Theory of the Anderson lattice at finite temperatures

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The theory of the heavy-fermion state in the Anderson lattice at absolute zero presented in the previous paper is extended to finite temperatures. This extension is systematically accomplished by using thermofield dynamics. The use of this formalism enables us to calculate the densities of states of the f electron and the conduction electron in the Anderson lattice at finite temperatures. An extremely sharp peak in each of the densities of states appears very near the Fermi level at low temperatures, along with a broad resonance peak outside the sharp peak. This narrow sharp peak corresponds to a heavy-quasifermion state. When the temperature increases, the sharp peak broadens and its height decreases due to a shortening of the quasifermion lifetime. This change may cause the crossover from the heavy-fermion state to the Kondo-impurity-like state observed in cerium and uranium compounds.

I. INTRODUCTION

Since the discovery of heavy-fermion systems in cerium and uranium compounds, extensive experimental and theoretical studies concerning their unusual properties have been done by many investigators. The following are some of the experimental results.[1] The specific-heat coefficients of these compounds are extremely large at low temperatures. The electrical resistivity in the systems exhibits a temperature dependence similar to that in Kondo-impurity systems at relatively high temperatures. However, at low temperatures, the resistivity is very small compared with that in Kondo-impurity systems and is proportional to the square of the temperature. This low-temperature state in the systems is called the heavy-fermion state or the coherent state. Some of the compounds show superconductivity in the heavy-fermion state.

Stimulated by the experimental results mentioned above, many theoretical studies have been made.[2] For treating the heavy-fermion systems, theoreticians usually use the following Anderson-lattice model. The f-electron ions whose f-electron energy levels are inside the conduction band are regularly placed at all lattice sites. The conduction electrons and the f electrons are mixed by the mixing interaction. The strong correlation interaction acts between f electrons when two f electrons sit on the same site. In a previous paper[3] (referred to as paper I hereafter), we used the following method to solve the Anderson-lattice problem at absolute zero. We assumed the Kondo regime where the f-electron levels are placed deeply below the Fermi level. In this regime, charge fluctuations are weak, and thus spin fluctuations dominantly contribute to the self-energies of electrons. Therefore, we set up coupled Dyson equations for the Green's functions for the electrons and the spin fluctuations. Between the self-energies and the vertex functions, there are various Ward-Takahashi relations which originate from the spin-rotational invariance. These Ward-Takahashi relations were utilized to relate the vertex functions to the self-

energies within the one-loop approximation. The Dyson equations which are approximated so as to satisfy these relations were solved numerically.

It has been shown that the unusual behavior of electrical resistivity, thermopower, specific heat, etc. in Kondo-impurity systems is explained in a unified manner by the resonance level appearing near the Fermi level.[4] The resonance level forms a peak in the density of states of the f electron near the Fermi level, when the density of states is calculated using an impurity Anderson model. It may be interesting to see how the resonance level is modified in the Anderson lattice. For this purpose we calculated the spectral density of the f-electron Green's function at absolute zero in paper I. The result is summarized as follows. When the wave number is fixed and the energy is changed, a very sharp peak appears near the Fermi level, corresponding to the quasifermion state. The energy dispersion of the quasifermion is very weak, indicating that the effective mass of the quasifermion is very heavy. Along with this sharp peak, a broad peak appears in a relatively high-energy region. This broad peak corresponds to the resonance level which is similar to the resonance level in the Anderson-impurity model.

Accordingly, we concluded that an essential difference of the electronic state in the Anderson lattice from that in the Kondo-impurity system is the appearance of the quasifermion state near the Fermi level. The fermion state may be responsible for the large coefficient of specific heat, the anomalous behavior of electrical resistivity, thermopower, and Hall effect, and also for superconductivity.

Our theory was restricted to absolute zero in paper I. In the present paper, to clarify the origin of the crossover between the heavy-fermion state and the impuritylike state at relatively high temperatures, we extend our theory to finite temperatures using the thermofield dynamics[5,6] which is a real-time formalism of quantum field theory at finite temperatures. A merit of the use of the thermofield dynamics is that there is no need to use the analytic continuation for obtaining dynamical quantities in contrast to the method of the temperature Green's function. The re-

sult of calculation is the following. The quasifermions even at the Fermi level have finite lifetimes at finite temperatures. As a result, the quasifermion level near the Fermi level rapidly changes to the resonance level as the temperature increases above a certain temperature. According to this change, the narrow sharp peak in the density of states near the Fermi level broadens and its height decreases as temperature increases. This change of the state near the Fermi level may cause the crossover from the heavy-fermion state to the Kondo-impurity-like state.

In Sec. II we give the formalism for the Anderson lattice at a finite temperature, and derive the Dyson equa-

tions for the self-energy, the spin fluctuations, and the vertex functions. In Sec. III we describe the procedure of solving the equations numerically and present the result of the calculation for the density of states of the f electron and the conduction electron. In Sec. IV the importance of the many-body effect in this system is especially emphasized.

II. FORMULATION

Let us consider the Anderson-lattice model described by the Hamiltonian

$$H = \sum_\sigma \int d^3x \{ \psi_\sigma^\dagger(x)\varepsilon(-\nabla^2)\psi_\sigma(x) + E_0\phi_\sigma^\dagger(x)\phi_\sigma(x) + V[\psi_\sigma^\dagger(x)\phi_\sigma(x) + \phi_\sigma^\dagger(x)\psi_\sigma(x)] + \tfrac{1}{2}U\phi_\sigma^\dagger(x)\phi_{-\sigma}^\dagger(x)\phi_{-\sigma}(x)\phi_\sigma(x) \} , \quad (2.1)$$

with

$$\varepsilon(-\nabla^2) = -\frac{1}{2m}\nabla^2 - \mu . \quad (2.2)$$

Here, $\psi_\sigma(x)$ and ϕ_σ are the Heisenberg fields, respectively, for the conduction electrons and f electrons, E_0 is the atomic f-electron level measured from the chemical potential μ, V is the mixing parameter, and U is the correlation energy between f electrons. Throughout this paper we use the units $\hbar = k_B = 1$. In the following calculations we utilize the formulation of thermofield dynamics (TFD)

to extend the theory for the Anderson lattice presented in paper I to that of finite temperature. In the TFD formalism the tilde Heisenberg fields which anticommute (commute) with the Heisenberg fields for fermions (bosons) are introduced to incorporate the temperature effect.[5,6] We denote these tilde Heisenberg fields for the conduction and f electrons, respectively, by $\tilde{\psi}_\sigma(x)$ and $\tilde{\phi}_\sigma(x)$. The system is then described by the total Hamiltonian,

$$\hat{H} = H - \tilde{H} , \quad (2.3)$$

where

$$\tilde{H} = \sum_\sigma \int d^3x \{ \tilde{\psi}_\sigma^\dagger(x)\varepsilon(-\nabla^2)\tilde{\psi}_\sigma(x) + E_0\tilde{\phi}_\sigma^\dagger(x)\tilde{\phi}_\sigma(x) + V[\tilde{\psi}_\sigma^\dagger(x)\tilde{\phi}_\sigma(x) + \tilde{\phi}_\sigma^\dagger(x)\tilde{\psi}_\sigma(x)] + \tfrac{1}{2}U\tilde{\phi}_\sigma^\dagger(x)\tilde{\phi}_{-\sigma}^\dagger(x)\tilde{\phi}_{-\sigma}(x)\tilde{\phi}_\sigma(x) \} . \quad (2.4)$$

Following Ref. 7, we define the thermal doublet:

$$\psi_\sigma^\alpha(x) = \begin{cases} \psi_\sigma(x) & \text{for } \alpha = 1 , \\ \tilde{\psi}_\sigma^\dagger(x) & \text{for } \alpha = 2 , \end{cases} \quad (2.5)$$

$$\phi_\sigma^\alpha(x) = \begin{cases} \phi_\sigma(x) & \text{for } \alpha = 1 , \\ \tilde{\phi}_\sigma^\dagger(x) & \text{for } \alpha = 2 . \end{cases} \quad (2.6)$$

Hamiltonian (2.3) leads to the following equations for ϕ_σ^α and ψ_σ^α:

$$[i\partial_t - \varepsilon(-\nabla^2)]\psi_\sigma^\alpha(x) = V\phi_\sigma^\alpha(x) , \quad (2.7)$$

$$(i\partial_t - E_0)\phi_\sigma^\alpha(x) = V\psi_\sigma^\alpha(x) + U\varepsilon^\alpha[\phi_{-\sigma}^\alpha(x)]^\dagger\phi_{-\sigma}^\alpha(x)\phi_\sigma^\alpha(x) , \quad (2.8)$$

where

$$\varepsilon^\alpha = \begin{cases} 1 & \text{for } \alpha = 1 , \\ -1 & \text{for } \alpha = 2 . \end{cases} \quad (2.9)$$

Now let us introduce the causal Green's functions for the f and conduction electrons:

$$g_\sigma^{\alpha\beta}(x - y) = \langle 0(\beta) | T\phi_\sigma^\alpha(x)[\phi_\sigma^\beta(y)]^\dagger | 0(\beta) \rangle$$

$$= \frac{i}{(2\pi)^4} \int d^4p \, g_\sigma^{\alpha\beta}(p)e^{ip(x-y)} , \quad (2.10)$$

$$C_\sigma^{\alpha\beta}(x - y) = \langle 0(\beta) | T\psi_\sigma^\alpha(x)[\psi_\sigma^\beta(y)]^\dagger | 0(\beta) \rangle$$

$$= \frac{i}{(2\pi)^4} \int d^4p \, C_\sigma^{\alpha\beta}(p)e^{ip(x-y)} , \quad (2.11)$$

where $| 0(\beta) \rangle$ is the temperature-dependent vacuum state, β being the inverse temperature, $1/T$. The equations for $g_\sigma^{\alpha\beta}$ and $C_\sigma^{\alpha\beta}$ can be derived using Eqs. (2.7) and (2.8):

$$(i\partial_t - E_0)g_\sigma^{\alpha\beta}(x-y) + iV^2 \sum_\gamma \int d^4z \, S_\sigma^{\alpha\gamma}(x-z)g_\sigma^{\gamma\beta}(z-y)$$

$$= i\delta^{(4)}(x-y) + U\varepsilon^\alpha \langle 0(\beta) \mid T[\phi_{-\sigma}^\alpha(x)]^\dagger \phi_{-\sigma}^\alpha(x)\phi_\sigma^\alpha(x)[\phi_\sigma^\beta(y)]^\dagger \mid 0(\beta) \rangle \ , \quad (2.12)$$

$$C_\sigma^{\alpha\beta}(x-y) = S_\sigma^{\alpha\beta}(x-y) - V^2 \int d^4z_1 d^4z_2 \sum_{\gamma_1,\gamma_2} S_\sigma^{\alpha\gamma_1}(x-z_1)g_\sigma^{\gamma_1\gamma_2}(z_1-z_2)S_\sigma^{\gamma_2\beta}(z_2-y) \ , \quad (2.13)$$

where $S_\sigma^{\alpha\beta}(x-y)$ is the unperturbed conduction-electron Green's function and is given by[6]

