the hybridization between f electrons and conduction electrons, and we adopt the effective hybridization energy V^* defined by Eq. (9) as such a

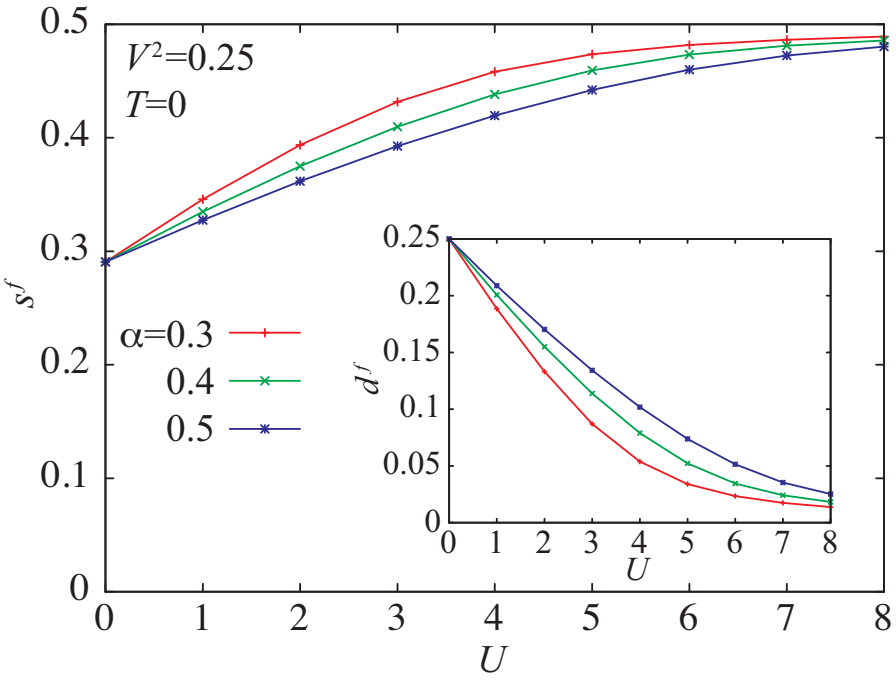

Fig. 2. (Color online) U dependences of the effective spin s^f of the f electron for several values of α (α = 0.3, 0.4, and 0.5) and V^2 = 0.25 at absolute zero. The inset shows the U dependences of the double occupancy d^f of the f electron.

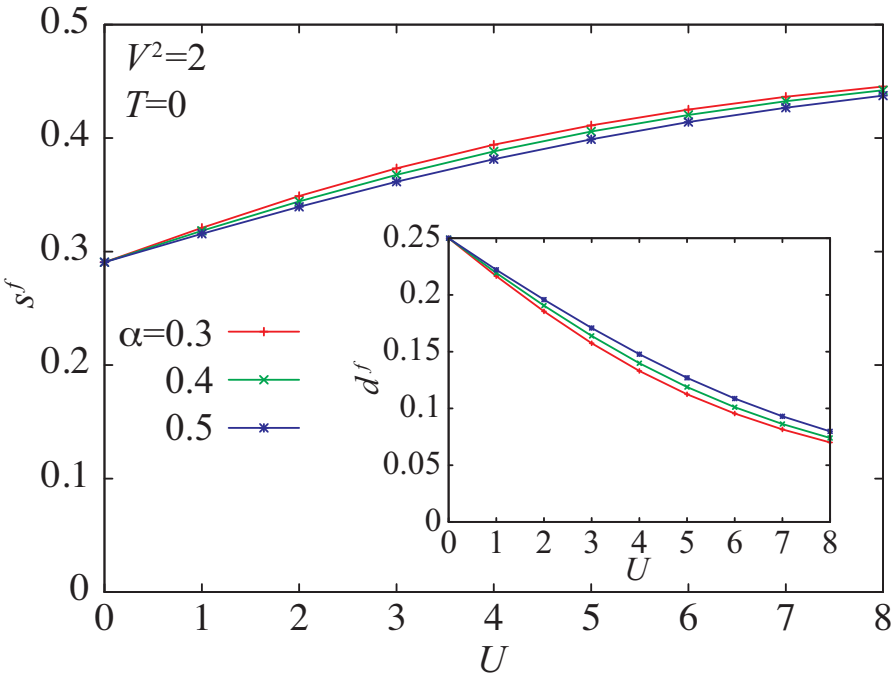

Fig. 3. (Color online) U dependences of the effective spin s^f of the f electron for several values of α (α = 0.3, 0.4, and 0.5) and V^2 = 2 at absolute zero. The inset shows the U dependences of the double occupancy d^f of the f electron.

