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Fluctuation effects on the mean-field approximation in the slave boson method for the Anderson lattice

Kikuo Harigaya
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

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Abstract. Applicability of the mean-field approximation is examined, when the slave boson technique is used for the SU(N_d) Anderson lattice model. The fluctuation component of the slave boson field is explicitly introduced and its interactions with electrons are studied. The self-energy parts are calculated up to the second order of the interactions without relying upon the usual $1/N_d$-expansion rule. Using perturbed propagators, we obtain modified self-consistency equations for the mean-field parameters. They are solved at the transition temperature and also at zero temperature. The transition temperature decreases by a certain factor when the fluctuation is incorporated. This factor mainly depends on the location of the atomic f level and the degeneracy N_d. We newly adopt this quantity as the quantitative measure of the fluctuation effects. It is confirmed that the mean-field theory is less affected by the fluctuation if the system is in the Kondo limit and the degeneracy is large. It is found that the fluctuation becomes more effective as the location of the atomic f level is closer to the Fermi level or the degeneracy of the orbital is smaller. The consequences for application of the mean-field theory to the real heavy-fermion compounds are discussed.

1. Introduction

In recent years, heavy-fermion systems have been attracting much interest, and intensive research has been performed experimentally [1, 2] and theoretically [3–5].

The experimental research [2] has found that there are material-independent properties in the heavy-fermion systems. In particular, in a temperature range $T < T_{coh}$, a coherent Kondo state is developed, and for $T > T_K$, the system behaves as if the scatterings from each magnetic ion are mutually independent, and the crossover between these two states is the main interest of the research. The temperature T_{coh} is a new characteristic temperature which has been suggested experimentally but has not been established theoretically yet. Nowadays, there are plenty of experimental data to be understood theoretically.

There have been many theoretical efforts [3]. A microscopic model for the heavy-fermion systems is believed to be the Anderson lattice model, which is a direct generalisation of the single-impurity Anderson model. There are several methods for studying this model. For example, the Coulomb interactions are taken into account with the help of perturbation methods [6], variational methods [7], quantum Monte Carlo research [8], the slave boson method [9–11], and so on.

In this paper, we study the SU(N_d) Anderson lattice, which is a generalised model of the infinite-U Anderson lattice in order that electronic states at each lattice site are N_d-fold degenerated [12]. We adopt the slave boson method, which was first introduced by Coleman [10] to avoid the complicated algebra of Hubbard's projection operator. The simplest approximation to the slave boson formalism is the mean-field approximation [9]. It has been found to explain some experimental properties successfully. For instance, the universal behaviour of the specific heat, the magnetic susceptibility and the resistivity are explained by interactions of electrons with the fluctuation particles [13, 14], and elastic anomalies at low temperatures are derived in the phenomenological theory [15]. The $1/N_d$-expansion rule has been applied to calculations. In contrast, there are some properties which cannot be explained by the usual $1/N_d$-treatment of the fluctuation. For example, some workers [16, 17] have tried to understand ordered states in the coherent Kondo states by incorporating fluctuation effects without relying upon the $1/N_d$-expansion method.

In the $1/N_d$-expansion theory, the mean-field parameters are assumed to be less affected by the fluctuation. However, interaction terms, which are of the higher order in the $1/N_d$-expansion theory, may give rise to large changes in mean-field parameters quantitatively. We examine this possibility in order to check applicability of the mean-field theory. In the present paper, we assume that the quantity $J\rho$ is small enough. Here, J is the Coqblin–Schrieffer coupling and ρ is the density of states of the conduction band. We calculate the self-energy parts of electrons and the slave bosons in the first order of $J\rho$, in other words in the second order of the interactions. Using perturbed propagators, we obtain the modified self-consistency equations for the mean-field parameters. Changes due to the fluctuation effects are considered. A reduction is found in the transition temperature. The factor of the reduction is determined by the position of the atomic f level and the degeneracy. We newly adopt this factor in order to measure the effects of the fluctuation. Although the phase transition is an artifact of the approximation scheme, it is also certain that the transition temperature characterises the energy scale of electrons in the mean theory. We use this concept. Applicability of the mean-field theory is discussed by relying upon the newly introduced parameter. It is found that the mean-field theory is less affected by the fluctuation if the system is in the Kondo limit and the degeneracy is large. This is a well known result in the $1/N_d$-expansion theories [18, 19]. In our theory, however, we can measure the degree of fluctuation effects quantitatively by the new parameter. The fluctuation is more effective as the location of the atomic f level is closer to the Fermi level or the degeneracy becomes smaller. The fluctuation effects on the mean-field parameters and some physical quantities are also discussed.

In section 2, we review the model and the mean-field approximation. In section 3, we calculate the second-order self-energy parts and give the modified self-consistency equations. The fluctuation effects on the mean-field results are derived. In section 4, a summary and discussion are presented.

2. Model and the mean-field theory

Coleman [10] introduced the slave boson method for the infinite-U Anderson model. A generalisation to the lattice system, in which electronic states at each lattice site are N_d-fold degenerated, is straightforward. The Hamiltonian [9, 11] is

$$\mathcal{H} = \sum_{im} (-E_f) f^\dagger_{im} f_{im} + \sum_{km} \varepsilon_k c^\dagger_{km} c_{km} + V \sum_{im} (b^\dagger_i c^\dagger_{im} f_{im} + f^\dagger_{im} c_{im} b_i) + \sum_i \lambda_i \Big(\sum_m f^\dagger_{im} f_{im} + b^\dagger_i b_i - 1 \Big) \tag{2.1}$$

where f_{im} denote an operator which annihilates a 4f electron with the z component of a spin m at the ith lattice site whose electronic level has the energy $-E_f$. The spin has the magnitude j, which gives the degeneracy $N_d = 2j + 1$. We take E_f to be positive, in this paper. The operator c_{km} annihilates conduction electrons with wavenumber $\boldsymbol{k}$ and the z component of the spin m. For simplicity, it is assumed that the spin of the conduction electrons has the same magnitude as the 4f electrons. The density of states of the conduction electrons, per site and one spin component, is assumed to be constant: $\rho = 1/2D$ at $-D < \varepsilon_k < D$, and zero otherwise. We define c_{im} by the relation $c_{im} = N^{-1/2} \sum_k \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_i)\, c_{km}$. The operator b_i annihilates a slave boson of the ith site. No more than one 4f electron number is introduced at the ith site. It is satisfied by the constraint

$$\sum_m f^\dagger_{im} f_{im} + b^\dagger_i b_i = 1 \tag{2.2}$$

for each site. It is taken into account in the Hamiltonian (2.1) with Lagrange's multiplier λ_i. Possible anisotropy in the mixing interaction V is neglected. The Fermi level is taken to be zero: $\mu = 0$.