$$S_\sigma^{\alpha\beta}(x-y) = \frac{i}{(2\pi)^4} \int d^4p \, S_\sigma^{\alpha\beta}(p)e^{ip(x-y)} \ , \quad (2.14)$$

with

$$S_\sigma^{\alpha\beta}(p) = \begin{vmatrix} \dfrac{C_F^2(p_0)}{p_0 - \varepsilon_p + i\eta} + \dfrac{d_F^2(p_0)}{p_0 - \varepsilon_p - i\eta} & \dfrac{-C_F(p_0)d_F(p_0)}{p_0 - \varepsilon_p + i\eta} + \dfrac{C_F(p_0)d_F(p_0)}{p_0 - \varepsilon_p - i\eta} \\[3mm] \dfrac{-C_F(p_0)d_F(p_0)}{p_0 - \varepsilon_p + i\eta} + \dfrac{C_F(p_0)d_F(p_0)}{p_0 - \varepsilon_p - i\eta} & \dfrac{d_F^2(p_0)}{p_0 - \varepsilon_p + i\eta} + \dfrac{C_F^2(p_0)}{p_0 - \varepsilon_p - i\eta} \end{vmatrix} \ , \quad (2.15)$$

where η is an infinitesimal positive number, and

$$C_F^2(p_0) = e^{p_0/T}/(e^{p_0/T} + 1), \quad d_F^2(p_0) = 1/(e^{p_0/T} + 1) \ , \quad (2.16)$$

$$\varepsilon_p = p^2/2m - \mu \ . \quad (2.17)$$

We note that the Green's function (2.15) can be rewritten in a more compact form:

$$S_\sigma^{\alpha\beta}(p) = \left[U_F(p_0) \begin{vmatrix} \dfrac{1}{p_0 - \varepsilon_p + i\eta} & 0 \\[3mm] 0 & \dfrac{1}{p_0 - \varepsilon_p - i\eta} \end{vmatrix} U_F^\dagger(p_0) \right]^{\alpha\beta} \ , \quad (2.18)$$

or

$$S_\sigma^{\alpha\beta}(p) = \frac{1}{p_0 - \varepsilon_p}\delta_{\alpha\beta} - i\pi\delta(p_0 - \varepsilon_p)[U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} \ , \quad (2.19)$$

where

$$U_F(p_0) = \begin{vmatrix} C_F(p_0) & d_F(p_0) \\ -d_F(p_0) & C_F(p_0) \end{vmatrix} \ , \quad (2.20)$$

$$\tau = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \ . \quad (2.21)$$

We define the f-electron self-energy function $\Sigma_\sigma^{\alpha\beta}(p)$ by the relation

$$U\varepsilon^\alpha \langle 0(\beta) \mid T[\phi_{-\sigma}^\alpha(x)]^\dagger \phi_{-\sigma}^\alpha(x)\phi_\sigma^\alpha(x)[\phi_\sigma^\beta(y)]^\dagger \mid 0(\beta) \rangle$$

$$= \sum_\gamma \frac{i}{(2\pi)^4} \int d^4p \, \Sigma_\sigma^{\alpha\gamma}(p)g_\sigma^{\gamma\beta}(p)e^{ip(x-y)} \ . \quad (2.22)$$

Then, substituting Eq. (2.22) into Eq. (2.12) and making a Fourier transformation, we obtain

$$\sum_\gamma [(p_0 - \varepsilon_p)\delta_{\alpha\gamma} - V^2 S_\sigma^{\alpha\gamma}(p) - \Sigma_\sigma^{\alpha\gamma}(p)]g_\sigma^{\gamma\beta}(p) = 1 \ . \quad (2.23)$$

Since the self-energy function can be separated into its real and imaginary parts in the following form from the requirement of its analyticity,[7]

$$\Sigma_\sigma^{\alpha\beta}(p) = \Sigma_{1\sigma}(p)\delta_{\alpha\beta} - i\Sigma_{2\sigma}(p)[U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} \ , \quad (2.24)$$

substitution of expression (2.24) into Eq. (2.23) yields the formal solution of the f-electron Green's function as follows:

$$g_\sigma^{\alpha\beta}(p) = g_{1\sigma}(p)\delta_{\alpha\beta} - ig_{2\sigma}(p)[U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} \ , \quad (2.25)$$

where

$$g_{1\sigma}(p) = \frac{p_0 - E_0 - \Sigma_{1\sigma}(p) - V^2/(p_0 - \varepsilon_p)}{[p_0 - E_0 - \Sigma_{1\sigma}(p) - V^2/(p_0 - \varepsilon_p)]^2 + \Sigma_{2\sigma}(p)^2} \ , \quad (2.26)$$

$$g_{2\sigma}(p) = \frac{\Sigma_{2\sigma}(p)}{[p_0 - E_0 - \Sigma_{1\sigma}(p) - V^2/(p_0 - \varepsilon_p)]^2 + \Sigma_{2\sigma}(p)^2} \ . \quad (2.27)$$

The Green's function for the conduction electron is also obtained from Eq. (2.13) as

$$C_\sigma^{\alpha\beta}(p) = S_\sigma^{\alpha\beta}(p) + V^2 \sum_{\gamma_1,\gamma_2} S_\sigma^{\alpha\gamma_1}(p)g_\sigma^{\gamma_1\gamma_2}(p)S_\sigma^{\gamma_2\beta}(p)$$

$$= C_{1\sigma}(p)\delta_{\alpha\beta} - iC_{2\sigma}(p)[U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} \ , \quad (2.28)$$

where

$$C_{1\sigma}(p) = \frac{p_0 - \varepsilon_p - \dfrac{V^2[p_0 - E_0 - \Sigma_{1\sigma}(p)]}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}}{\left[p_0 - \varepsilon_p - \dfrac{V^2[p_0 - E_0 - \Sigma_{1\sigma}(p)]}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}\right]^2 + \left[\dfrac{V^2\Sigma_{2\sigma}(p)}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}\right]^2} , \tag{2.29}$$

$$C_{2\sigma}(p) = \frac{\dfrac{V^2\Sigma_{2\sigma}(p)}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}}{\left[p_0 - \varepsilon_p - \dfrac{V^2[p_0 - E_0 - \Sigma_{1\sigma}(p)]}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}\right]^2 + \left[\dfrac{V^2\Sigma_{2\sigma}(p)}{[p_0 - E_0 - \Sigma_{1\sigma}(p)]^2 + \Sigma_{2\sigma}(p)^2}\right]^2} . \tag{2.30}$$

Let us consider the Kondo regime where f-electron energy levels are deeply below the Fermi level. In this regime spin fluctuations dominantly contribute to the many-body correction to the f-electron self-energy at low temperatures. Therefore, we set up the Dyson equation for the self-energy function in terms of the spin-fluctuation and f-electron Green's functions. To do so let us define the spin-fluctuation Green's function at a temperature T as

$$\Delta^{\alpha\beta}(x - y) = \langle 0(\beta) | T\sigma_+^\alpha(x)\sigma_-^\beta(y) | 0(\beta) \rangle = \frac{i}{(2\pi)^4} \int d^4p \, \Delta^{\alpha\beta}(q)e^{iq(x-y)} , \tag{2.31}$$

where

$$\sigma_+^\alpha(x) = \varepsilon^\alpha[\phi_\uparrow^\alpha(x)]^\dagger\phi_\downarrow^\alpha(x) \quad \text{and} \quad \sigma_-^\alpha(x) = \varepsilon^\alpha[\phi_\downarrow^\alpha(x)]^\dagger\phi_\uparrow^\alpha(x) . \tag{2.32}$$

The vertex functions $\Gamma_{+\delta}^{ab}(p;q;r)$ and $\Gamma_{-\delta}^{ab}(p;q;r)$ are introduced by expressing the three-point functions as

$$\langle 0(\beta) | T\sigma_+^\alpha(x)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger | 0(\beta) \rangle$$

$$= \left[\frac{i}{(2\pi)^4}\right]^2 \int d^4p \, d^4q \left[\varepsilon^\alpha g_\uparrow^{\beta\alpha}(p)g_\downarrow^{\alpha\gamma}(p+q) - \sum_{\delta,a,b} \Delta^{\alpha\delta}(q)\Gamma_{+\delta}^{ab}(p;q;p+q)g_\uparrow^{\beta a}(p)g_\downarrow^{b\gamma}(p+q)\right]e^{ipx_1 + iqx - i(p+q)x_2} , \tag{2.33}$$

$$\langle 0(\beta) | T\sigma_-^\alpha(x)\phi_\downarrow^\beta(x_1)[\phi_\downarrow^\gamma(x_2)]^\dagger | 0(\beta) \rangle$$

$$= \left[\frac{i}{(2\pi)^4}\right]^2 \int d^4p \, d^4q \left[\varepsilon^\alpha g_\downarrow^{\beta a}(p+q)g_\uparrow^{\alpha\gamma}(p) - \sum_{\delta,a,b} \Delta^{\delta\alpha}(q)\Gamma_{-\delta}^{ab}(p+q;q;p)g_\downarrow^{\beta a}(p+q)g_\uparrow^{b\gamma}(p)\right]e^{i(p+q)x_1 - iqx - ipx_2} . \tag{2.34}$$

We note that the two-particle Green's function (2.22) can be expressed in terms of the above three-point functions:

$$\varepsilon^\alpha\langle 0(\beta) | T[\phi_{-\sigma}^\alpha(x)]^\dagger\phi_{-\sigma}^\alpha(x)\phi_\sigma^\alpha(x)[\phi_\sigma^\beta(y)]^\dagger | 0(\beta) \rangle = \begin{cases} -\langle 0(\beta) | T\sigma_-^\alpha(x)\phi_\uparrow^\alpha(x)[\phi_\uparrow^\beta(y)]^\dagger | 0(\beta) \rangle & \text{for } \sigma = \uparrow , \\ -\langle 0(\beta) | T\sigma_+^\alpha(x)\phi_\downarrow^\alpha(x)[\phi_\downarrow^\beta(y)]^\dagger 0(\beta) \rangle & \text{for } \sigma = \downarrow . \end{cases} \tag{2.35}$$

Therefore, substituting the three-point functions (2.33) and (2.34) into (2.35), and using the relation (2.22), we obtain the equations for the self-energy functions,

$$\Sigma_\uparrow^{\alpha\beta}(p) = Un_\downarrow^f\delta_{\alpha\beta} + U\left[\frac{i}{(2\pi)^4}\right]\int d^4q \sum_{\delta,a} \Delta^{\delta\alpha}(q)\Gamma_{-\delta}^{\alpha\beta}(p+q;q;p)g_\downarrow^{\alpha a}(p+q) , \tag{2.36}$$

$$\Sigma_\downarrow^{\alpha\beta}(p) = Un_\uparrow^f\delta_{\alpha\beta} + U\left[\frac{i}{(2\pi)^4}\right]\int d^4q \sum_{\delta,a} \Delta^{\alpha\delta}(q)\Gamma_{+\delta}^{\alpha\beta}(p-q;q;p)g_\uparrow^{\alpha a}(p-q) , \tag{2.37}$$

where we used the relation

$$n_{\uparrow,\downarrow}^f = -\left[\frac{i}{(2\pi)^4}\right]\int d^4q \, \varepsilon^\alpha g_{\uparrow,\downarrow}^{\alpha\alpha}(q)e^{ip_0 0^+} . \tag{2.38}$$