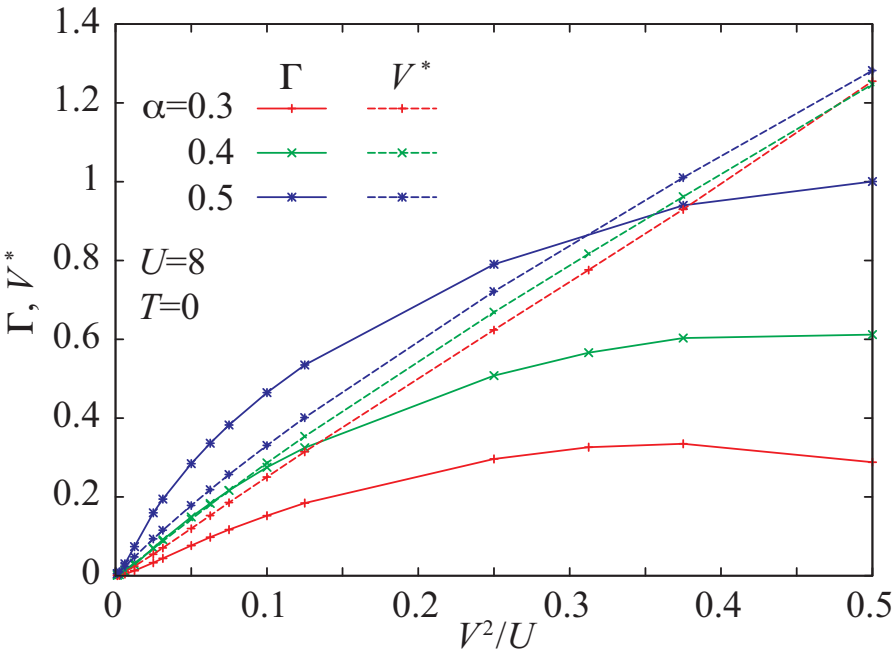

Fig. 4. (Color online) V^2/U dependences of Γ and V^* for several values of α (α = 0.3, 0.4, and 0.5) and U = 8 at absolute zero. The solid and dashed lines indicate Γ and V^*, respectively.

characteristic energy. Figure 4 shows the V^2/U dependences of Γ and V^* for several values of α.

For $\alpha = 0.5$, the parameter region can be separated into two: a region for $V^2/U \lesssim 0.3$ in which $\Gamma > V^*$ and a region for $V^2/U \gtrsim 0.3$ in which $\Gamma < V^*$. We call the systems in the former and latter regions type A and type B, respectively. Since Γ is larger than V^* in the type A system, there should be a temperature region in which the quasiparticle picture still holds although the effective hybridization is lost. Thus, it is expected in the type A system that the quasiparticle state, which almost consists of only conduction electrons, will exist in the above temperature region. In the type B system, however, the quasiparticle state without the effective hybridization cannot be formed because the temperature corresponding to V^* is higher than that corresponding to Γ.

Actually, in Fig. 5, one can confirm that a crossover occurs in the type A system from the quasiparticle state formed in the hybridization band between f electrons and conduction electrons to the state that almost consists of only conduction electrons. At $T = 0$, a clear Fermi surface of the hybridization band can be seen.[8)] As temperature increases, the intensity at the original Fermi surface at $T = 0$ is gradually suppressed. Finally, the spectrum has a high intensity along the Fermi surface of conduction electrons, which do not have the original hybridization with f-electrons at the highest temperature.[9)] The crossover occurs in a narrow