The mean-field approximation [9, 11] for the slave bosons assumes that

$$\langle b_i \rangle_{\mathrm{mf}} = \langle b^\dagger_i \rangle_{\mathrm{mf}} = r_{\mathrm{mf}} \qquad \langle b^\dagger_i b_i \rangle_{\mathrm{mf}} = r^2_{\mathrm{mf}} \tag{2.3a}$$

and site-independent Lagrange's multiplier

$$\lambda_i = \lambda \qquad \text{for all } i. \tag{2.3b}$$

The definition of the mean-field ground state is summarised in the appendix. The mean-field Hamiltonian becomes

$$\mathcal{H}_{\mathrm{mf}} = \sum_{im} \tilde{E}_f f^\dagger_{im} f_{im} + \sum_{km} \varepsilon_k c^\dagger_{km} c_{km} + r_{\mathrm{mf}} V \sum_{im} (f^\dagger_{im} c_{im} + c^\dagger_{im} f_{im}) + \lambda_{\mathrm{mf}} N (r^2_{\mathrm{mf}} - 1) \tag{2.4}$$

where $\tilde{E}_f = -E_f + \lambda_{\mathrm{mf}}$. The mixing interaction is effectively reduced by the factor r_{mf}; so r_{mf} is frequently called the reduction factor.

To diagonalise $\mathcal{H}_{\mathrm{mf}}$, we introduce the finite temperature electron propagator of a matrix form

$$\mathbf{G}_m(\tau, \boldsymbol{k}) = \begin{bmatrix} G_{fm}(\tau, \boldsymbol{k}) A_m(\tau, \boldsymbol{k}) \\ A^*_m(\tau, \boldsymbol{k}) G_{cm}(\tau, \boldsymbol{k}) \end{bmatrix} \tag{2.5a}$$

$$= \begin{bmatrix} -\langle T_\tau f_{km}(\tau) f^\dagger_{km}(0) \rangle_{\mathrm{mf}} & -\langle T_\tau f_{km}(\tau) c^\dagger_{km}(0) \rangle_{\mathrm{mf}} \\ -\langle T_\tau c_{km}(\tau) f^\dagger_{km}(0) \rangle_{\mathrm{mf}} & -\langle T_\tau c_{km}(\tau) c^\dagger_{km}(0) \rangle_{\mathrm{mf}} \end{bmatrix}. \tag{2.5b}$$

It is readily calculated, and its Fourier transform satisfies

$$\mathbf{G}^{-1}_m(\mathrm{i}\omega, \boldsymbol{k}) = \begin{bmatrix} \mathrm{i}\omega - \tilde{E}_f & -r_{\mathrm{mf}} V \\ -r_{\mathrm{mf}} V & \mathrm{i}\omega - \varepsilon_k \end{bmatrix} \tag{2.6}$$

where ω is the odd Matsubara frequency. Since $\mathbf{G}_m$ is spin independent, we suppress the suffix m. Also, we put $A^* = A$, since r_{mf} can be taken to be a real number.

The spectrum of the quasi-particle is derived with the help of the relation $\det[\mathbf{G}^{-1}(E(\boldsymbol{k}), \boldsymbol{k})] = 0$ to be

$$E_\pm(\boldsymbol{k}) = \tfrac{1}{2}[\varepsilon_k + \tilde{E}_f \pm \sqrt{(\varepsilon_k - \tilde{E}_f)^2 + 4r^2_{\mathrm{mf}} V^2}]. \tag{2.7}$$

The number n_f, of f electrons per site is calculated with the help of equation (2.6), at $T = 0$, and turns out to be

$$n_f = (N_d/2D)\{r^2_{\mathrm{mf}} V^2/\tilde{E}_f + \tfrac{1}{2}[D + \tilde{E}_f - \sqrt{(D + \tilde{E}_f)^2 + 4r^2_{\mathrm{mf}} V^2}]\}. \tag{2.8a}$$

The number n_c of conduction electrons, is

$$n_c = (N_d/4D)[D - \tilde{E}_f + \sqrt{(D + \tilde{E}_f)^2 + 4r^2_{\mathrm{mf}} V^2}]. \tag{2.8b}$$

In the heavy-fermion systems, it is assumed that the electronic states are less than half filled, and the numbers of electrons satisfy $n_f \leqslant 1$ and $n_c \simeq N_d/2$. Occupancy of the f state, which is close to unity, is realised by the smallness of r_{mf}^2 in equation (2.8*a*). The value of n_c is easily evaluated if the relation $D \gg \tilde{E}_f, r_{mf}V$ is considered in equation (2.8*b*). Hereafter, we consider the case of the limit $n_f \rightarrow 1$.

The mean-field approximation gives the free energy per site

$$F_{mf} = -N_d \frac{T}{N} \sum_{\omega k} \log[(i\omega - \varepsilon_k)(i\omega - \tilde{E}_f) - r_{mf}^2 V^2] + \lambda_{mf}(r_{mf}^2 - 1). \tag{2.9}$$

The values of r_{mf} and λ_{mf} are determined by the self-consistency equation

$$\begin{aligned}\frac{\partial F_{mf}}{\partial r_{mf}} &= 2N_d \frac{T}{N} \sum_{\omega k} \frac{r_{mf} V^2}{(i\omega - \varepsilon_k)(i\omega - \tilde{E}_f) - r_{mf}^2 V^2} + 2 r_{mf} \lambda_{mf} \\ &= 2N_d V \frac{T}{N} \sum_{\omega k} A(i\omega, \boldsymbol{k}) + 2 r_{mf} \lambda_{mf} = 0\end{aligned} \tag{2.10}$$

and the constraint (2.2).