The equation for the spin-fluctuation Green's function can be constructed with the use of the three-point functions by noticing the relation

$$\langle 0(\beta) | T\sigma_+^\alpha(x)\sigma_-^\beta(y) | 0(\beta) \rangle = -\langle 0(\beta) | T\sigma_+^\alpha(x)\phi_\downarrow^\beta(t_y,\mathbf{y})[\phi_\downarrow^\beta(t_y + 0, \mathbf{y})]^\dagger | 0(\beta) \rangle\varepsilon^\beta , \tag{2.39}$$

or

$$\langle 0(\beta) | T\sigma_+^\alpha(x)\sigma_-^\beta(y) | 0(\beta) \rangle = -\langle 0(\beta) | T\sigma_-^\beta(y)\phi_\uparrow^\alpha(t_y,\mathbf{y})[\phi_\uparrow^\alpha(t_y + 0, \mathbf{y})]^\dagger | 0(\beta) \rangle\varepsilon^\alpha . \tag{2.40}$$

Using the relations (2.31), (2.33), and (2.34), we thus have

$$
\Delta^{\alpha\beta}(q) = -\left[\frac{i}{(2\pi)^4}\right]\int_c d^4p\ \varepsilon^\alpha g_\uparrow^{\beta\alpha}(p)g_\uparrow^{\alpha\beta}(p+q)\varepsilon^\beta + \left[\frac{i}{(2\pi)^4}\right]\int_c d^4p \sum_{a,b,\delta}\Delta^{\alpha\delta}(q)\Gamma_{+\delta}^{ab}(p;q;p+q)g_\uparrow^{\beta a}(p)g_\uparrow^{b\beta}(p+q)\varepsilon^\beta\ ,
$$

(2.41)

or

$$
\Delta^{\alpha\beta}(q) = -\left[\frac{i}{(2\pi)^4}\right]\int_c d^4p\ \varepsilon^\alpha g_\uparrow^{\alpha\beta}(p)g_\uparrow^{\beta\alpha}(p+q)\varepsilon^\beta + \left[\frac{i}{(2\pi)^4}\right]\int_c d^4p \sum_{a,b,\delta}\Delta^{\delta\alpha}(q)\Gamma_{-\delta}^{ab}(p+q;q;p)g_\uparrow^{b\beta}(p)g_\uparrow^{\beta a}(p+q)\varepsilon^\beta\ .
$$

(2.42)

Here, the integration path c is taken in the upper half-plane of complex p_0, i.e., $\mathrm{Im}\,p_0 > 0$. Equations (2.41) and (2.42) indicate the relation for the vertices:

$$
\Gamma_{+\delta}^{ab}(p;q;p+q) = \Gamma_{-\delta}^{ab}(p+q;q;p)\ .
$$

(2.43)

Equations (2.36), (2.37), (2.41), and (2.42) provide a set of coupled equations to determine the f-electron and spin-fluctuation Green's functions when the vertex functions are given.

As discussed in paper I, we approximate the vertex function in Eqs. (2.36) and (2.37) in the following way:

$$
U\Gamma_{\pm\delta}^{ab}(p\pm q;q;p) \simeq U\Gamma_{\pm\delta}^{ab}(p_F;0;p_F) = \lambda_r^2\delta_{a\delta}\delta_{b\delta}\ ,
$$

(2.44)

where $p_F = (0,\mathbf{p}_F)$, $\mathbf{p}_F$ being the Fermi momentum, and λ_r is the renormalized coupling constant. Then Eqs. (2.36) and (2.37) become, respectively,

$$
\Sigma_\uparrow^{\alpha\beta}(p) = Un\{\delta_{\alpha\beta} + \lambda_r^2\left[\frac{i}{(2\pi)^4}\right]\int d^4q\ \Delta^{\beta\alpha}(q)g_\uparrow^{\alpha\beta}(p+q)\ ,
$$

(2.45)

$$
\Sigma_\uparrow^{\alpha\beta}(p) = Un\{\delta_{\alpha\beta} + \lambda_r^2\left[\frac{i}{(2\pi)^4}\right]\int d^4q\ \Delta^{\alpha\beta}(q)g_\uparrow^{\beta\alpha}(p-q)\ .
$$

(2.46)

Let us proceed to the discussion about the equation for $\Delta^{\alpha\beta}(q)$. As discussed in paper I, to maintain the correct low-energy behavior of $\Delta^{\alpha\beta}(q)$ in an approximate calculation, the spin-rotational invariance of the system should not be violated. Therefore we seek an approximation for $\Delta^{\alpha\beta}(q)$ which is consistent with the approximation done for the self-energy functions (2.45) and (2.46) in a sense that the spin-rotational invariance of the system is maintained. To do so, the vertex functions $\Gamma_{\pm\delta}^{ab}$ in Eqs. (2.41) and (2.42) approximated so as to satisfy the Ward-Takahashi relations which stem from the spin-rotational invariance of the system. For deriving the Ward-Takahashi relations, we add the following symmetry-breaking terms to the total Hamiltonian (2.3):

$$
-\sum_\alpha\{\tfrac{1}{2}h_s\varepsilon^\alpha[\psi^\alpha(x)]^\dagger\sigma_3\psi^\alpha(x) + \tfrac{1}{2}h_f\varepsilon^\alpha[\phi^\alpha(x)]^\dagger\sigma_3\phi^\alpha(x)\}\ ,
$$

(2.47)

where σ_3 is the Pauli matrix. In the presence of the above terms the following equation for the three-point functions (2.33) can be derived:

$$
(-i\partial_t + h_f)\langle 0(\beta)\,|\,T\sigma_+^\alpha(x)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle = i\delta_{\alpha\beta}\delta^{(4)}(x-x_1)\varepsilon^\alpha g_\uparrow^{\alpha\gamma}(x_1-x_2) - i\delta_{\alpha\gamma}\delta^{(4)}(x-x_2)\varepsilon^\alpha g_\uparrow^{\beta\alpha}(x_1-x_2)
$$

$$
- V\varepsilon^\alpha\langle 0(\beta)\,|\,T\{[\phi_\uparrow^\alpha(x)]^\dagger\psi_\uparrow^\alpha(x)
$$

$$
- [\psi_\uparrow^\alpha(x)]^\dagger\phi_\uparrow^\alpha(x)\}\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle\ .
$$

(2.48)

If it is noted that

$$
\langle 0(\beta)\,|\,T[\phi_\uparrow^\alpha(x)]^\dagger\psi_\uparrow^\alpha(x)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle = -iV\int d^4z\sum_\gamma S_\uparrow^{\alpha\gamma}(x-z)\langle 0(\beta)\,|\,T[\phi_\uparrow^\alpha(x)]^\dagger\phi_\uparrow^\gamma(z)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle\ ,
$$

(2.49)

$$
\langle 0(\beta)\,|\,T[\psi_\uparrow^\alpha(x)]^\dagger\phi_\uparrow^\alpha(x)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle = -iV\int d^4z\sum_\gamma\langle 0(\beta)\,|\,T[\phi_\uparrow^\gamma(z)]^\dagger\phi_\uparrow^\alpha(x)\phi_\uparrow^\beta(x_1)[\phi_\uparrow^\gamma(x_2)]^\dagger\,|\,0(\beta)\rangle S_\uparrow^{\gamma\alpha}(z-x)\ ,
$$

(2.50)

a Fourier transformation of the two-particle Green's function appearing on the right-hand side of Eq. (2.48) is expressed as

$$\langle 0(\beta) \mid T\{[\phi_\uparrow^\alpha(x)]^\dagger \psi_\uparrow^\alpha(x) - [\psi_\uparrow^\alpha(x)]^\dagger \phi_\uparrow^\alpha(x)\} \phi_\uparrow^\beta(x_1)[\phi_\downarrow^\gamma(x_2)]^\dagger \mid 0(\beta)\rangle$$

$$= V\left[\frac{i}{(2\pi)^4}\right] \int d^4p \, d^4q \left[\frac{-q_0 + h_s + \varepsilon_{p+q} - \varepsilon_p}{(p_0 + q_0 - \varepsilon_{p+q} - \frac{1}{2}h_s)(p_0 - \varepsilon_p + \frac{1}{2}h_s)} g_\uparrow^{\beta\alpha}(p) g_\downarrow^{\alpha\gamma}(p+q)\right.$$

$$+ \left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{-q_0 + h_s + \varepsilon_{k+q} - \varepsilon_k}{(k_0 + q_0 - \varepsilon_{k+q} - \frac{1}{2}h_s)(k_0 - \varepsilon_k + \frac{1}{2}h_s)}$$

$$\times \sum_{\gamma_1,\gamma_2} \sum_{\delta_1,\delta_2} g_\uparrow^{\beta\gamma_1}(p) g_\downarrow^{\alpha\gamma_2}(k+q) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\gamma_1\gamma_2;\delta_1\delta_2}(p, k+q; p+q; k)$$

$$\left. \times g_\downarrow^{\delta_1\gamma}(p+q) g_\uparrow^{\delta_2\alpha}(k)\right] e^{ipx_1 + iqx - i(p+q)x_2} \,. \tag{2.51}$$

Here, we introduced the vertex function with four f-electron external points $\Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\gamma\gamma';\delta\delta}(p,q;r,s)$. Substitution of Eqs. (2.33) and (2.51) into Eq. (2.48) gives

$$g_\uparrow^{-1}(p)^{\alpha\beta} - g_\downarrow^{-1}(p+q)^{\alpha\beta} = -(q_0 - h_f)\delta_{\alpha\beta} + (q_0 - h_f)\sum_\delta \Pi^\delta(q)\Gamma_{+\delta}^{\alpha\beta}(p;q;p+q) + V^2[S_\downarrow^{\alpha\beta}(p+q) - S_\uparrow^{\alpha\beta}(p)]$$

$$+ V^2\left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{-q_0 + h_s + \varepsilon_{k+q} - \varepsilon_k}{(k_0 + q_0 - \varepsilon_{k+q} - \frac{1}{2}h_s)(k_0 - \varepsilon_k + \frac{1}{2}h_s)}$$

$$\times \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k+q) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a;\beta b}(p, k+q; p+q, k) \,, \tag{2.52}$$

where

$$\Pi^\delta(q) = \sum_\gamma \varepsilon^\gamma \Delta^{\gamma\delta}(q) \,. \tag{2.53}$$

As shown in Appendix A, this equation leads to the following Ward-Takahashi relations in the limit of $q \to 0$ and $h_s = h_f \to 0$:

$$\left[\frac{\partial \Sigma_{\uparrow,\downarrow}^{\alpha\beta}(p)}{\partial h_f}\right]_{h=0} = \pm \frac{1}{2}\Delta_0 \sum_\delta \Gamma_{+\delta}^{\alpha\beta}(p;0;p) \,, \tag{2.54}$$

$$\left[\frac{\partial \Sigma_{\uparrow,\downarrow}^{\alpha\beta}(p)}{\partial h_s}\right]_{h=0} = -\frac{1}{2}\left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{V^2}{(k_0 - \varepsilon_k)^2} \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k) g_\uparrow^{b\gamma}(k) \Gamma^{\alpha a,\beta b}(p,k;p,k) \,, \tag{2.55}$$

$$\left[\frac{\partial \Sigma_{\uparrow,\downarrow}^{\alpha\beta}(p)}{\partial p_0}\right]_{h=0} = \Delta_0 \sum_\delta \Gamma_{+\delta}^{\alpha\beta}(p;0;p) - \left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{V^2}{(k_0 - \varepsilon_k)^2} \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a,\beta b}(p,k;p,k) \,, \tag{2.56}$$

$$\left[\frac{\partial \Sigma_{\uparrow,\downarrow}^{\alpha\beta}(p)}{\partial \mathbf{p}}\right]_{h=0} = \left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{V^2}{(k_0 - \varepsilon_k)^2} \left[\frac{\partial \varepsilon_k}{\partial \mathbf{k}}\right] \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a,\beta b}(p,k;p,k) \,, \tag{2.57}$$

where

$$\Delta_0 = \Pi^\delta(0) \,, \tag{2.58}$$

which is independent of δ. The signs $+$ and $-$ in Eq. (2.54) and $-$ and $+$ in Eq. (2.55) are taken for the spin suffices $\uparrow$ and $\downarrow$ of the self-energy respectively.