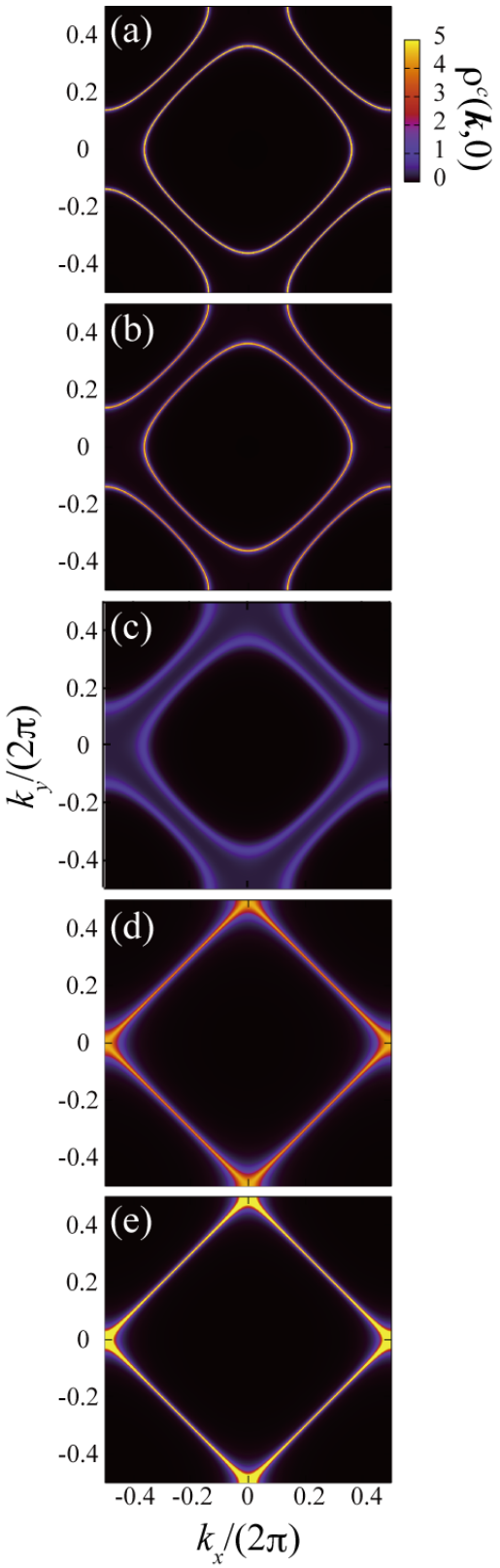

Fig. 5. (Color online) Temperature dependence of the conduction-electron component of the spectral intensity $\rho^c(\boldsymbol{k}, 0)$ at $\varepsilon = 0$ for $V^2 = 0.25$, $U = 8$, and $\alpha = 0.5$ (type A system: see text) at (a) $T = 0$, (b) 0.02, (c) 0.04, (d) 0.08, and (e) 0.16.

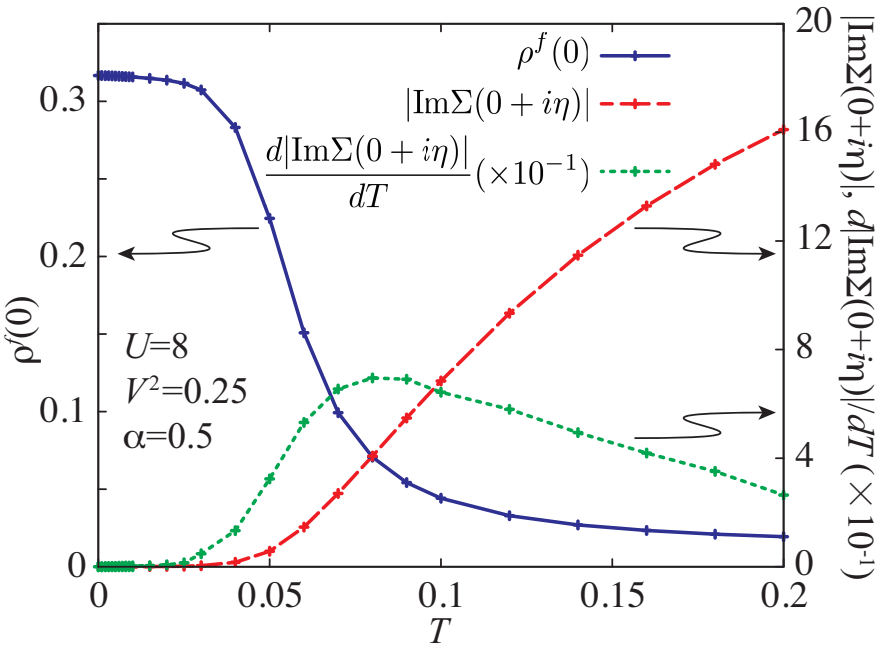

Fig. 6. (Color online) Temperature dependences of the quasiparticle peak height $\rho^f(0)$, the imaginary part $|\mathrm{Im}\Sigma(0+i\eta)|$ of the self-energy, and temperature derivative $d|\mathrm{Im}\Sigma(0+i\eta)|/dT$ of the imaginary part of the self-energy for $V^2 = 0.25$, $U = 8$, and $\alpha = 0.5$ (type A system).