Next, we derive the transition temperature T_c^{mf} from equation (2.10). From the constraint (2.2), we obtain $n_f = 1$ at $T = T_c^{mf}$. This relation can be written as

$$\frac{N_d}{2D} \int_{-D}^{D} d\varepsilon_k \, T_c^{mf} \sum_{\omega} G_f(i\omega, \boldsymbol{k})|_{r=0} = N_d f_{mf}(\tilde{E}_f) = 1 \tag{2.11}$$

where $f_{mf}(x) = 1/[\exp(x/T_c^{mf}) + 1]$. It is rewritten as

$$\tilde{E}_f = T_c^{mf} \log(N_d - 1). \tag{2.12}$$

Equation (2.10) is transformed into

$$\frac{N_d V^2}{2D\lambda_{mf}} \int_{-D}^{D} d\varepsilon_k \frac{f_{mf}(\varepsilon_k) - f_{mf}(\tilde{E}_f)}{\varepsilon_k - \tilde{E}_f} + 1 = 0. \tag{2.13}$$

Performing integration and using equation (2.12), we obtain

$$\begin{aligned}&2D\lambda_{mf}/N_d V^2 + \frac{N_d - 2}{2N_d} \log[(D - \tilde{E}_f)/(D + \tilde{E}_f)] \\ &\qquad + \log[\pi T_c^{mf}/2\gamma(N_d)\sqrt{D^2 - \tilde{E}_f^2}] = 0\end{aligned} \tag{2.14}$$

where we define $\gamma(N_d)$ as

$$\begin{aligned}\log\left(\frac{\pi}{4\gamma(N_d)}\right) &= \frac{1}{4T_c^{mf}} \int_{-\infty}^{\infty} d\varepsilon \log\left|\frac{\varepsilon}{2T_c^{mf}}\right| \operatorname{sech}^2\left(\frac{\varepsilon + \tilde{E}_f}{2T_c^{mf}}\right) \\ &= \int_{-\infty}^{\infty} dx \log|x| \frac{2\exp(2x)(N_d - 1)}{[\exp(2x)(N_d - 1) + 1]^2}.\end{aligned} \tag{2.15}$$

Note that $\log[\gamma(N_d = 2)] \simeq 0.577$ is Euler's constant. Equation (2.14) can be rewritten as

$$\begin{aligned}T_c^{mf} &= [2\gamma(N_d)\sqrt{D^2 - \tilde{E}_f^2}/\pi][(D + \tilde{E}_f)/(D - \tilde{E}_f)]^{(N_d - 2)/2N_d} \\ &\qquad \times \exp[-(2D/N_d V^2)(E_f + \tilde{E}_f)].\end{aligned} \tag{2.16}$$

We perform iterations in equations (2.16). Setting $T_c^{mf} = 0$ on the right-hand side, we obtain the first approximation of T_c^{mf} from the left-hand side. After the second iteration, we obtain

$$T_c^{mf} = [2\gamma(N_d)/\pi]T_K(N_d - 1)^{-[4\gamma(N_d)DT_K]/\pi N_d V^2} \tag{2.17}$$

where T_K is the Kondo temperature: $T_K = D\exp(-2DE_f/N_dV^2)$. Here, we have neglected the small quantities of the order of $(T_K/D)^2$ in the coefficient of T_K. The quantity DT_K/N_dV^2 in the exponent is small enough. So equation (2.17) is a good approximation for T_c^{mf}. The coefficient of T_K is very close to unity: for example, $T_c^{mf} = 1.134T_K$ for $N_d = 2$. Then, the system in the mean-field theory shows a phase transition around the temperature T_K. It is well known that this transition is an artifact of the mean-field approximation. However, it is also certain that T_c^{mf} is a kind of characteristic energy scale of the mean-field theory. In the next section, a decrease in the transition temperature will be adopted in order to measure fluctuation effects on the system.

The quantity λ_{mf} has the value, at $T = T_c^{mf}$,

$$\lambda_{mf} = E_f + T_c^{mf}\log(N_d - 1) \sim E_f \tag{2.18}$$

which can be readily derived from equation (2.12).

We estimate parameters at $T = 0$. Equation (2.10) mainly gives the value of λ_{mf} [9, 11]. This equation is transformed into

$$\frac{N_dV^2}{2D\lambda_{mf}}\int_{E_-(\mathrm{bot})}^{0} \mathrm{d}E_-(\boldsymbol{q})\frac{1}{\tilde{E}_f - E_-(\boldsymbol{q})} = 1 \tag{2.19}$$

where

$$E_-(\mathrm{bot}) = E_-(\boldsymbol{k})|_{\varepsilon_k=-D}$$
$$\simeq -D + (1-n_f)(-V^2/D + \tilde{E}_fV^2/D^2 - \tilde{E}_f^2V^2/D^3) + O(\tilde{E}_f^3/D^2) \tag{2.20}$$

in the limit $r_{mf}^2 = 1 - n_f \ll 1$. After integration, equation (2.19) becomes

$$\tilde{E}_f = [D + \tilde{E}_f + (1-n_f)(V^2/D - \tilde{E}_fV^2/D^2 + \tilde{E}_f^2V^2/D^3)]\exp[-2D(E_f + \tilde{E}_f)/N_dV^2]. \tag{2.21}$$

Assuming that $\tilde{E}_f \ll E_f$, we perform the iterations twice as in equation (2.16). Then, we obtain

$$\tilde{E}_f = T_K(1 - 2DT_K/N_dV^2 + T_K/D) + (1-n_f)(V^2T_K/D^2)(1 - 4DT_K/N_dV^2) \tag{2.22}$$

where $1 - 2DT_K/N_dV^2 + T_K/D$ and $1 - 4DT_K/N_dV^2$ are within an accuracy of the order T_K/D and DT_K/N_dV^2, respectively. Equation (2.22) means that the effective f level is located slightly above the Fermi level and that λ_{mf} has the magnitude $\lambda_{mf} \sim E_f + T_K$ at $T = 0$.

The value of r_{mf} can be obtained from the constraint [9, 11]

$$n_f = 1 - r_{mf}^2 = \frac{N_d}{2D}\int_{E_-(\mathrm{bot})}^{0} \mathrm{d}E_-(\boldsymbol{q})\frac{r_{mf}^2V^2}{[\tilde{E}_f - E_-(\boldsymbol{q})]^2}. \tag{2.23}$$

After integration, equation (2.23) is transformed into

$$1 - n_f = [\![1 + (N_dV^2/2D)\{E_-(\mathrm{bot})/\tilde{E}_f[E_-(\mathrm{bot}) - \tilde{E}_f]\}]\!]^{-1}. \tag{2.24}$$

Substituting equations (2.20) and (2.22) into equation (2.24), we obtain

$$r_{mf}^2 = 1 - n_f = (2DT_K/N_dV^2)(1 - 4DT_K/N_dV^2 + 2T_K/D). \tag{2.25}$$

As $n_f \to 1$, we obtain $T_K \to 0$. This means that the atomic f level $-E_f$ must be far enough from the Fermi level. Substituting equation (2.25) into equation (2.22), we obtain

$$\tilde{E}_f = T_K[1 - 2DT_K/N_dV^2 + (1 + 2/N_d)T_K/D]. \tag{2.26}$$

The second and third terms are within an accuracy of $O(DT_K/N_dV^2)$ and $O(T_K/D)$, respectively.