Let us now determine the vertex function $\Gamma_{+\delta}^{\alpha\beta}(p;q;p+q)$, using Eq. (2.52) and the Ward-Takahashi relations (2.54)–(2.57). Following paper I, we approximate the last term on the right-hand side of Eq. (2.52) by its form for small q:

$$V^2\left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{-q_0 + h_s + \varepsilon_{k+q} - \varepsilon_k}{(k_0 + q_0 - \varepsilon_{k+q} - \frac{1}{2}h_s)(k_0 - \varepsilon_k + \frac{1}{2}h_s)} \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k+q) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a;\beta b}(p, k+q; p+q, k)$$

$$\simeq (-q_0 + h_s)\left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{V^2}{(k_0 - \varepsilon_k)^2} \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a;\beta b}(p,k;p,k)$$

$$+ \mathbf{q} \cdot \left[\frac{i}{(2\pi)^4}\right] \int d^4k \frac{V^2}{(k_0 - \varepsilon_k)^2} \left[\frac{\partial \varepsilon_k}{\partial \mathbf{k}}\right] \sum_{a,b,\gamma} g_\downarrow^{\gamma a}(k) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{\alpha a;\beta b}(p,k;p,k) \,. \tag{2.59}$$

Here, we assumed $h_s \simeq 0$. The integrals on the right-hand side of (2.59) can be replaced by the derivatives of the self-energy function (2.55) and (2.57):

$$V^2 \left[\frac{i}{(2\pi)^4} \right] \int d^4 k \frac{-q_0 + h_s + \varepsilon_{k+q} - \varepsilon_k}{(k_0 + q_0 - \varepsilon_{k+q} - \frac{1}{2}h_s)(k_0 - \varepsilon_k + \frac{1}{2}h_s)} \sum_{a,b,\gamma} g_\uparrow^{\gamma a}(k+q) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\downarrow\uparrow}^{a\alpha;\beta b}(p, k+q; p+q, k)$$

$$\simeq 2(q_0 - h_s) \left[\frac{\partial \Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_s} \right]_{h=0} + \mathbf{q} \cdot \left[\frac{\partial \Sigma_\uparrow^{\alpha\beta}(p)}{\partial \mathbf{p}} \right]_{h=0} . \tag{2.60}$$

Substituting Eq. (2.60) into Eq. (2.52), we find the approximate equation for the vertex function $\Gamma_{+\delta}^{\alpha\beta}(p; q; p+q)$:

$$(q_0 - h_f) \sum_\delta \Pi^\delta(q) \Gamma_{+\delta}^{\alpha\beta}(p; q; p+q) \simeq g_\uparrow^{-1}(p)^{\alpha\beta} - g_\downarrow^{-1}(p+q)^{\alpha\beta} + (q_0 - h_f) \delta_{\alpha\beta} - V^2 [S_\uparrow^{\alpha\beta}(p+q) - S_\uparrow^{\alpha\beta}(p)]$$

$$- 2(q_0 - h_f) \left[\frac{\partial \Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_s} \right]_{h=0} - \mathbf{q} \cdot \left[\frac{\partial \Sigma_\uparrow^{\alpha\beta}(p)}{\partial \mathbf{p}} \right]_{h=0} . \tag{2.61}$$

As can easily be checked, the vertex function $\Gamma_{+\delta}^{\alpha\beta}$ given in the above equation satisfies the Ward-Takahashi relation (2.54). This Ward-Takahashi relation is a result of the spin-rotational invariance of the system as shown in Ref. 8, so that the use of Eq. (2.61) for the vertex function in Eq. (2.41) leads to the approximate equation for $\Delta^{\alpha\beta}(q)$ which does not break the spin-rotational invariance. Thus we have the following equation for the spin-fluctuation Green's function:

$$(q_0 - h_f) \Pi^\beta(q) = M_f - V^2 \left[\frac{i}{(2\pi)^4} \right] \int_c d^4 p \frac{-q_0 + h_s + \varepsilon_{p+q} - \varepsilon_p}{(p_0 + q_0 - \varepsilon_{p+q} - \frac{1}{2}h_s)(p_0 - \varepsilon_p + \frac{1}{2}h_s)} \sum_\alpha g_\uparrow^{\beta\alpha}(p) g_\downarrow^{\alpha\beta}(p+q)\varepsilon^\beta$$

$$- 2(q_0 - h_f) \left[\frac{i}{(2\pi)^4} \right] \int_c d^4 p \sum_{a,b} g_\uparrow^{\beta a}(p) \left[\frac{\partial \Sigma_\uparrow^{ab}(p)}{\partial h_s} \right]_{h=0} g_\downarrow^{b\beta}(p+q)\varepsilon^\beta$$

$$- \mathbf{q} \cdot \left[\frac{i}{(2\pi)^4} \right] \int_c d^4 p \sum_{a,b} g_\uparrow^{\beta a}(p) \left[\frac{\partial \Sigma_\uparrow^{ab}(p)}{\partial \mathbf{p}} \right]_{h=0} g_\downarrow^{b\beta}(p+q)\varepsilon^\beta . \tag{2.62}$$

In deriving Eq. (2.62) we used the relation

$$\frac{i}{(2\pi)^4} \int_c d^4 p [g_\uparrow^{\beta\beta}(p+q) - g_\uparrow^{\beta\beta}(p)] \varepsilon^\beta = n_\uparrow^f - n_\downarrow^f = M_f . \tag{2.63}$$

When the limit of $h_f, h_s \to 0$ is taken in Eq. (2.62), we should be careful with the real part of $\Pi^\beta(q)$, especially in its static limit, since the real part has a pole term, $M_f/(q_0 - h_f)$. The limit of $h_f, h_s \to 0$ should follow after the static limit $q_0 \to 0$ is taken in calculating $\Pi^\beta(0)$ (see Appendix B). The equation along with Eq. (2.45) or (2.46) provides a set of coupled equations to determine the self-energy and the spin-fluctuation Green's function. In Sec. III those equations are approximately solved.

III. NUMERICAL CALCULATION

To solve the coupled equations (2.45), (2.46), and (2.62), we introduce the following spectral representations for $g_\sigma^{\alpha\beta}(p)$ and $\Delta^{\alpha\beta}(q)$,[6,7]

$$g_\sigma^{\alpha\beta}(p) = \int dw \, \rho_\sigma(w, \mathbf{p}) [U_F(w)(p_0 - w + i\delta\tau)^{-1} U_F^\dagger(w)]^{\alpha\beta} , \tag{3.1}$$

$$\Delta^{\alpha\beta}(q) = \int dw \, D(w, \mathbf{q}) [U_B(w)\tau(q_0 - w + i\delta\tau)^{-1} U_B^\dagger(w)]^{\alpha\beta} , \tag{3.2}$$

where $\rho_\sigma(w, \mathbf{p})$ and $D(w, \mathbf{q})$ are the spectral functions. We assumed that the spin-fluctuation Green's function is bosonlike. Then the matrix $U_B(w)$ is given by[6,7]

$$U_B(w) = \begin{bmatrix} C_B(w) & d_B(w) \\ d_B(w) & C_B(w) \end{bmatrix} , \tag{3.3}$$

with

$$C_B^2(w) = e^{w/T}/(e^{w/T} - 1) \quad \text{and} \quad d_B^2(w) = 1/(e^{w/T} - 1) . \tag{3.4}$$

Substituting the expressions (3.1) and (3.2) into Eqs. (2.45) and (2.46), we rewrite the equations for the self-energies as follows:

$$\Sigma_{\uparrow,\downarrow}^{\alpha\beta}(p) = U n_{\downarrow,\uparrow}^f \delta_{\alpha\beta} + \int dw \, \tilde{\Sigma}_{2\uparrow,\downarrow}(w, \mathbf{p}) [U_F(w)(p_0 - w + i\delta\tau)^{-1} U_F^\dagger(w)]^{\alpha\beta} , \tag{3.5}$$

where

$$\tilde{\Sigma}_{2\uparrow,\downarrow}(p) = \lambda_r^2 \int dq_0 \int \frac{d\mathbf{q}}{(2\pi)^3} \rho_{\downarrow,\uparrow}(p \pm q) D(q) \left[\frac{1}{e^{q_0/T} - 1} + \frac{1}{e^{(q_0 \pm p_0)/T} + 1} \right] . \tag{3.6}$$

Note that the right-hand side of Eq. (3.5) can be divided into the real and imaginary parts as

$$\Sigma^{\alpha\beta}_{\uparrow,\uparrow}(p) = \left[U n^f_{\downarrow,\uparrow} + \int dw \frac{1}{p_0 - w} \tilde{\Sigma}_{2\uparrow,\downarrow}(w,\mathbf{p}) \right] \delta_{\alpha\beta} - i\pi \tilde{\Sigma}_{2\uparrow,\downarrow}(p) [U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} . \tag{3.7}$$

Comparing this with Eq. (2.24), we find

$$\Sigma_{1\sigma}(p) = U n^f_{\downarrow,\uparrow} + \int dw \frac{1}{p_0 - w} \tilde{\Sigma}_{2\sigma}(w,\mathbf{p}) , \tag{3.8}$$

$$\Sigma_{2\sigma}(p) = \pi \tilde{\Sigma}_{2\sigma}(p) . \tag{3.9}$$

In the case of no external field the self-energy does not depend on the spin direction, so we drop the spin indices hereafter.