temperature region and it is reflected in the temperature dependence of the quasiparticle peak height $\rho^f(0)$ or the imaginary part $|\mathrm{Im}\Sigma(0+i\eta)|$ of the self-energy that corresponds to the inverse of the quasiparticle lifetime.[2)] As temperature increases, the quasiparticle peak height rapidly decreases, as shown in Fig. 6. The behavior reflects a rapid increase in the scattering rate with increasing temperature. One can regard the temperature around which the temperature derivative of $|\mathrm{Im}\Sigma(0+i\eta)|$ peaks as the crossover temperature. It is shown in Fig. 7 that the Fermi surface structure also changes markedly at approximately the crossover temperature.

On the other hand, in the type B system, the separation of components of f electrons and conduction electrons in the hybridization band does not occur up to the highest temperature shown in Fig. 8. Although there exists a clear Fermi surface of the hybridization band at $T = 0$, it loses its intensity and the entire structure of the Fermi surface does not change as temperature increases. The quasiparticle states in the hybridization band become ambiguous before the effective hybridization between f electrons and conduction electrons is lost, as shown in Fig. 8(e), which should be compared with Fig. 7(b). In the type B system, thus, a quasiparticle state that consists only of the conduction-electron component does not exist. In the case of $\alpha = 0.3$, Γ is always smaller than V^* in the entire V^2/U range, as shown in Fig. 4, and there exists only the type B system.

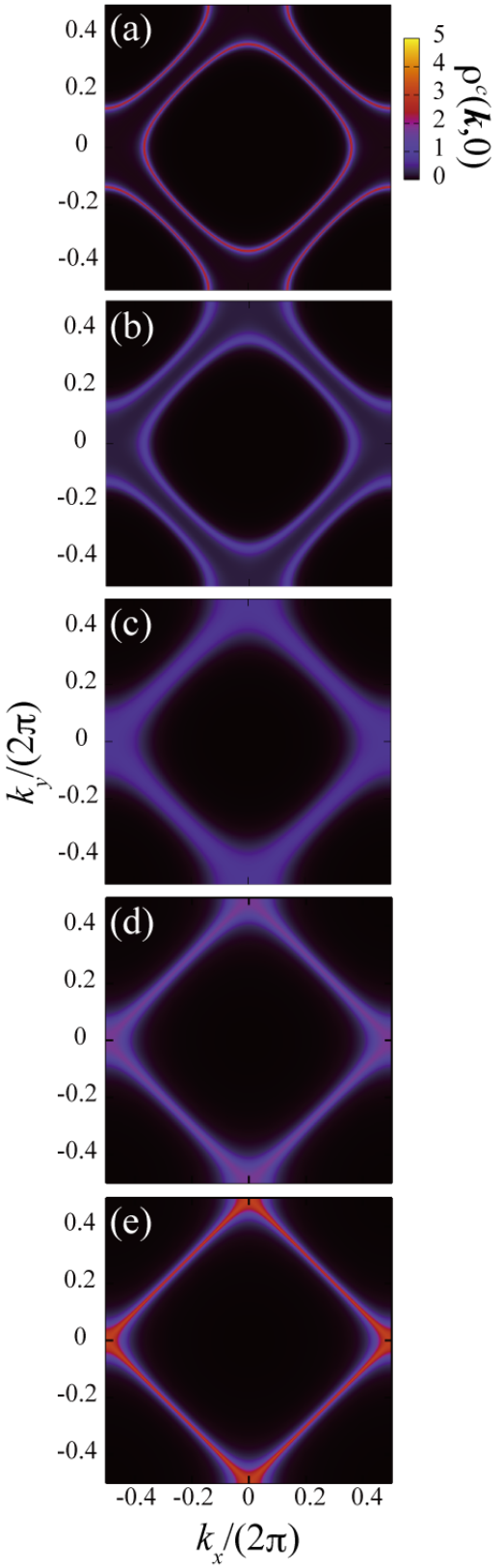

Fig. 7. (Color online) Fine temperature dependence of the conduction-electron component of the spectral intensity $\rho^c(\boldsymbol{k}, 0)$ at $\varepsilon = 0$ for $V^2 = 0.25$, $U = 8$, and $\alpha = 0.5$ (type A system) at (a) $T = 0.03$, (b) 0.04, (c) 0.05, (d) 0.06, and (e) 0.07.