The number of conduction electrons is evaluated as

$$n_c = (N_d/2D)[0 - E_-(\text{bot})] \simeq (N_d/2)[1 + r_{\text{mf}}^2(V^2/D^2 - \tilde{E}_f V^2/D^3)]$$
$$\simeq (N_d/2)\{1 + (2T_K/N_d D)(1 - 4DT_K/N_d V^2) + O[(T_K/D)^2]\}. \quad (2.27)$$

The number of the conduction electrons is larger than $N_d/2$. This is due to the mixing interaction V.

The effective mass at the Fermi level is given by

$$m^*/m = \{[\partial E_-(\boldsymbol{k})/\partial \varepsilon_k]|_{E_-(\boldsymbol{k})=0}\}^{-1} = 1 + r_{\text{mf}}^2 V^2/\tilde{E}_f^2 \sim 2D/N_d T_K. \quad (2.28)$$

Therefore, m^* is greatly enhanced. These heavy quasi-particles have been believed to give rise to the experimentally observed heavy Fermi liquid state or the coherent Kondo state.

3. Effects of the second-order fluctuation

We define the fluctuation field β_i as

$$b_i = r + \beta_i. \quad (3.1)$$

The accompanying particles are called β-bosons. The parameter r is to be determined self-consistently so as to minimise the free energy. The Hamiltonian (2.1) is rewritten

$$\mathcal{H} = \mathcal{H}_{\text{mf}} + \mathcal{H}_{\text{int}} \quad (3.2a)$$

$$\mathcal{H}_{\text{mf}} = \sum_{im} \tilde{E}_f f_{im}^\dagger f_{im} + \sum_{km} \varepsilon_k c_{km}^\dagger c_{km} + rV \sum_{im} (f_{im}^\dagger c_{im} + c_{im}^\dagger f_{im})$$
$$+ \lambda \sum_k \beta_k^\dagger \beta_k + \lambda N(r^2 - 1) \quad (3.2b)$$

$$\mathcal{H}_{\text{int}} = \frac{V}{\sqrt{N}} \sum_{kpm} (f_{k+pm}^\dagger c_{km} \beta_p + \beta_p^\dagger c_{km}^\dagger f_{k+pm}) + r\lambda\sqrt{N}(\beta_0^\dagger + \beta_0) \quad (3.2c)$$

where β_0 is the annihilation operator of the zero-momentum β-boson.

Using $\mathcal{H}_{\text{mf}}$, we define the non-interacting β-boson propagator by

$$D(\tau) = -\langle T_\tau \beta_k(\tau) \beta_k^\dagger(0)\rangle_{\text{mf}}. \quad (3.3)$$

Since it does not depend on $\boldsymbol{k}$, we denote it as $D(\tau)$. Its Fourier transform is

$$D(\mathrm{i}\nu) = 1/(\mathrm{i}\nu - \lambda) \quad (3.4)$$

where ν is the even Matsubara frequency.

The mean-field propagators G_f, G_c and A in this section are derived from equation (2.6), if r_{mf} and λ_{mf} are replaced by r and λ, respectively. They are diagrammatically represented in figure 1, together with $D(\mathrm{i}\nu)$.

The general formula for the free energy is

$$F = -T \log[\![\text{Tr}\{\exp[-(1/T)(\mathcal{H}_{\text{mf}} + \mathcal{H}_{\text{int}})]\}]\!]. \quad (3.5)$$

The explicit r-derivative of equation (3.5) gives the minimisation condition of the free energy:

$$\frac{\partial F}{\partial r} = V \sum_{im} \langle f_{im}^\dagger c_{im} + c_{im}^\dagger f_{im}\rangle + \lambda\sqrt{N}\langle \beta_0^\dagger + \beta_0\rangle + 2r\lambda N = 0 \quad (3.6)$$

where $\langle \ldots \rangle$ denotes the thermal average. In order to overcome the Bose condensation of the fluctuation, the condition

$$\langle \beta_0^\dagger \rangle = \langle \beta_0 \rangle = 0 \quad (3.7)$$

is needed. Then the general expression of the self-consistency equation turns out to be

$$N_d V \frac{T}{N} \sum_{\omega k} \bar{A}(\mathrm{i}\omega, \boldsymbol{k}) + r\lambda = 0 \quad (3.8)$$

where $\bar{A}(\mathrm{i}\omega, \boldsymbol{k})$ is the exactly perturbed propagator of $A(\mathrm{i}\omega, \boldsymbol{k})$.

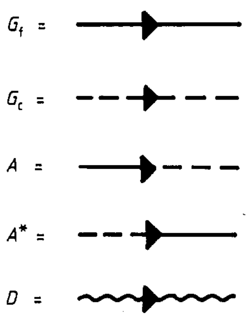

Figure 1. Diagrammatic representations of propagators: ——, f-electron propagator; – – –, conduction electron propagator; ∿∿∿, β-boson propagator. The line of the anomalous propagator A is composed of f-electron and conduction electron lines.

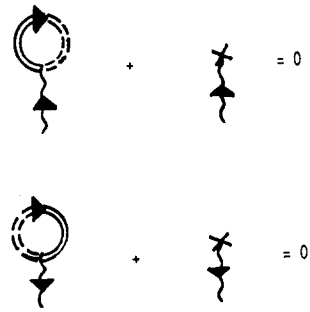

Figure 2. Diagrammatic expression of the general self-consistency condition. The double lines denote the exactly perturbed propagator $\bar{A}$ $(\mathrm{i}\omega, \boldsymbol{k})$.

The meaning of the self-consistency equation (3.8) is that the spontaneous creation and annihilation processes of zero-momentum β-bosons cancel with the vacuum fluctuation processes of electrons. The situation is illustrated in figure 2. The cross in the diagram means the last term of equation (3.2*c*). We must not include these processes in the diagrams in order to construct a consistent theory.

In this section, we regard $V^2/D\lambda$ as the small expansion parameter, and the self-energy parts of electrons and β-bosons are calculated up to the second order in $\mathcal{H}_{\mathrm{int}}$, since $D(\mathrm{i}\nu)$ has a denominator which involves a large λ: $\lambda \sim E_f \gg T_K$. Note that $V^2/D\lambda \sim J\rho$, where the Coqblin–Schrieffer coupling J has a magnitude of $J \sim V^2/E_f$. Usually, the $1/N_d$-expansion method has been used to take the fluctuation into account. However, it is known that interaction terms which do not obey the rule of the $1/N_d$-expansion method may give rise to important contributions in some cases. For example, some workers [16, 17] have considered possible ordered states in the coherent Kondo state without the $1/N_d$-rule. They may also affect the mean-field parameters quantitatively. In this section, we examine the applicability of the mean-field theory by including all the second-order interaction effects.