In the following numerical calculations we choose a renormalized f-electron level

$$\tilde{E}_0 = E_0 + \Sigma_1(0,\mathbf{p}_F) \big|_{T=0} \tag{3.10}$$

as a parameter, where the second term is the real part of the self-energy at the Fermi level and at absolute zero. Since the bare f level always appears through the combination of $E_0 + \Sigma_1(p)$ in our theory, as seen in Eqs. (2.26), (2.27), (2.29), and (2.30), this combination is written as

$$E_0 + \Sigma_1(p) = \tilde{E}_0 + \tilde{\Sigma}_1(p) , \tag{3.11}$$

with

$$\tilde{\Sigma}_1(p) = \Sigma_1(p) - \Sigma_1(0,\mathbf{p}_F) \bigg|_{T=0}$$
$$= \int dw \left[\frac{1}{p_0 - w} \tilde{\Sigma}_2(w,\mathbf{p}) + \frac{1}{w} \tilde{\Sigma}_2(w,\mathbf{p}_F) \right]_{T=0} . \tag{3.12}$$

In the above the temperature dependence of the f-electron number is assumed to be neglected. If the imaginary part of the self-energy function is known, the real part of the self-energy is calculated from Eq. (3.12) and thus the f- and conduction-electron Green's functions are obtained.

To solve Eq. (3.6) we will try to make an iterative calculation. In the present paper, the lowest-order calculation is performed in the following. Following paper I, as the zeroth-order spectral function for the f-electron Green's function we consider the Hartree-Fock spectral function in which the Hartree-Fock f level $E_0 + U n^f_\sigma$ is replaced by the renormalized f level $\tilde{E}_0$:

$$\rho(w,\mathbf{p}) \sim \rho_0(w,\mathbf{p}) = \delta(w - \tilde{E}_0 - V^2/(w - \varepsilon_p)) . \tag{3.13}$$

Thus, using the spectral function (3.13) for the f-electron Green's function in Eq. (2.62), we calculate the spectral function for the spin-fluctuation Green's function from Eq. (2.62). To do so, we first calculate the derivatives of the self-energy function in Eq. (2.62). In this stage of the iterative calculation the derivatives are obtained as

$$\left[\frac{\partial \Sigma^{ab}_\uparrow(p)}{\partial h_s} \right]_{h=0} = U \left[\frac{\partial n^f_\downarrow}{\partial h_s} \right]_{h=0} \delta_{ab} - \int dw \frac{1}{w} \left[\frac{\partial}{\partial h_s} \tilde{\Sigma}_2(w,\mathbf{p}_F) \right]_{h=0} = -\frac{1}{2} U_s^* \chi_s \delta_{ab} , \tag{3.14}$$

$$\left[\frac{\partial \Sigma_\uparrow(p)}{\partial \mathbf{p}} \right]_{h=0} = 0 , \tag{3.15}$$

where

$$\chi_s = -2 \left[\frac{\partial n^f_\downarrow}{\partial h_s} \right]_{h=0} , \tag{3.16}$$

$$U_s^* = U - \frac{1}{\chi_s} \int dw \frac{1}{w} \left[\frac{\partial}{\partial h_s} \tilde{\Sigma}_2(w,\mathbf{p}_F) \right]_{h=0} . \tag{3.17}$$

The explicit expression for χ_s and some discussion on the parameter U_s^* are given in Appendix B. Therefore, Eq. (2.62) is reduced to

$$(q_0 - h_f)\Pi^\beta(q) = M_f + \left[\frac{i}{(2\pi)^4} \right] \int_c d^4p \left[U_s^* \chi_s (q_0 - h_f) - V^2 \frac{-q_0 + h_s + \varepsilon_{p+q} - \varepsilon_p}{(p_0 + q_0 - \varepsilon_{p+q} - \frac{1}{2}h_s)(p_0 - \varepsilon_p + \frac{1}{2}h_s)} \right]$$
$$\times \sum_\alpha g^{\beta\alpha}_\uparrow(p) g^{\alpha\beta}_\downarrow(p+q) \varepsilon^\beta . \tag{3.18}$$

Thus, using the spectral representation (3.1) for the f-electron Green's function in (3.18), we find

$$(q_0-h_f)\Pi^\beta(q)=M_f+\int dw\,[U_s^*\chi_s(q_0-h_f)A(w,\mathbf{q})-V^2B(w,\mathbf{q})]\sum_\alpha \varepsilon^\alpha[U_B(w)\tau(q_0-w+i\delta\tau)^{-1}U_B^\dagger(w)]^{\alpha\beta}\,,\tag{3.19}$$

where

$$A(w,\mathbf{q})=\int dp_0\int \frac{d\mathbf{p}}{(2\pi)^3}\rho_\uparrow(p_0,\mathbf{p})\rho_\downarrow(p_0+w,\,\mathbf{p}+\mathbf{q})\left[\frac{1}{e^{(p_0+w)/T}+1}-\frac{1}{e^{p_0/T}+1}\right],\tag{3.20}$$

$$B(w,\mathbf{q})=\int dp_0\int \frac{d\mathbf{p}}{(2\pi)^3}\frac{-w+h_s+\varepsilon_{p+q}-\varepsilon_p}{(p_0+w-\varepsilon_{p+q}-\tfrac12 h_s)(p_0-\varepsilon_p+\tfrac12 h_s)}\rho_\uparrow(p_0,\mathbf{p})\rho_\downarrow(p_0+w,\,\mathbf{p}+\mathbf{q})\left[\frac{1}{e^{(p_0+w)/T}+1}-\frac{1}{e^{p_0/T}+1}\right].\tag{3.21}$$

In obtaining Eq. (3.19) we used the formula[6]

$$\frac{i}{(2\pi)^4}\int_c d^4p\,\varepsilon^\alpha g_\uparrow^{\beta\alpha}(p)g_\uparrow^{\alpha\beta}(p+q)\varepsilon^\beta=\int dw\,A(w,\mathbf{q})[U_B(w)\tau(q_0-w+i\delta\tau)^{-1}U_B^\dagger(w)]^{\alpha\beta}\,,\tag{3.22}$$

$$\frac{i}{(2\pi)^4}\int d^4p\frac{-q_0+h_s+\varepsilon_{p+q}-\varepsilon_p}{(p_0+q_0-\varepsilon_{p+q}-\tfrac12 h_s)(p_0-\varepsilon_p+\tfrac12 h_s)}\varepsilon^\alpha g_\uparrow^{\beta\alpha}(p)g_\uparrow^{\alpha\beta}(p)\varepsilon^\beta=\int dw\,B(w,\mathbf{q})[U_B(w)\tau(q_0-w+i\delta\tau)^{-1}U_B^\dagger(w)]^{\alpha\beta}\,.\tag{3.23}$$

Noting the definition (2.53) for $\Pi^\beta(q)$ and using the spectral representation (3.2), we derive the equation for $D(q)$ from Eq. (3.19) in the limit of $h_s,h_f\to 0$ as

$$D(q)=\int dp_0\int \frac{d\mathbf{p}}{(2\pi)^3}\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(p_0+q_0-\varepsilon_{p+q})(p_0-\varepsilon_p)}\right]\rho_0(p)\rho_0(p+q)\left[\frac{1}{e^{(p_0+q_0)/T}+1}-\frac{1}{e^{p_0/T}+1}\right].\tag{3.24}$$

In further calculations we shall confine ourselves to the region of low-temperature where the system exhibits the behavior of heavy fermions and calculate the self-energy functions up to second order in T. To make the low-temperature expansion, it is convenient that the integrals (3.6) and (3.24) are rewritten with the changes of integral variable as

$$\tilde\Sigma_2(p)=\lambda_r^2\int dq_0\int\frac{d\mathbf{q}}{(2\pi)^3}\rho_0(p+q)D(q)[\Theta(q_0)-\Theta(q_0+q_0)]$$

$$+T\int_0^\infty dz\,\lambda_r^2\int\frac{d\mathbf{q}}{(2\pi)^3}\left[\frac{1}{e^z+1}[\rho_0(p_0+Tz,\,\mathbf{p}+\mathbf{q})D(Tz,\mathbf{q})-\rho(p_0-Tz,\,\mathbf{p}+\mathbf{q})D(-Tz,\mathbf{q})]\right.$$

$$\left.+\frac{1}{e^z+1}[\rho(Tz,\,\mathbf{p}+\mathbf{q})D(Tz-p_0,\,\mathbf{q})-\rho(-Tz,\,\mathbf{p}+\mathbf{q})D(-Tz-p_0,\,\mathbf{q})]\right],\tag{3.25}$$

$$D(q)=\int dp_0\int \frac{d\mathbf{p}}{(2\pi)^3}\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(p_0+q_0-\varepsilon_{p+q})(p_0-\varepsilon_p)}\right]\rho_0(p)\rho_0(p+q)[\Theta(p_0)-\Theta(p_0+q_0)]$$

$$+T\int_0^\infty dz\frac{1}{e^z+1}\int\frac{d\mathbf{p}}{(2\pi)^3}\left[\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(Tz+q_0-\varepsilon_{p+q})(Tz-\varepsilon_p)}\right]\rho_0(Tz,\mathbf{p})\rho_0(Tz+q_0,\,\mathbf{p}+\mathbf{q})\right.$$

$$-\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(-Tz+q_0-\varepsilon_{p+q})(-Tz-\varepsilon_p)}\right]\rho_0(-Tz,\mathbf{p})\rho_0(-Tz+q_0,\,\mathbf{p}+\mathbf{q})$$

$$-\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(Tz-\varepsilon_{p+q})(Tz-q_0-\varepsilon_p)}\right]\rho_0(Tz-q_0,\,\mathbf{p})\rho_0(Tz,\,\mathbf{p}+\mathbf{q})$$

$$\left.+\left[U_s^*\chi_s-\frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(-Tz-\varepsilon_{p+q})(-Tz-q_0-\varepsilon_p)}\right]\rho_0(-Tz-q_0,\,\mathbf{p})\rho_0(-Tz,\,\mathbf{p}+\mathbf{q})\right].\tag{3.26}$$

The first terms on the right-hand side of Eqs. (3.25) and (3.26) give, respectively, the values of $\tilde\Sigma_2(p)$ and $D(q)$ at absolute zero. Expansion of the integrands in Eqs. (3.25) and (3.26) with respect to T gives the low-temperature expansion of the self-energy and the spectral function of the spin-fluctuation Green's function. For simplicity of the numerical calculations, we evaluate the temperature-dependent terms in Eqs. (3.25) and (3.26) in the low-energy region, i.e., $p_0\sim 0$ for $\tilde\Sigma_2(p)$ and $q_0\sim 0$ for $D(q)$. After some calculations, we obtain the following results up to second order in temperature:

$$\tilde{\Sigma}_2(p) \simeq \lambda_r^2 \int dq_0 \int \frac{d\mathbf{q}}{(2\pi)^3} \rho_0(p+q)D(q)[\Theta(q_0)-\Theta(q_0+p_0)] + \tfrac{1}{2}\lambda_r^2(\pi T)^2 \frac{\partial}{\partial q_0} \left[\int \frac{d\mathbf{q}}{(2\pi)^3}\rho_0(p+q)D(q) \right]\Bigg|_{q_0=0} , \qquad (3.27)$$

$$D(q) \simeq \int dp_0 \int \frac{d\mathbf{p}}{(2\pi)^3} \left[U_s^* \chi_s - \frac{V^2(-q_0+\varepsilon_{p+q}-\varepsilon_p)}{q_0(p_0+q_0-\varepsilon_{p+q})(p_0-\varepsilon_p)} \right] \rho_0(p)\rho_0(p+q)[\Theta(p_0)-\Theta(p_0+q_0)] . \qquad (3.28)$$