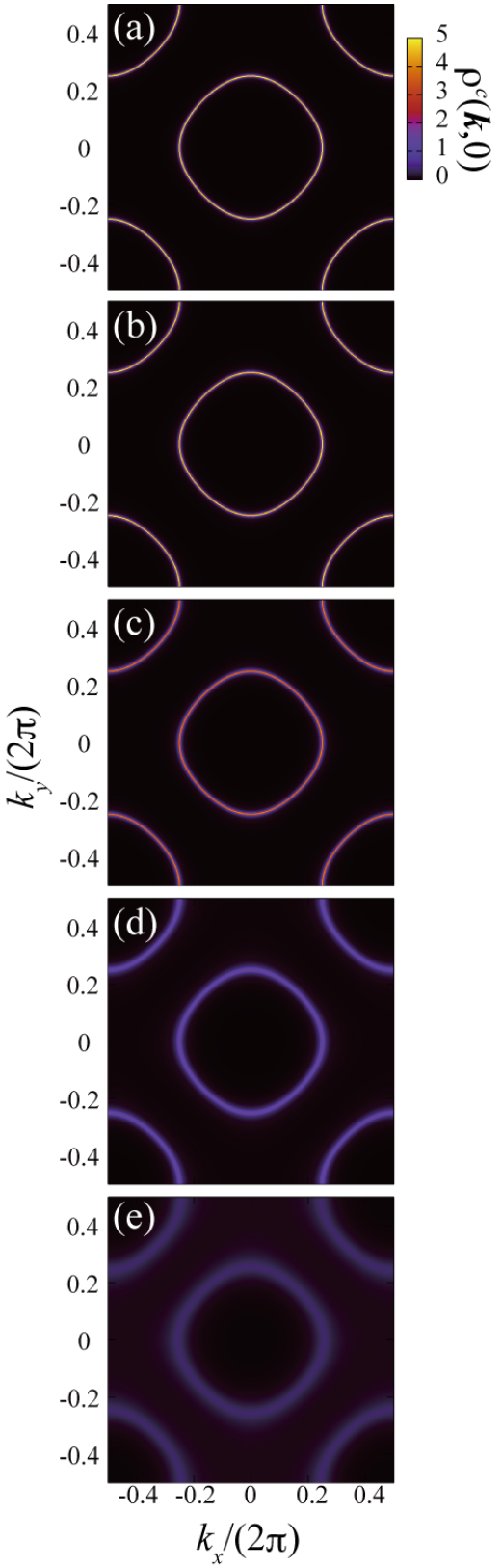

Fig. 8. (Color online) Temperature dependence of the conduction-electron component of the spectral intensity $\rho^c(\boldsymbol{k}, 0)$ at $\varepsilon = 0$ for $V^2 = 2$, $U = 8$, and $\alpha = 0.5$ (type B system: see text) at (a) $T = 0$, (b) 0.02, (c) 0.04, (d) 0.08, and (e) 0.16.