The second-order self-energy parts of electrons are given in the matrix form

$$\boldsymbol{\Sigma}(\mathrm{i}\omega) = \begin{bmatrix} \Sigma_f(\mathrm{i}\omega) & 0 \\ 0 & \Sigma_c(\mathrm{i}\omega) \end{bmatrix} \tag{3.9}$$

where

$$\Sigma_f(\mathrm{i}\omega) = -V^2 \frac{T}{N} \sum_{\nu \boldsymbol{q}} G_c(\mathrm{i}\omega - \mathrm{i}\nu, \boldsymbol{q}) D(\mathrm{i}\nu) = \frac{V^2}{2D} \sum_{\sigma=\pm} \int_{E_\sigma(\mathrm{bot})}^{E_\sigma(\mathrm{top})} \mathrm{d}E_\sigma(\boldsymbol{q}) \frac{n(\lambda) + f(-E_\sigma(\boldsymbol{q}))}{\mathrm{i}\omega - \lambda - E_\sigma(\boldsymbol{q})} \tag{3.10a}$$

$$\Sigma_c(\mathrm{i}\omega) = -V^2 \frac{T}{N} \sum_{\nu \boldsymbol{q}} G_f(\mathrm{i}\omega + \mathrm{i}\nu, \boldsymbol{q}) D(\mathrm{i}\nu) = \frac{V^2}{2D} \sum_{\sigma=\pm} \int_{E_\sigma(\mathrm{bot})}^{E_\sigma(\mathrm{top})} \mathrm{d}E_\sigma(\boldsymbol{q}) \frac{r^2 V^2}{[E_\sigma(\boldsymbol{q}) - \tilde{E}_f]^2} \frac{n(\lambda) + f(E_\sigma(\boldsymbol{q}))}{\mathrm{i}\omega + \lambda - E_\sigma(\boldsymbol{q})} \tag{3.10b}$$

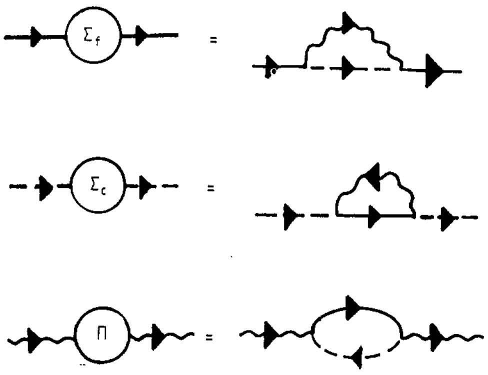

Figure 3. The self-energy parts of the second-order fluctuation.

$E_\sigma(\text{top}) = E_\sigma(\varepsilon_k = D)$, $E_\sigma(\text{bot}) = E_\sigma(\varepsilon_k = -D)$, $f(x) = 1/[\exp(x/T)+1]$ and $n(x) = 1/[\exp(x/T)-1]$. The diagrammatic representations are shown in figure 3.

The perturbed propagator $\tilde{\mathbf{G}}$ satisfies the Dyson equation

$$\tilde{\mathbf{G}}(\mathrm{i}\omega, \boldsymbol{k}) = \mathbf{G}(\mathrm{i}\omega, \boldsymbol{k}) + \mathbf{G}(\mathrm{i}\omega, \boldsymbol{k})\boldsymbol{\Sigma}(\mathrm{i}\omega, \boldsymbol{k})\tilde{\mathbf{G}}(\mathrm{i}\omega, \boldsymbol{k}). \tag{3.11}$$

The solution is

$$\tilde{\mathbf{G}}^{-1}(\mathrm{i}\omega, \boldsymbol{k}) = \begin{bmatrix} \mathrm{i}\omega - \tilde{E}_\mathrm{f} - \Sigma_\mathrm{f} & -rV \\ -rV & \mathrm{i}\omega - \varepsilon_k - \Sigma_\mathrm{c} \end{bmatrix}. \tag{3.12}$$

We give the β-boson's self-energy part $\Pi(\mathrm{i}\nu, \boldsymbol{k})$ in figure 3. It is explicitly written

$$\begin{aligned}\Pi(\mathrm{i}\nu, \boldsymbol{k}) &= N_\mathrm{d} V^2 \frac{T}{N} \sum_{\omega \boldsymbol{q}} G_\mathrm{f}(\mathrm{i}\omega + \mathrm{i}\nu, \boldsymbol{k}+\boldsymbol{q}) G_\mathrm{c}(\mathrm{i}\omega, \boldsymbol{q}) \\ &= \frac{N_\mathrm{d} V^2}{2D} \sum_{\sigma,\tau=\pm} \int_{E_\sigma(\text{bot})}^{E_\sigma(\text{top})} \mathrm{d}E_\sigma(\boldsymbol{q}) \frac{r^2 V^2}{[\tilde{E}_\mathrm{f} - E_\tau(\boldsymbol{k}+\boldsymbol{q})]^2 + r^2 V^2} \\ &\quad \times \frac{f(E_\sigma(\boldsymbol{q})) - f(E_\tau(\boldsymbol{k}+\boldsymbol{q}))}{\mathrm{i}\nu + E_\sigma(\boldsymbol{q}) - E_\tau(\boldsymbol{k}+\boldsymbol{q})}.\end{aligned} \tag{3.13}$$

The perturbed propagator becomes

$$D(\mathrm{i}\nu, \boldsymbol{k}) = 1/[\mathrm{i}\nu - \lambda - \Pi(\mathrm{i}\nu, \boldsymbol{k})]. \tag{3.14}$$

The self-consistency equation within the second-order perturbation is obtained by setting $\bar{A} = \tilde{A}$ in equation (3.8). It has the form

$$N_\mathrm{d} V \frac{T}{N} \sum_{\omega k} \frac{rV}{[\mathrm{i}\omega - \tilde{E}_\mathrm{f} - \Sigma_\mathrm{f}(\mathrm{i}\omega)][\mathrm{i}\omega - \varepsilon_k - \Sigma_\mathrm{c}(\mathrm{i}\omega)] - r^2 V^2} + r\lambda = 0. \tag{3.15}$$

The explicit λ-derivative of equation (3.5) gives the constraint

$$\frac{\partial F}{\partial \lambda} = \sum_{im} \langle f_{im}^\dagger f_{im} \rangle + \sum_k \langle \beta_k^\dagger \beta_k \rangle + r\sqrt{N} \langle \beta_0^\dagger + \beta_0 \rangle + N(r^2 - 1) = 0. \tag{3.16}$$

Taking into account condition (3.7) and including the second-order self-energy parts, we obtain

$$N_\mathrm{d} \frac{T}{N} \sum_{\omega k} \tilde{G}_\mathrm{f}(\mathrm{i}\omega, \boldsymbol{k}) - \frac{T}{N} \sum_{\nu k} \tilde{D}(\mathrm{i}\nu, \boldsymbol{k}) + r^2 = 1. \tag{3.17}$$

For simplicity, we perform the static approximation for the self-energy parts. Also, possible imaginary parts due to the interactions are not considered. This is sufficient for the aim of this paper; we discuss the low-temperature properties of the heavy Fermi liquid by the mean-field theory.