The integrals in Eqs. (3.27) and (3.28) can be evaluated by following the procedure given in paper I. Using the numerical results for $\tilde{\Sigma}_2(p)$, we can calculate the Green's functions for the f and conduction electrons from Eqs. (2.25)–(2.30), (3.11), and (3.12). The spectral functions and the density of states of the electrons are obtained from the Green's functions in the following way. Since the spectral representation for the f-electron Green's function (3.1) is rewritten in the form

$$g^{\alpha\beta}(p) = \int dw \frac{\delta_{\alpha\beta}}{p_0-w}\rho(w,\mathbf{p}) - i\pi\rho(p)[U_F(p_0)\tau U_F^\dagger(p_0)]^{\alpha\beta} , \qquad (3.29)$$

the spectral function $\rho(p)$ is given by

$$\rho(p) = \frac{1}{\pi} g_2(p) . \qquad (3.30)$$

Here, we used the relation (2.25). The density of states of the f electrons is obtained by summing the spectral function over the momentum $\mathbf{p}$ space:

$$N_f(p_0) = \frac{1}{\pi} \sum_\mathbf{p} g_2(p_0,\mathbf{p}) . \qquad (3.31)$$

In the same way we obtain the density of states for the conduction electrons as

$$N_s(p_0) = \frac{1}{\pi} \sum_\mathbf{p} C_2(p_0,\mathbf{p}) . \qquad (3.32)$$

Let us now present the numerical results. We chose the normalized quantities, $\tilde{E}_0/\xi_{p_F}$, V/ξ_{p_F}, $U_s^*\rho_s(\xi_{p_F})$, $\lambda_r\rho_s(\xi_{p_F})$, and D/ξ_{p_F} as parameters, where

$$\rho_s(\xi_{p_F}) = (2m^3)^{1/2}\xi_{p_F}^{1/2}/(2\pi)^2 ,$$

$\xi_{p_F} = \mathbf{p}_F^2/2m$, and $D = \mathbf{p}_c^2/2m$, $\mathbf{p}_c$ being the cutoff momentum. The definition of the Fermi momentum $\mathbf{p}_F$ is given in paper I. In the following numerical calculations we present the results for two cases of the parameter $\tilde{E}_0 = -0.003$ and 0.003. The values of the other parameters are fixed as $V/\xi_{p_F} = 0.02$, $U_s^*\rho_s(\xi_{p_F}) = 0.02$, $\lambda_r\rho_s(\xi_{p_F}) = 1.0$, and $D/\xi_p = 1.5$. In these choices we suppose the cases in which $\xi_{p_F} \sim 10^4$ K, $V \sim 10^2$ K, $D \sim 10^4$ K, and the renormalized f level is very close to the Fermi level. For the selection of the values λ_r and U_s^*, see Appendix B. First, we show the f-electron spectral function near the Fermi level at two different temperatures, $T/\xi_{p_F} = 0$ and 0.002 in the case of $\tilde{E}_0 = -0.003$. In Fig. 1(a) the energy dependence of the spectral function at absolute zero is plotted for three different momentums. The spectral function has a sharp peak near the Fermi level and a resonance peak above it. Since the position of the

sharp peak varies with momentum and its width becomes infinitesimal at $\mathbf{p} = \mathbf{p}_F$, the sharp peaks correspond to quasiparticle excitations, so that our system behaves as a Fermi liquid at the low-energy region. As shown in paper I, the effective mass m^* of the quasiparticle can be estimated from the dispersion of the sharp peak and is obtained to be $|m^*/m| \sim 400$ in the present case. Thus, the choice of the above parameter values leads to a heavy-fermion state in the Anderson-lattice system. The result for a finite-temperature case is given in Fig. 1(b). As seen in the figure, we have two peaks also at this temperature. The peak near the Fermi level is, however, much broader than that at absolute zero. Furthermore, the peak has a finite width even in the case of $\mathbf{p} = \mathbf{p}_F$. This change is caused by a large magnitude of the imaginary part of the self-energy even at the Fermi level at a higher temperature. This fact indicates that the heavy-quasifermion state which is well defined at very low temperatures becomes unstable and changes to a resonance state as temperature increases. We further note that the position and the shape of the resonance peak centered on the Fermi level are almost independent of momentum. This means that the spatial correlation of the resonance state is very weak and then the resonance state is almost localized on the lattice sites, in contrast with the quasifermion state. Therefore, the resonance state which is changed from the quasifermion state is similar to that in a single-impurity Kondo system. As is well known, heavy-fermion systems show a crossover effect from a heavy-fermion state to an impurity Kondo-like state with increasing temperature. The temperature variation shown above in the f-electron spectral function corresponds to the crossover effect observed in heavy-fermion systems.

Obtaining the spectral function, we can calculate the density of states from Eqs. (3.31) and (3.32). We show the result for the f-electron system near the Fermi level in Fig. 2 for several temperatures. The values of the parameters are the same as those in Fig. 1. We see a very sharp peak centered on the Fermi level and a broad peak above it at $\tilde{T} = 0.0005$. As understood from the f-electron spectral function shown in Fig. 1(a), this sharp peak originates from the heavy-quasifermion levels around the Fermi level, so the peak width gives the quasifermion bandwidth, i.e., an energy scale of the coherence. As temperature increases the sharp peak broadens and its height decreases. This temperature variation of the f-electron density of states is induced by the crossover effect from the heavy-fermion state to the Kondo-impurity-like resonance state. The width of the resonance peak at higher temperatures gives a measure of the resonance state without coherence. Thus, from the result of the temperature variation of the f-electron density of states, we may speculate that the two characteristic energy scales exist at low temperatures in
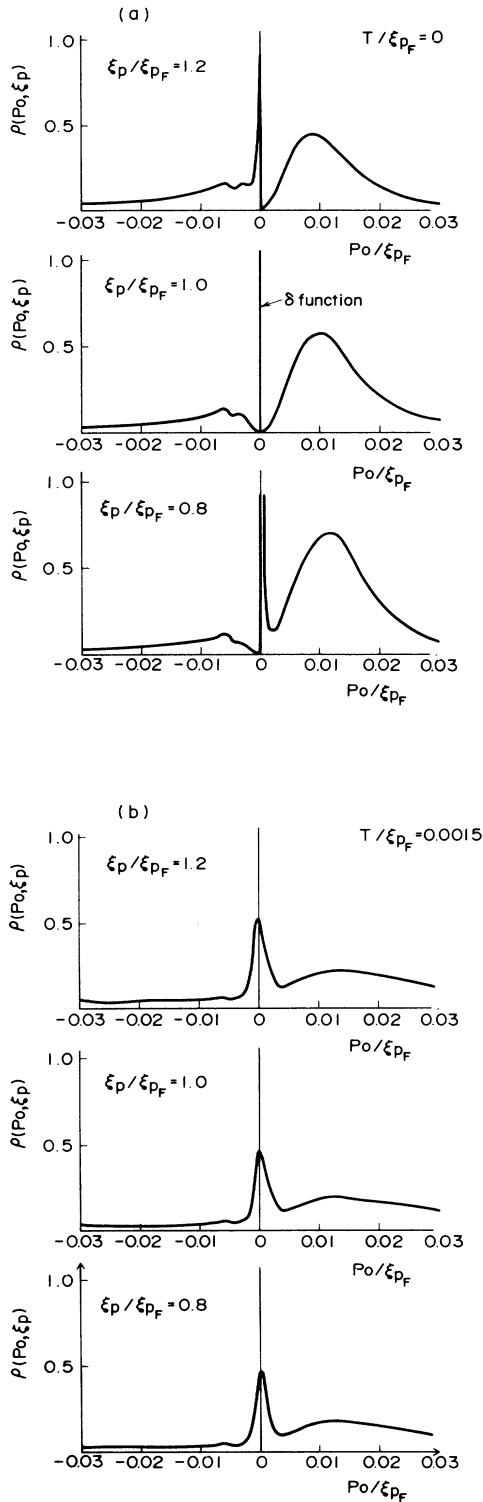
FIG. 2. Energy dependence of the f-electron density of states for several temperatures. The following values of the parameters are used: $\bar{E}_0/\xi_{p_F} = -0.003$, $V/\xi_{p_F} = 0.02$, $\lambda_r \rho_s(\xi_{p_F}) = 1.0$, $U_s^* \rho_s(\xi_{p_F}) = 0.02$, and $D/\xi_{p_F} = 1.5$.
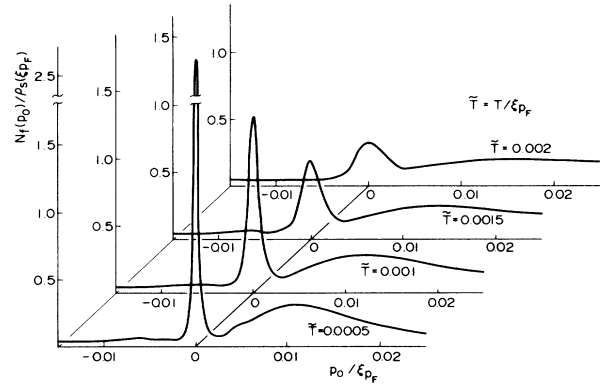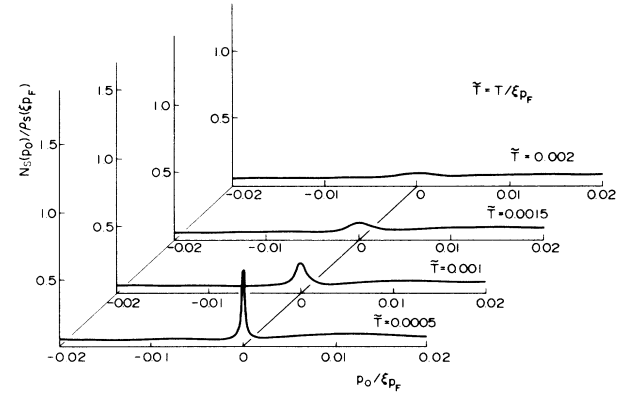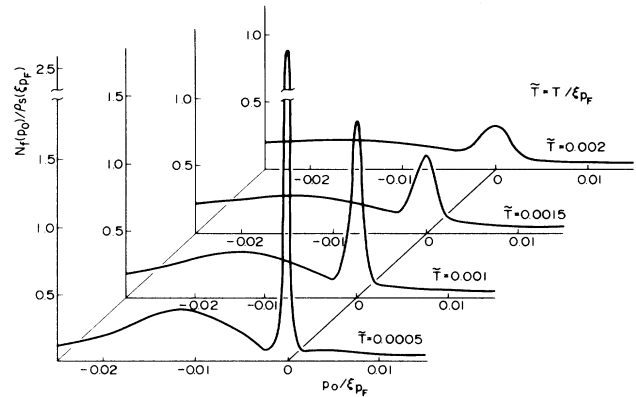

FIG. 3. Energy dependence of the conduction-electron density of states for several temperatures. The following values of the parameters are used: $\bar{E}_0/\xi_{p_F} = -0.003$, $V/\xi_{p_F} = 0.02$, $\lambda_r \rho_s(\xi_{p_F}) = 1.0$, $U_s^* \rho_s(\xi_{p_F}) = 0.02$, and $D/\xi_{p_F} = 1.5$.