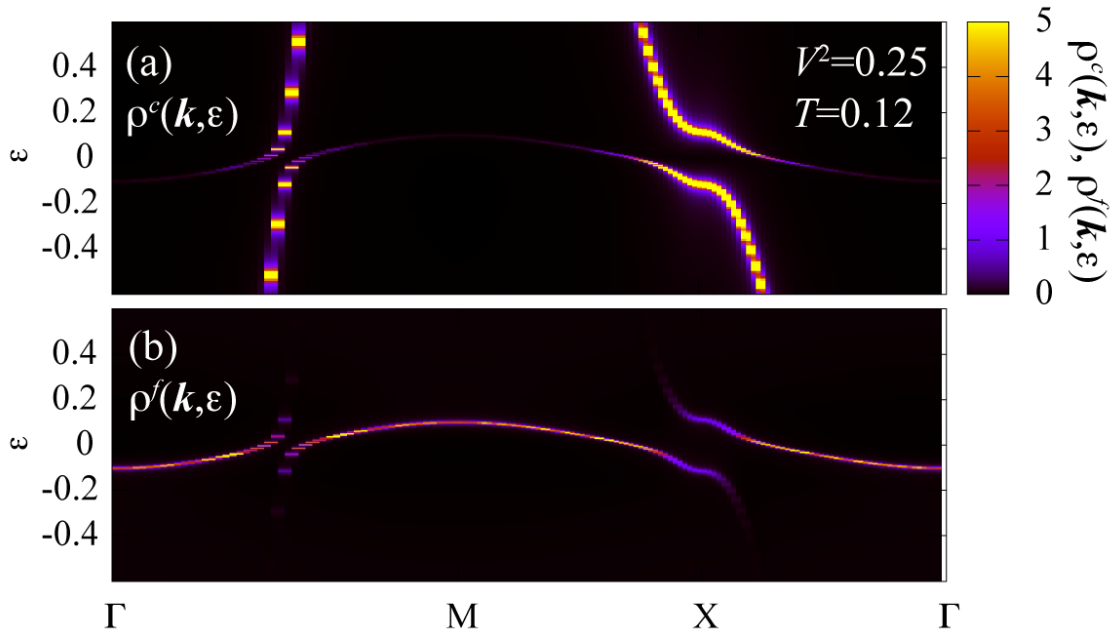

Fig. 9. (Color online) (a) Conduction-electron component $\rho^c(\boldsymbol{k}, \varepsilon)$ and (b) f-electron component $\rho^f(\boldsymbol{k}, \varepsilon)$ of the spectral functions near the Fermi level $\varepsilon = 0$ along the symmetric line in the first Brillouin zone for $V^2 = 0.25$, $U = 8$, and $\alpha = 0.5$ at $T = 0$. The horizontal and vertical lines indicate the wave number $\boldsymbol{k}$ along the symmetric line of the first Brillouin zone and the energy ε, respectively.

Let us concentrate on the spectral functions $\rho^c(\boldsymbol{k}, \varepsilon)$ and $\rho^f(\boldsymbol{k}, \varepsilon)$ of both type A and B systems. At absolute zero, the conduction electron and f electron hybridize, forming a hybridization band. Both components of the conduction electron and f electron have almost the same intensity near the Fermi level $\varepsilon = 0$ (Fig. 9). At a temperature higher than that corresponding to the effective hybridization V^*, the energy dispersion of the conduction-electron component becomes almost the same as that of the conduction band without the f electron [Fig. 10(a)]. The f-electron component of the spectrum loses its intensity at approximately the Fermi level and only the intensity without a strong dispersion in the high-energy region remains [Fig. 10(b)]. In the type B system, however, the f-electron component of the spectrum has a dispersive intensity near the Fermi level even at the highest temperature (Fig. 11). This shows that the separation of the conduction-electron component and f-electron component does not occur up to a temperature higher than that corresponding to Γ in the type B system.

4. Summary and Discussion

In summary, we have calculated the spectral functions of the PAM on the square lattice and have investigated their temperature dependence by the dynamical mean-field approach.