A new dispersion relation of the electrons is obtained from $\det[\tilde{\mathbf{G}}^{-1}(E^*(\boldsymbol{k}), \boldsymbol{k})] = 0$ to be

$$E^*_{\pm}(\boldsymbol{k}) = \tfrac{1}{2}(\varepsilon_k + \Sigma_c(0) + \tilde{E}_f + \Sigma_f(0) \pm \sqrt{[\varepsilon_k + \Sigma_c(0) - \tilde{E}_f - \Sigma_f(0)]^2 + 4r^2V^2}). \tag{3.18}$$

We derive a new expression for the transition temperature T_c. At $T = T_c$, the self-energy parts have simpler forms:

$$\Sigma_f(\mathrm{i}\omega) = \frac{V^2}{2D}\int_{-D}^{D} \mathrm{d}\varepsilon_q \frac{n_c(\lambda) + f_c(-\varepsilon_q)}{\mathrm{i}\omega - \lambda - \varepsilon_q} \tag{3.19a}$$

and

$$\Sigma_c(\mathrm{i}\omega) = V^2[n_c(\lambda) + f_c(\tilde{E}_f)]/(\mathrm{i}\omega + \lambda - \tilde{E}_f) \tag{3.19b}$$

where $f_c(x) = 1/[\exp(x/T_c) + 1]$ and $n_c(x) = 1/[\exp(x/T_c) - 1]$. The quantity $n_c(\lambda)$ is exponentially small since $\lambda \sim E_f$. We can neglect $n_c(\lambda)$. In equation (3.19*a*), the denominator in the integrand varies weakly around the Fermi level. We can evaluate this integration at $T = 0$. In the static approximation, we obtain

$$\Sigma_f(0) = (V^2/2D)\log[\lambda/(D + \lambda)] \tag{3.20a}$$

and

$$\Sigma_c(0) = V^2 f_c(\tilde{E}_f)/(\lambda - \tilde{E}_f). \tag{3.20b}$$

The constraint (3.17) becomes $n_f + n_c[\lambda + \Pi(0, k_F)] = 1$, where $n_f = N_d f_c[\tilde{E}_f + \Sigma_f(0)]$. The number $n_c(\lambda + \Pi)$ of β-bosons is exponentially small. We neglect this term hereafter. Then, we obtain

$$\tilde{E}_f + \Sigma_f(0) = T_c \log(N_d - 1). \tag{3.21}$$

Comparing equation (3.21) with equation (2.12), it is found that λ is changed by the value of the magnitude $-\Sigma_f(0)$.

We write the self-consistency equation (3.15) in the form

$$\frac{N_d V^2}{2D\lambda}\int_{-D}^{D} \mathrm{d}\varepsilon_k \frac{f_c(\varepsilon_k + \Sigma_c) - f_c(\tilde{E}_f + \Sigma_f)}{\varepsilon_k - \tilde{E}_f - \Sigma_f(0) + \Sigma_c(0)} + 1 = 0. \tag{3.22}$$

Performing the integral as in section 2 and using the relation (3.21), we obtain

$$\begin{aligned} T_c = {} & [2\gamma(N_d)/\pi]\sqrt{D^2 - [\tilde{E}_f + \Sigma_f(0) - \Sigma_c(0)]^2} \\ & \times \{[D + \tilde{E}_f + \Sigma_f(0) - \Sigma_c(0)]/[D - \tilde{E}_f - \Sigma_f(0) + \Sigma_c(0)]\}^{(N_d-2)/2N_d} \\ & \times \exp[-(2D/N_d V^2)(E_f + \tilde{E}_f)]. \end{aligned} \tag{3.23}$$

After the second iteration process, we get

$$T_c = [2\gamma(N_d)/\pi]\kappa T_K (N_d - 1)^{-4\gamma(N_d)D\kappa T_K/\pi N_d V^2} \tag{3.24}$$

where

$$\kappa = \exp[2D\Sigma_f(0)/N_d V^2] \tag{3.25}$$

and small terms of the order of $\tilde{E}_f/D$, $\Sigma_f(0)/D$ and $\Sigma_c(0)/D$ in the coefficient of κT_K are neglected. The magnitude of κ is evaluated with the help of equations (3.20a) and (3.21) to be

$$\kappa \simeq [E_f/(D+E_f)]^{1/N_d}. \tag{3.26}$$

Then, we find that

$$T_c/T_c^{mf} \simeq \kappa(N_d-1)^{-4\gamma(N_d)D(\kappa-1)T_K/\pi N_d V^2}. \tag{3.27}$$

The transition temperature decreases at least by the factor κ. We shall regard this factor κ as the measure of applicability of the mean-field approximation.

Next, we derive the values of parameters at $T=0$. The constraint (3.17) becomes $n_f + r^2 = 1$, since $n(\lambda+\Pi)=0$. Equation (3.15) becomes

$$\frac{N_d V^2}{2D\lambda}\int_{E^*_-(\text{bot})}^{0} dE^*_-(q)\frac{1}{\tilde{E}_f+\Sigma_f(0)-E^*_-(q)}=1 \tag{3.28}$$

where

$$E^*_-(\text{bot}) = E^*_-(k)|_{\varepsilon_k=-D}$$
$$\simeq -D+\Sigma_c(0)+(1-n_f)\{-V^2/D+[\tilde{E}_f+\Sigma_f(0)-\Sigma_c(0)]V^2/D^2\}. \tag{3.29}$$