FIG. 4. Energy dependence of the f-electron density of states for several temperatures. The following values of the parameters are used: $\bar{E}_0/\xi_{p_F} = 0.003$, $V/\xi_{p_F} = 0.02$, $\lambda_r \rho_s(\xi_{p_F}) = 1.0$, $U_s^* \rho_s(\xi_{p_F}) = 0.02$, and $D/\xi_{p_F} = 1.5$.
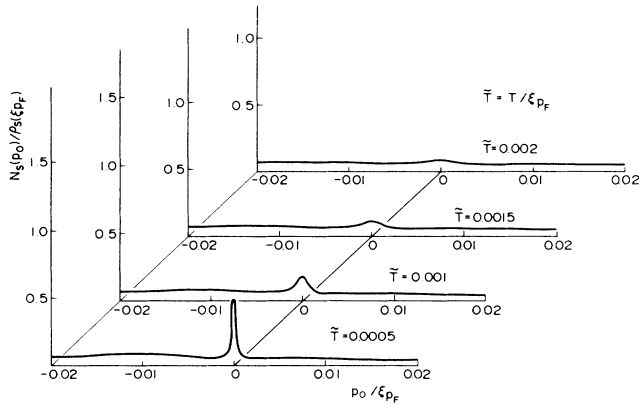
FIG. 1. Energy dependence of the f-electron spectral function at two different temperatures, (a) $\bar{T} = 0$ and (b) $\bar{T} = 0.002$. The following values of the parameters are used: $\bar{E}_0/\xi_{p_F} = -0.003$, $V/\xi_{p_F} = 0.02$, $\lambda_r \rho_s(\xi_{p_F}) = 1.0$, $U_s^* \rho_s(\xi_{p_F}) = 0.02$, and $D/\xi_{p_F} = 1.5$.

FIG. 5. Energy dependence of the conduction-electron density of states for several temperatures. The following values of the parameters are used: $\bar{E}_0/\xi_{P_F}=0.003$, $V/\xi_{P_F}=0.02$, $\lambda_r\rho_s(\xi_{P_F})=1.0$, $U_s^*\rho_s(\xi_{P_F})=0.02$, and $D/\xi_{P_F}=1.5$.

the Anderson lattice. In Fig. 3 we plot the density of states of conduction electrons near the Fermi level for several temperatures. As seen in the figure, the sharp peak corresponding to the heavy-fermion state appears also in the conduction-electron channel, although its intensity is weaker than that in the f-electron channel. The
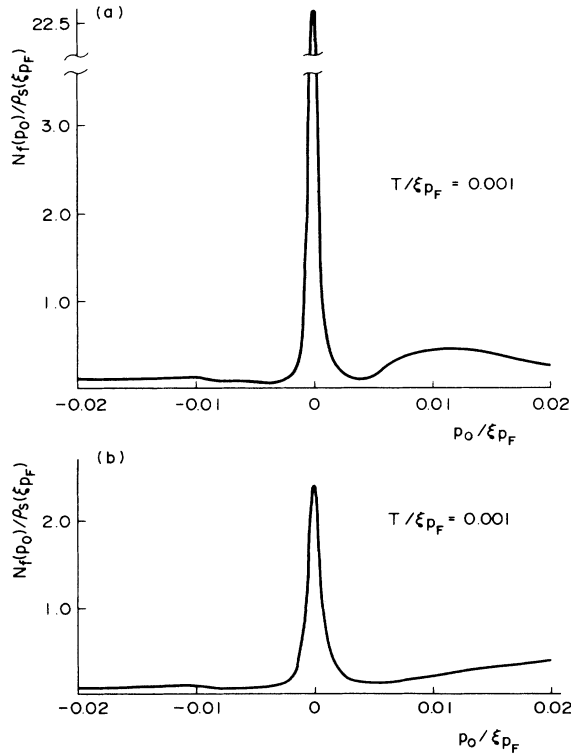

FIG. 6. Mixing-parameter dependence of the f-electron density of states at temperature $T/\xi_{P_F}=0.001$. The following values of the parameters are used: $\bar{E}_0/\xi_{P_F}=-0.005$, $\lambda_r\rho_s(\xi_{P_F})=1.0$, $U_s^*\rho_s(\xi_{P_F})=0.02$, $D/\xi_{P_F}=1.5$, and (a) $V/\xi_{P_F}=0.02$, (b) $V/\xi_{P_F}=0.03$.

temperature variation of the density of the states of the conduction electrons is similar to that of the f electrons.

In Figs. 4 and 5 the results for another choice of parameter values are presented. A positive value of $\bar{E}_0$, $\bar{E}_0/\xi_{P_F}=0.003$, is taken and values of the other parameters are unchanged. The structure of the density of states and their temperature dependence are similar to those in the previous case, except that the broad resonance level appears below the Fermi level.

Finally, the dependence of the f-electron density of states on the mixing parameter is shown in Fig. 6. For the small mixing parameter [Fig. 6(a)] the heavy-fermion peak is sharp and very high, and the broad resonance peak is close to the heavy-fermion peak. On the other hand, when the mixing parameter is larger [Fig. 6(b)], the peak height is lower and the resonance peak is shifted away from the Fermi level.

IV. DISCUSSION AND SUMMARY

In this paper we calculated the density of states of the Anderson lattice near the Fermi level, taking account of the effect of the spin fluctuations in a one-loop approximation, and investigated the temperature variation of the heavy-fermion state. In paper I we discussed the nature of the low-energy excited states in the Anderson lattice in a metallic case on the basis of the calculated result of the f-electron spectral function at absolute zero. We found a well-defined quasiparticle state very near the Fermi level and a resonance state outside the quasifermion state. The effective mass of the quasiparticle is very large when the renormalized f level $\bar{E}_0$ is close to the Fermi level. According to this fact, we claimed that the heavy-fermion state or the so-called coherent state in the Anderson lattice at low temperatures can be characterized by the existence of the well-defined heavy quasiparticle states in the vicinity of the Fermi level. As shown in Sec. III, the present calculation shows that a very sharp peak centered on the Fermi level appears in the density-of-states curve. This sharp peak corresponds to the heavy quasiparticle state. The states outside the sharp peak are not single-particle-like, but are resonance states because these states have short lifetime. The characteristic energy scale associated with the coherence may be obtained from the quasiparticle bandwidth, so the width of the sharp peak in the f-electron density of states at absolute zero gives a measure of coherence energy.

To obtain a better understanding of the heavy-fermion state, let us compare the present result of the density of states with that in the Hartree-Fock approximation. In Fig. 7 we plotted the density of states of the f electron in the Hartree-Fock approximation along with that calculated for a temperature $\bar{T}=0.0003$ in Sec. III. The parameter values used in both cases are the same. As seen in Fig. 7, the density of states in the present calculation is much smaller than that in the Hartree-Fock approximation and has a peak at the Fermi level. On the other hand, in the Hartree-Fock approximation the hybridization gap lies near the Fermi level and no peak structure appears at the Fermi level. We note that the value of the density of states at the Fermi level in the present calcula-
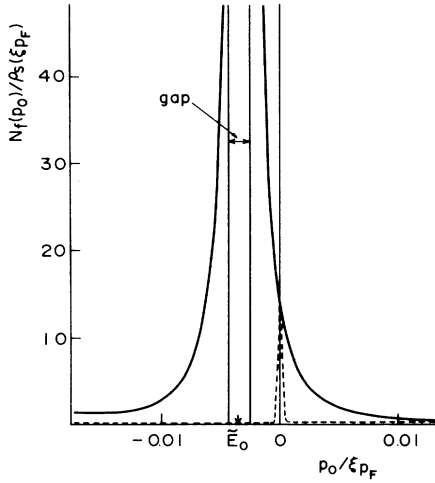
FIG. 7. f-electron density of states for the values of the following parameters: $\bar{E}_0/\xi_{p_F} = -0.003$, $V/\xi_{p_F} = 0.02$, $\lambda_r \rho_s(\xi_{p_F}) = 1.0$, $U_s^* \rho_s(\xi_{p_F}) = 0.02$, and $D/\xi_{p_F} = 1.5$. The solid line represents the result in the Hartree-Fock approximation. The dashed line represents the result in the present calculation.

tion is very close to that of the Hartree-Fock approximation. This is due to the fact that the imaginary part of the self-energy vanishes at the Fermi level at absolute zero and the momentum dependence of the real part of the self-energy is very weak. As the energy is far away from the Fermi level, the imaginary part of the self-energy rapidly increases, as shown in paper I. As a result, the density of states dramatically decreases from its value at the Fermi level. The number of states around the Fermi level is much smaller than those in the Hartree-Fock approximation. This result implies that most of the f-electron states lie in the energy region deeply below the Fermi level, although our calculation of the density of states is limited to the region near the Fermi level. This feature of the density of states does not contradict the fact of the large electronic specific heat in the heavy-fermion systems, since the electronic specific heat is related not directly to the bare f electrons but to the large excitation density of quasiparticles. The excitation density is approximately given by $N_f(p_0)/z(\mathbf{p}_F)$, where $z(\mathbf{p}_F)$ is the wave-function

renormalization constant and is expressed by $[1 - \partial\Sigma(p_0, p_F)/\partial p_0 \,|\,]^{-1}$. Since $z(\mathbf{p}_F)$ is very small in heavy-fermion systems, the excitation density is very large.

The quasiparticle state cannot be well defined at finite temperatures greater than the coherence energy. As shown in Sec. III, this can be seen in the temperature variation of the f-electron spectral function, i.e., the quaiparticle peak changes to a resonance peak with a small temperature increase. As a result, the levels around the Fermi level consist of the resonance levels at high temperatures, which are similar to those in the single-impurity Kondo state. Associated with this change, the sharp peak in the f-electron density-of-states curve broadens and its height decreases. We consider that it is this change in the electronic states that causes the crossover from the heavy-fermion state to the single-impurity-Kondo-like state observed in the heavy-fermion compounds. To confirm our understanding for the crossover effect in the Anderson-lattice system, it is desirable to calculate physical quantities such as resistivity, so we are planning to calculate the temperature variation of the resistivity on the basis of our theory.

ACKNOWLEDGMENTS

APPENDIX A

In this appendix we derive the Ward-Takahashi relations (2.54)–(2.57) from Eq. (2.52).