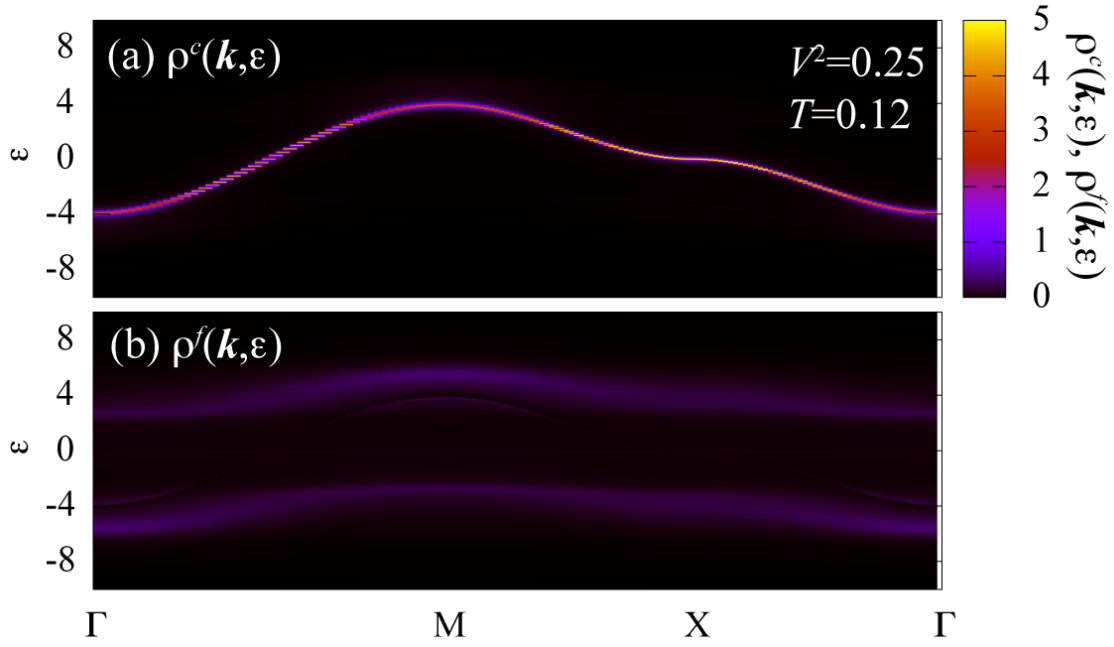

Fig. 10. (Color online) (a) Conduction-electron component $\rho^c(\boldsymbol{k}, \varepsilon)$ and (b) f-electron component $\rho^f(\boldsymbol{k}, \varepsilon)$ of the spectral functions along the symmetric line in the first Brillouin zone for $V^2 = 0.25$, $U = 8$, and $\alpha = 0.5$ at $T = 0.12$.

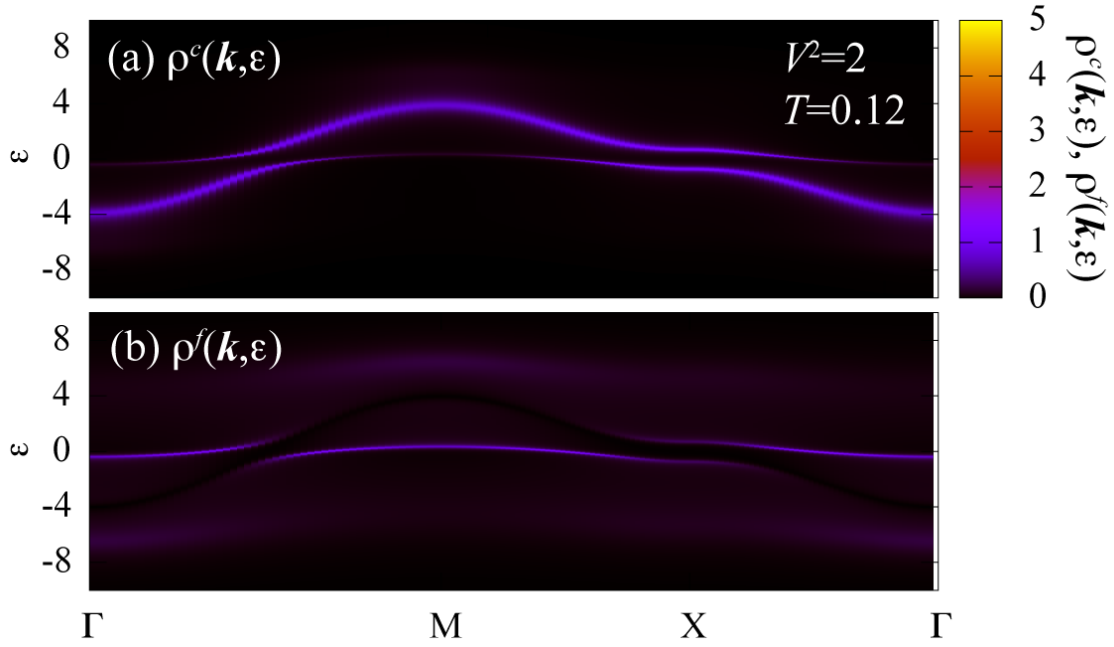

Fig. 11. (Color online) (a) Conduction-electron component $\rho^c(\boldsymbol{k}, \varepsilon)$ and (b) f-electron component $\rho^f(\boldsymbol{k}, \varepsilon)$ of the spectral functions along the symmetric line in the first Brillouin zone for $V^2 = 2$, $U = 8$, and $\alpha = 0.5$ at $T = 0.12$.