Equation (3.28) is transformed into

$$E_f^* = [D+E_f^*-\Sigma_c(0)+(1-n_f)(V^2/D-E_f^*V^2/D^2)]$$
$$\times \exp\{-2D[E_f+E_f^*-\Sigma_f(0)]/N_dV^2\} \tag{3.30}$$

where $E_f^* = \tilde{E}_f + \Sigma_f(0)$. We perform the iterations twice and obtain

$$E_f^* = \kappa T_K[1+T_K/D-(2DT_K/N_dV^2)\kappa]$$
$$+(1-n_f)(V^2T_K/D^2)\kappa[1+O(T_K/D)+O(2DT_K/N_dV^2)]. \tag{3.31}$$

The quantity $\Sigma_c(0)$ mainly contributes to the higher-order terms in the term $1+O(T_K/D)+O(2DT_K/N_dV^2)$ in equation (3.31). From equation (3.31), the parameter λ is evaluated as

$$\lambda \simeq E_f - \Sigma_f(0) + \kappa T_K. \tag{3.32}$$

The coefficient κ has the magnitude

$$\kappa \sim [E_f/(D+E_f)]^{1/N_d} \tag{3.33}$$

at $T=0$, too. This can be estimated from the expression

$$\Sigma_f(0) = -(V^2/2D)\log\{[E_+(\text{top})+\lambda][E_-(\text{top})+\lambda]/[E_+(\text{bot})+\lambda]\lambda\} \tag{3.34}$$

with the dominant term approximation, $E_+(\text{top}) \sim D$, $E_+(\text{bot}) \sim \tilde{E}_f + r^2V^2/D$ and $E_-(\text{top}) \sim \tilde{E}_f - r^2V^2/D$. The magnitude of λ changes at least by the self-energy part $\Sigma_f(0)$.

The value of r is obtained from the constraint

$$n_f = 1-r^2 = \frac{N_d}{2D}\int_{E^*_-(\text{bot})}^{0} dE^*_-(k)\frac{r^2V^2}{[\tilde{E}_f+\Sigma_f(0)-E^*_-(k)]^2}. \tag{3.35}$$

The calculation is parallel to that in section 2. The result is

$$r^2 = 1-n_f = (2DT_K/N_dV^2)\kappa[1+(\kappa+1)T_K/D-(4DT_K/N_dV^2)\kappa]. \tag{3.36}$$

Then, from equations (2.25) and (3.36) we obtain

$$r^2/r^2_{mf} \sim \kappa. \tag{3.37}$$

This means that the value of the order parameter r is decreased by the factor $\sqrt{\kappa}$.

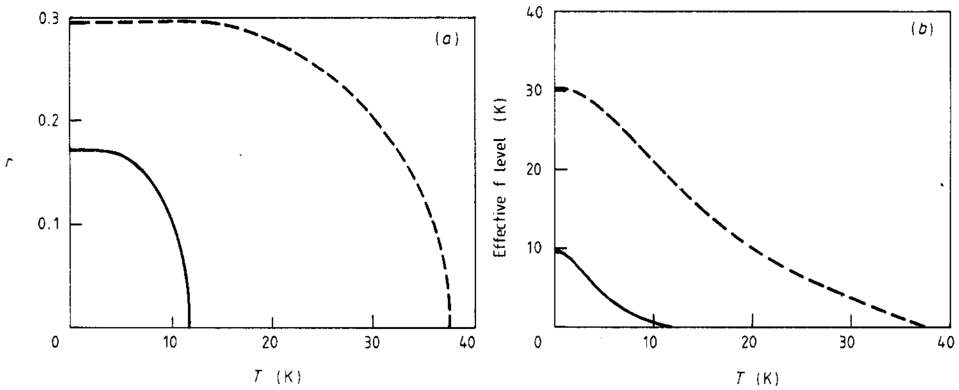

Figure 4. Numerical results for the parameters: (*a*) the mean-field *r*; (*b*) the effective f level ($\tilde{E}_f$ in the mean-field theory and $\tilde{E}_f + \Sigma_f$ in section 3) (the parameters are $N_d = 2$, $D = 2 \times 10^4$ K, $V = 2500$ K and $E_f = 2000$ K): ---, results of the mean field theory; ——, solutions of equations (3.15) and (3.17).

The number of conduction electrons is

$$n_c = (N_d/2)[0 - E_-^*(\text{bot})]$$
$$\simeq N_d/2\{1 - \Sigma_c(0)/D + (2T_K/N_dD)\kappa[1 - (4DT_K/N_dV^2)\kappa]\} \qquad (3.38)$$

where $\Sigma_c(0)$ is explicitly given by

$$\Sigma_c(0) = (r^2V^4/2D)\{E_-(\text{bot})/\tilde{E}_f(\tilde{E}_f - \lambda)[\tilde{E}_f - E_-(\text{bot})]$$
$$+ [1/(\tilde{E}_f - \lambda)^2] \log|\lambda[\tilde{E}_f - E_-(\text{bot})]/\tilde{E}_f[\lambda - E_-(\text{bot})]|\}. \qquad (3.39)$$

We find that n_c is mainly changed by the quantity $-N_d\Sigma_c/2D$, and T_K in equation (2.27) changes into κT_K.

We evaluate the effective mass at the Fermi level, as in equation (2.28), to find

$$m^*/m = 1 + r^2V^2/[\tilde{E}_f + \Sigma_f(0)]^2 \sim (2D/N_dT_K)(1/\kappa). \qquad (3.40)$$

The ratio is larger than that in the mean-field theory. The heavy quasi-particles have a weaker itinerancy character. Since T_c is decreased, the temperature range of the ordered phase is reduced and f electrons have a stronger localisation character at $T = 0$.

In order to confirm the above estimations, we numerically solve the self-consistency condition (3.15) and the constraint (3.17) and compare the solutions with those of the mean-field theory in figure 4. The parameters are $N_d = 2$, $D = 2 \times 10^4$ K, $V = 2500$ K and $E_f = 2000$ K. Usually, the magnitude $E_f \sim D$ is assumed. We, however, take that value in order to see fluctuation effects clearly. We obtain $T_c^{\text{mf}} = 37.6$ K and $T_c = 11.7$ K. Then the numerical estimation for κ is $11.7/37.6 = 0.311$. The theoretical first-order estimation is $[E_f/(D + E_f)]^{1/2} = 0.302$. Two values agree remarkably. Also, we numerically confirm the theory from the points that *r* is decreased by the factor $\sqrt{\kappa}$ and that the effective f level $\tilde{E}_f + \Sigma_f$ has the value $\kappa(-E_f + \lambda_{\text{mf}})$ at $T = 0$ K.