From Eq. (2.23) we note that the inverse f-electron Green's function in the presence of the term (2.47) is given by

$$g_\sigma^{-1}(p)^{\alpha\beta} = (p_0 - E_0 - \tfrac{1}{2}h_f\sigma_3)\delta_{\alpha\beta} - V^2 S_\sigma^{\alpha\beta}(p) - \Sigma_\sigma^{\alpha\beta}(p) \ .$$

$$(A1)$$

Substituting the Green's function (A1) into Eq. (2.52), we have the following relation between the self-energy function and the vertex functions:

$$\Sigma_\uparrow^{\alpha\beta}(p+q) - \Sigma_\uparrow^{\alpha\beta}(p) = (q_0 - h_f) \sum_\delta \Pi^\delta(q) \Gamma_{+\delta}^{\alpha\beta}(p;q;p+q)$$

$$+ V^2 \left[\frac{i}{(2\pi)^4} \right] \int d^4k \frac{-q_0 + h_s + \varepsilon_{k+q} - \varepsilon_k}{(k_0 + q_0 - \varepsilon_{k+q} - \tfrac{1}{2}h_s)(k_0 - \varepsilon_k + \tfrac{1}{2}h_s)}$$

$$\times \sum_{a,b,\gamma} g_\uparrow^{\gamma a}(k+q) g_\uparrow^{b\gamma}(k) \Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{aa;\beta b}(p, k+q;p+q, k) \ .$$

$$(A2)$$

First, we take the limit $q \to 0$. In this limit Eq. (A2) is reduced to

$$\Sigma_\uparrow^{\alpha\beta}(p)-\Sigma_\downarrow^{\alpha\beta}(p)=h_f\Delta_0\sum_\delta \Gamma_{+\delta}^{\alpha\beta}(p;q;p+q)$$

$$-h_s V^2\left[\frac{i}{(2\pi)^4}\right]\int d^4k\frac{1}{(k_0-\varepsilon_k-\frac{1}{2}h_s)(k_0-\varepsilon_k+\frac{1}{2}h_s)}\sum_{a,b,\gamma}g_\uparrow^{\gamma a}(k)g_\uparrow^{b\gamma}(k)\Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{\gamma a;\beta b}(p,k;p,k)\ . \tag{A3}$$

Here, Δ_0 is defined by the relation (2.58). When only linear terms with respect to h_f and h_s are retained, Eq. (A3) is reduced to

$$\Sigma_\uparrow^{\alpha\beta}(p)-\Sigma_\downarrow^{\alpha\beta}(p)=2h_f\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_f}\right]_{h=0}+2h_s\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_s}\right]_{h=0}$$

$$=-2h_f\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial h_f}\right]_{h=0}-2h_s\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial h_s}\right]_{h=0}$$

$$=h_f\Delta_0\sum_\delta \Gamma_{+\delta}^{\alpha\beta}(p;0;p)-h_s\left[\frac{i}{(2\pi)^4}\right]\int d^4k\frac{V^2}{(k_0-\varepsilon_k)^2}\sum_{a,b,\gamma}g_\uparrow^{\gamma a}(k)g_\uparrow^{b\gamma}(k)\Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{\alpha a;\beta b}(p,k;p,k)\ . \tag{A4}$$

This relation indicates the Ward-Takahashi relations (2.54) and (2.55) in the limit of $h_f,h_s\to 0$:

$$\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_f}\right]_{h=0}=-\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial h_f}\right]_{h=0}=\frac{1}{2}\Delta_0\sum_\delta \Gamma_{+\delta}^{\alpha\beta}(p;0;p)\ , \tag{A5}$$

$$\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial h_s}\right]_{h=0}=-\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial h_s}\right]_{h=0}$$

$$=-\frac{1}{2}\left[\frac{i}{(2\pi)^4}\right]\int d^4k\frac{V^2}{(k_0-\varepsilon_k)^2}\sum_{a,b,\gamma}g_\uparrow^{\gamma a}(k)g_\uparrow^{b\gamma}(k)\Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{\alpha a;\beta b}(p,k;p,k)\ . \tag{A6}$$

Furthermore, noting the relation in the case of $q\to 0$,

$$\Sigma_\downarrow^{\alpha\beta}(p+q)-\Sigma_\uparrow^{\alpha\beta}(p)=[\Sigma_\downarrow^{\alpha\beta}(p+q)-\Sigma_\downarrow^{\alpha\beta}(p)]-[\Sigma_\uparrow^{\alpha\beta}(p)-\Sigma_\downarrow^{\alpha\beta}(p)]$$

$$=q_0\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial p_0}\right]+\mathbf{q}\cdot\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial\mathbf{p}}\right]-[\Sigma_\uparrow^{\alpha\beta}(p)-\Sigma_\downarrow^{\alpha\beta}(p)]\ , \tag{A7}$$

we obtain the Ward-Takahashi relations (2.56) and (2.57) from Eq. (A2) in the limit of $q,h_f,h_f\to 0$:

$$\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial p_0}\right]_{h=0}=\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial p_0}\right]_{h=0}$$

$$=\Delta_0\sum_\delta\Gamma_{+\delta}^{\alpha\beta}(p;0;p)-\left[\frac{i}{(2\pi)^4}\right]\int d^4k\frac{V^2}{(k_0-\varepsilon_k)^2}\sum_{a,b,\gamma}g_\uparrow^{\gamma a}(k)g_\uparrow^{b\gamma}(k)\Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{\alpha a;\beta b}(p,k;p,k)\ , \tag{A8}$$

$$\left[\frac{\partial\Sigma_\downarrow^{\alpha\beta}(p)}{\partial\mathbf{p}}\right]_{h=0}=\left[\frac{\partial\Sigma_\uparrow^{\alpha\beta}(p)}{\partial\mathbf{p}}\right]_{h=0}$$

$$=\left[\frac{i}{(2\pi)^4}\right]\int d^4k\frac{V^2}{(k_0-\varepsilon_k)^2}\left[\frac{\partial\varepsilon_k}{\partial\mathbf{k}}\right]\sum_{a,b,\gamma}g_\uparrow^{\gamma a}(k)g_\uparrow^{b\gamma}(k)\Gamma_{\uparrow\downarrow,\uparrow\uparrow}^{\alpha a;\beta b}(p,k;p,k)\ . \tag{A9}$$

APPENDIX B

In this appendix the explicit expression for χ_s used in the numerical calculations and some discussions on the renormalized parameters U_s^* and λ_r are given. We consider the case of absolute zero in the following, since we need only the values of those quantities at absolute zero for the calculation of the self-energy function up to second order in temperature.

Let us first obtain the equation for Δ_0 at $T=0$ K from Eq. (2.62), taking the limit $q\to 0$:

$$-h_f\Delta_0=M_f-h_s\left[\frac{i}{(2\pi)^4}\right]\int_c d^4p\frac{V^2}{(p_0-\varepsilon_p+\frac{1}{2}h_s)(p_0-\varepsilon_p-\frac{1}{2}h_s)}g_\uparrow(p)g_\downarrow(p)$$

$$+2h_s\left[\frac{i}{(2\pi)^4}\right]\int_c d^4p\,g_\uparrow(p)\left[\frac{\partial\Sigma_\uparrow(p)}{\partial h_s}\right]_{h=0}g_\downarrow(p)\ . \tag{B1}$$

Here, we dropped the off-diagonal components such as $g_\sigma^{12}(p)$ and $\Sigma_\sigma^{12}(p)$, and replaced $g_\sigma^{11}(p)$ and Σ_σ^{11} by $g_\sigma(p)$ and $\Sigma_\sigma(p)$, which are the f-electron Green's function and self-energy function at absolute zero, respectively, since the off-diagonal components vanish at absolute zero and the (1,1) components are equal to those of absolute zero. As shown in paper I, M_f is written as

$$M_f = -h_f\Delta_0 + h_s\chi_s \ . \tag{B2}$$

Substituting the relation (B2) into Eq. (B1), we have the following equation in the limit of $h_s, h_f \to 0$:

$$\chi_s = \left[\frac{i}{(2\pi)^4}\right] \int_c d^4p \frac{V^2}{(p_0 - \varepsilon_p)^2} g_\uparrow(p) g_\downarrow(p)$$
$$-2\left[\frac{i}{(2\pi)^4}\right] \int_c d^4p\, g_\uparrow(p) \left[\frac{\partial \Sigma_\uparrow(p)}{\partial h_s}\right]_{h=0} g_\downarrow(p) \ . \tag{B3}$$

When the approximations (3.13) and (3.14) are used, Eq. (B3) is reduced to

$$\chi_s = R + U_s^* Q \chi_s \ , \tag{B4}$$

where

$$R = \frac{V^2}{\tilde{E}_0^2 + V^2}\rho_s(\xi_{p_F}) \ , \tag{B5}$$

$$Q = \frac{V^4}{\tilde{E}_0^2(\tilde{E}_0^2 + V^2)}\rho_s(\xi_{p_F}) \ , \tag{B6}$$

$\rho_s(\xi_{p_F})$ being the density of states of the bare conduction band at the energy $\xi_{p_F} = p_F^2/2m$. Thus, χ_s is determined to be

$$\chi_s = R/(1 - U_s^* Q) \ . \tag{B7}$$

Let us next consider the relation given by Eq. (2.32) in paper I:

$$\chi_s = \left[\frac{i}{(2\pi)^4}\right] \int d^4p \frac{V^2}{(p_0 - \varepsilon_p - \frac{1}{2}h_s)(p_0 - \varepsilon_p + \frac{1}{2}h_s)}$$
$$\times[1 - \Delta_0\Gamma_+(p;0;p)]g_\uparrow(p)g_\downarrow(p) \ . \tag{B8}$$

When the approximate spectral function (3.13) is used for the Green's functions in (B8), the vertex function $\Gamma_+(p;0;p)$ should be taken to be a constant from the consideration of the Ward-Takahashi relation (2.54), because in this case the self-energy function is independent of p. Therefore, we can replace the vertex function in Eq. (B8) by the renormalized coupling constant λ_r. Thus we have the relation in the limit of $h_s, h_f \to 0$:

$$\chi_s = R(1 - \lambda_r\Delta_0) \ . \tag{B9}$$

Δ_0 can be obtained from Eqs. (B7) and (B9) as

$$\Delta_0 = -(U_s^*/\lambda_r)Q/(1 - U_s^* Q) \ . \tag{B10}$$

To see the relation between U_s^* and λ_r, we consider the Ward-Takahashi relation (2.55). When the approximate spectral function (3.13) is used, we can approximately estimate the integral at absolute zero as

$$\left[\frac{\partial \Sigma_\uparrow(0,\mathbf{p}_F)}{\partial h_s}\right]_{h=0} \sim -\frac{1}{2}\Gamma_{\uparrow\downarrow}R \ , \tag{B11}$$

where $\Gamma_{\uparrow\downarrow}$ is the value of the vertex function at the Fermi level, so that the use of the relation (3.14) yields

$$U_s^* \sim \Gamma_{\uparrow\downarrow}R/\chi_s = \Gamma_{\uparrow\downarrow}(1 - U_s^* Q) \ , \tag{B12}$$

and this relation leads to the estimation

$$U_s^* \sim \Gamma_{\uparrow\downarrow}/(1 + \Gamma_{\uparrow\downarrow}Q) \ . \tag{B13}$$

Let us consider the case that the renormalized f level $\tilde{E}_0$ is very close to the Fermi level, i.e., $\tilde{E}_0 \sim 0$ and $V/|\tilde{E}_0| \gg 1$. In this case, as seen from Eq. (B6), Q is very large and

$$Q \sim O((V/\tilde{E}_0)^2\rho_s(\xi_{p_F})) \ .$$

Therefore, if we assume $\Gamma_{\uparrow\downarrow} \sim \lambda_r$, we find the relation

$$U_s^* \ll \lambda_r \ . \tag{B14}$$

Therefore, the choice of the values of U_s^* and λ_r used in Sec. III, i.e., $U_s^*\rho_s(\xi_{p_F}) = 0.02$ and $\lambda_r\rho_s(\xi_{p_F}) = 1.0$, is reasonable.

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