The half-width Γ of the central peak of the DOS spectrum, which reflects the lifetime of the quasiparticle, and the effective hybridization energy V^* have been compared. We have found that the c-f separated state without the effective hybridization is not apparent at high temperature in the type B system with a smaller Γ than V^*, while the well-defined conduction-electron-like dispersion relation separated from the degree of freedom of the f electron at a temperature higher than that corresponding to V^* has been found in the type A system with larger Γ than V^*. The crossover behavior in the type A system in a narrow temperature range at approximately the crossover temperature corresponds to that reported in Ref. 2. In the simple picture of the electronic state of the heavy-fermion system, it might be considered that the c-f separated state always occurs at a temperature higher than that corresponding to the effective hybridization energy. In this study, however, it has been pointed out that there is a condition under which the c-f separated state occurs at high temperature, and not all systems with the c-f hybridization have the well-defined c-f separated state that loses the effective hybridization.

It has been assumed in the present calculation that the f electron has the energy dispersion in contrast to the conventional PAM with $\alpha = 0$ in order to realize the metallic ground state even if the system has the particle-hole symmetry. If one considers the conventional PAM without any f-electron dispersions under the particle-hole symmetry, the system has a hybridization gap at the Fermi level. Even in the interacting system, the hybridization gap is guaranteed to open on the basis of Luttinger's theorem,[10] and this situation is considered as a theoretical model of the Kondo insulator/semiconductor.[11,12] The magnitude Δ of the energy gap between the valence and conduction bands is estimated in the quasiparticle picture at absolute zero as $\Delta \simeq 2(V^*)^2/D$ for $Z \ll 1$. In this situation, a quantity corresponding to Γ in Sect. 3 should be Δ, and then $\Gamma/D \sim \Delta/D \simeq 2(V^*/D)^2 \ll V^*/D$ holds, that is, $\Gamma \ll V^*$ for $Z \ll 1$. A situation similar to the above corresponds to the type B system in the present results in the case of $\alpha = 0.3$. Thus, the artificiality of the particle-hole symmetry of the model might cause the present result that only the type B system exists in the case of $\alpha = 0.3$ even though it seems that the f-electron localization becomes stronger with decreasing α. Although α is the artificial parameter introduced to realize the metallic ground state under the particle-hole symmetry and the parameter is not essential for reproducing the heavy-quasiparticle state at low temperature, it is expected that the type A system in the present result for $\alpha = 0.5$ with a small V^2/U is a typical model of a realistic heavy-fermion system. It is also expected that the present condition of the existence of the crossover will be general in the hybridization model because a similar temperature dependence of the spectral function and crossover behavior are

observed in the system on another type of lattice without any singularities in the density of states (not shown here in detail).[13)]

It will be left as a future work to systematically investigate the condition of the existence of the crossover from the heavy-quasiparticle state at low temperature to the clear c-f separated state at high temperature in a simple but more general model of the heavy-fermion system. We believe that the condition of $\Gamma \gg V^*$ is an essential and reasonable condition for the existence of the crossover between the above two states in general heavy-fermion systems.

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References

1) For a review, see, e.g., A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1997).

2) J. H. Shim, K. Haule, and G. Kotliar, Science **318**, 1615 (2007).

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

4) G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. **78**, 865 (2006).

5) X. Y. Zhang, M. Rozenberg, and G. Kotliar, Phys. Rev. Lett. **70**, 1666 (1993).

6) Although the effect of the f-orbital bandwidth itself on the magnetic correlation in a heavy-fermion model has recently been studied [A. Euverte, S. Chiesa, R. T. Scalettar, and G. G. Batrouni, Phys. Rev. B **88**, 235123 (2013)], the dispersiveness of the f electron is not essential to the present study, as mentioned below.

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

8) Note that the form of the Fermi surface is unchanged by the interaction between electrons under the local approximation of the self-energy.

9) Strictly speaking, the Fermi surface should be defined at absolute zero, and the expression "the Fermi surface at finite temperature" is used only for convenience and is not correct.

10) J. M. Luttinger, Phys. Rev. **119**, 1153 (1960); J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960); R. M. Martin, Phys. Rev. Lett. **48**, 362 (1982).

11) G. Aeppli and Z. Fisk, Comments Condens. Matter Phys. **16**, 155 (1992).

12) P. Riseborough, Adv. Phys. **49**, 257 (2000).

13) We have confirmed a similar temperature dependence of the spectral function of the system with the semicircle density of states for free conduction electrons. The semicircle density of states corresponds to that of the system on the Bethe lattice with a limit of infinite connectivity; it has no singularity in contrast to the system on the square lattice.