4. Summary and discussion

The second-order perturbation due to the fluctuation has been found to decrease the transition temperature by the factor $\kappa \sim [E_f/(D + E_f)]^{1/N_d}$ from its value of the mean-field theory. The values of the mean field *r* and the effective f level, at $T = 0$, decrease by the factors $\sqrt{\kappa}$ and κ, respectively. Also, we have found that the effective mass of quasi-particles at $T = 0$ increases by the factor κ^{-1}. These results imply that the mean-field ground state is more or less affected by the fluctuation. The effects of the fluctuation appear more strongly for the system with smaller N_d.

It is also shown that T_c does not change so drastically in the system with larger N_d. In particular, $\kappa \to 1$ as $N_d \to \infty$. This coincides with the usual assumption that the mean-field theory is a good starting point when the fluctuation is treated making use of the $1/N_d$-expansion method [12].

The factor κ, which is the measure of the applicability, also depends on the parameter E_f. In the limit $n_f \to 1$, the quantity r approaches zero, i.e. $T_K \to 0$. This implies that the atomic f level $-E_f$ becomes deep enough. (E_f is comparable with D.) Thus the factor κ is not very small. This confirms the assumption that the mean-field theory would be a good first approximation if the system is in the Kondo limit. However, as n_f becomes much smaller than unity, the value of E_f decreases and κ becomes very small. Thus the mean-field solution is more unreliable as the occupancy of the f state decreases. It would be desirable to find a new method which does not depend on the mean-field theory, even using the slave boson method, for these situations.

We have considered fluctuation effects by the second-order perturbation method. Higher-order interaction effects can be taken into account by a self-consistent renormalisation method. We believe that the results do not change qualitatively if the quantity $J\rho$ can be regarded as sufficiently small.

For real Ce compounds, $N_d = 14$ when all the 4f orbitals are degenerate, and $N_d =$ 6 or 8 when there are spin–orbit interactions. The value of N_d is smaller if the crystalline-field splitting is effective at low temperatures. Usually, an N_d-value of 2 or 4 is assumed in the coherent Kondo state, and the Kondo limit $E_f \sim D$ is taken. It would be dangerous to consider that the factor κ is very close to unity. It might be necessary to apply another method in this situation.

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Appendix: definition of the mean field

In this appendix, we describe the definition of the mean-field ground state and the thermal average for the slave boson and the β-boson in detail.

A1. Ground state

The coherent state for the slave boson b_i is

$$|r\rangle = \exp\left(-\frac{r^2}{2}\right) \sum_{n=0}^{\infty} \frac{r^n}{n!} (b_i^\dagger)^n \,|0\rangle = \exp\left(-\frac{r^2}{2}\right) \exp(r b_i^\dagger)\,|0\rangle \qquad \text{(A1.1)}$$

where r is a positive real number. Since $|r\rangle$ has the properties $b_i|r\rangle = r|r\rangle$ and

$b_i^\dagger b_i|r\rangle = r^2|r\rangle$, we obtain

$$\langle r|b_i^\dagger b_i|r\rangle = r^2 \quad (\text{A1.2}a)$$

$$\langle r|b_i|r\rangle = \langle r|b_i^\dagger|r\rangle = r. \quad (\text{A1.2}b)$$

With these relations, the mean-field ground state is defined as $|r\rangle$ for all the lattice site i.

The β-boson $\beta_i = b_i - r$ has the properties

$$\beta_i|r\rangle = (b_i - r)|r\rangle = 0 \quad (\text{A1.3}a)$$

$$(\beta_i^\dagger\beta_i)(1/\sqrt{n!})(\beta_i^\dagger)^n|r\rangle = n(1/\sqrt{n!})(\beta_i^\dagger)^n|r\rangle. \quad (\text{A1.3}b)$$

Then, $|r\rangle$ is the vacuum state for the β-boson and off-diagonal matrix elements vanish in the Fock space spanned by $\Pi_i\ (\beta_i^\dagger)^{n_i}/\sqrt{n_i!}\ |r\rangle (n_i = 0, 1, 2, \ldots)$.

We consider the Hamiltonian

$$\mathcal{H} = \lambda \sum_i \beta_i^\dagger\beta_i. \quad (\text{A1.4})$$

To derive perturbative corrections to the mean-field theory, it is reasonable to define the β-boson propagator in the form

$$D(t, \boldsymbol{k}) = -\mathrm{i}\langle r|T\beta_{\boldsymbol{k}}(t)\beta_{\boldsymbol{k}}^\dagger(0)\,|r\rangle. \quad (\text{A1.5})$$

Using the Hamiltonian (A1.4), we derive the Fourier transform of equation (A1.5) to obtain

$$D(\nu, \boldsymbol{k}) = 1/(\nu - \lambda + \mathrm{i}\delta). \quad (\text{A1.6})$$

A2. Finite temperatures

We denote the thermal average over the states $\Pi_i\ (\beta_i^\dagger)^n i/\sqrt{n_i!}\ |r\rangle\ (n_i = 0, 1, 2, \ldots)$ as $\langle\ \rangle_{\mathrm{mf}}$. Then, we get

$$\langle\beta_i^\dagger\beta_i\rangle_{\mathrm{mf}} = \mathrm{Tr}[\beta_i^\dagger\beta_i \exp(-\mathcal{H}/T)]/\mathrm{Tr}[\exp(-\mathcal{H}/T)] = 1/[\exp(\lambda/T) - 1] \quad (\text{A2.1}a)$$

$$\langle\beta_i\rangle_{\mathrm{mf}} = \langle\beta_i^\dagger\rangle_{\mathrm{mf}} = 0 \quad (\text{A2.1}b)$$

where $\mathcal{H}$ is the Hamiltonian (A1.4). Also, we obtain

$$\langle b_i^\dagger b_i\rangle_{\mathrm{mf}} = r^2 + \langle\beta_i^\dagger\beta_i\rangle_{\mathrm{mf}} \quad (\text{A2.2}a)$$

$$\langle b_i\rangle_{\mathrm{mf}} = \langle b_i^\dagger\rangle_{\mathrm{mf}} = r. \quad (\text{A2.2}b)$$

The corresponding definition of the propagator in equation (A1.5) is

$$D(\tau, \boldsymbol{k}) = -\langle T_\tau\beta_{\boldsymbol{k}}(\tau)\beta_{\boldsymbol{k}}^\dagger(0)\rangle_{\mathrm{mf}}. \quad (\text{A2.3})$$

Its Fourier transform is

$$D(\mathrm{i}\nu, \boldsymbol{k}) = 1/(i\nu - \lambda) \quad (\text{A2.4})$$

where ν is the even Matsubara frequency. This form has been used in the text.

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