

# Superconductivity from magnetic order for Van Vleck metals

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For Van Vleck metals such as Pr, it is shown in a previous paper that the indirect electron-electron interaction  $V$ , mediated by the virtual excitation of the crystal field singlet ground state through the  $s$ - $f$  exchange interaction, can give rise to superconductivity. With increase of the  $s$ - $f$  exchange interaction or the Van Vleck susceptibility,  $V$  increases and makes the superconducting transition temperature  $T_c$  increase. Conversely, when  $V$  is beyond the critical value  $V_M$ , magnetic order appears at a finite temperature  $T_M$ . In this case, a problem arises in whether  $T_c$  lies above or below  $T_M$ . This paper shows that, except for the very vicinity of  $V_M$ , the superconductivity appears below  $T_M$  contrary to the conclusion of the BCS approximation. This is due to the depairing effect by the scattering of the conduction electrons accompanied by the excitation of the singlet ground state. The phase diagram is obtained by assuming the free electron band and the orthorhombic crystal field. [S0163-1829(97)02801-4]

## I. INTRODUCTION

For non-Kramers ions such as Pr, the crystal field (CF) leads to a singlet ground state by lifting the  $(2J+1)$ -fold degeneracy of the ground multiplet. A process, in which one electron virtually excites this CF singlet ground state through the  $s$ - $f$  exchange interaction and the other electron turns it back, brings an effective interaction  $V$  between these two conduction electrons.<sup>1</sup>  $V$  is proportional to the square of the  $s$ - $f$  exchange interaction and the Van Vleck susceptibility, and acts as a repulsive short-range interaction near the Fermi surface. Furthermore, two electrons distant from each other also interact indirectly through the conduction electron spin fluctuation. This indirect interaction, which is denoted as  $\tilde{V}$ , is represented by the random-phase-approximation (RPA) susceptibility for  $f$  electrons. Some components of its partial wave expansion turn attractive.

Following the spin-fluctuation-mediated pairing theory for liquid <sup>3</sup>He, heavy fermion systems and high- $T_c$  superconductors,<sup>2-7</sup> we have proposed a pairing mechanism due to this interaction.<sup>8</sup> Recently we have shown by solving the Eliashberg equations in Ref. 9, which is hereafter referred to as [I], that the superconductivity by the present mechanism can still survive in the presence of the depairing effect, although  $T_c$  is strongly reduced. This depairing effect is mainly due to the mass enhancement of the conduction electrons which is also induced by the virtual excitation of the CF singlet ground state.

With increase of the  $s$ - $f$  exchange interaction or decrease of the CF splitting, the bare effective interaction  $V$  becomes strong. When  $V$  increases beyond the critical value  $V_M$ ,  $\tilde{V}$  diverges at a finite temperature  $T_M$  to induce the magnetic order. In this situation, a problem arises concerning the coexistence or competition of the superconductivity with the magnetic order. Especially, when  $T$  approaches  $T_M$  from above,  $\tilde{V}$  increases and it seems that the superconductivity is induced at a finite temperature  $T_c$  which lies above  $T_M$ . Pr metal and its metallic compounds show magnetic order. It is due to the moment induced from the CF singlet ground state or sometimes substantially by the nuclear spins. For ex-

ample, Pr<sub>3</sub>Tl turns ferromagnetic at 11 K,<sup>10</sup> Pr metal turns antiferromagnetic at 60 mK,<sup>11</sup> and PrNi<sub>5</sub> shows a ferromagnetic order at 0.4 mK.<sup>12</sup> These latter two are mainly by the nuclear spins. However, we have no examples of superconductors with  $T_c$  above  $T_M$ . To clarify this discrepancy of the expectation with the behavior of the real substances and to obtain the correct superconducting transition temperature  $T_c$  in the presence of the magnetic order are the purposes of the present paper.

To this end, in place of treating the realistic system, we assume for simplicity in this paper the free electron band for the conduction electrons, for which ferromagnetic order may appear. By extending the theory in [I], we calculate  $T_c$  in the case where ferromagnetic order occurs. In Sec. II, we calculate  $T_M$  and the magnetization of the  $f$  electron system in the mean-field approximation. Then, we derive the RPA susceptibility for  $f$  electrons in the presence of the magnetic order. In Sec. III, we set up the Eliashberg equations in the presence of the magnetic order. In Sec. IV, on the basis of them, we investigate  $T_c$ . It is shown that except for the very vicinity of  $V_M$ ,  $T_c$  does appear not above but below  $T_M$ . Conclusion and discussion are given in the last section.

## II. MAGNETIC ORDERING TEMPERATURE AND MAGNETIZATION

We describe the system by the Hamiltonian,

$$\begin{aligned}
 H = & \sum_{\mathbf{k}, \alpha} \varepsilon_{\mathbf{k}} a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} \\
 & + \sum_{i,n} E_n |i,n\rangle \langle i,n| - \frac{\tilde{J}}{2N} \sum_i \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} \\
 & \times \sum_{\alpha, \alpha'} a_{\mathbf{k}'\alpha'}^\dagger \boldsymbol{\sigma}_{\alpha'\alpha} \cdot \mathbf{J}_i a_{\mathbf{k}\alpha}, \quad (1)
 \end{aligned}$$

where  $|i,n\rangle$  represents the  $n$ th crystalline field state at site  $i$  with energy  $E_n$ .  $\tilde{J}$  is the  $s$ - $f$  exchange coupling constant

multiplied by  $(g_J - 1)$ .  $\mathbf{J}_i$  is the total angular momentum of the ground multiplet at the  $i$ th site.

To focus ourselves to the problem concerning the relation between the superconductivity and the magnetic order, we simplify real systems by assuming the free electron band for the conduction electrons and the orthorhombic CF expressed as

$$\sum_{i,n} E_n |i,n\rangle \langle i,n| = \sum_i [DJ_{ix}^2 + dJ_{iy}^2], \quad (2)$$

with  $J=1$  and  $D > d > 0$ .

Under these assumptions, ferromagnetic order can occur in parallel with the  $z$  axis. In the presence of the ferromagnetic order the internal field appears, so that the vector potential should be introduced. However, we neglect for simplicity the terms involving the vector potential which is related to the effect of the orbital motion. Therefore, we limit ourselves to the effect of the magnetic order which appears in the spins. Then, the mean-field Hamiltonian is written as

$$\begin{aligned} H_0^{\text{MF}} &= H_c^{\text{MF}} + V^{\text{MF}}, \\ H_0^{\text{MF}} &= H_c^{\text{MF}} + H_{\text{crystal}}^{\text{MF}} = \sum_{\mathbf{k},\alpha} \bar{\varepsilon}_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} \\ &+ \sum_i \left[ DJ_{ix}^2 + dJ_{iy}^2 - \frac{\tilde{J}}{2} \langle \sigma_z \rangle J_{iz} \right], \\ V^{\text{MF}} &= -\frac{\tilde{J}}{2} \sum_i \left[ \frac{1}{2} (\sigma_{i+} J_{i-} + \sigma_{i-} J_{i+}) \right. \\ &\left. + (\sigma_{iz} - \langle \sigma_z \rangle) (J_{iz} - \langle J_z \rangle) \right], \quad (3) \end{aligned}$$

where

$$\begin{aligned} \bar{\varepsilon}_{\mathbf{k}\alpha} &= \varepsilon_{\mathbf{k}} \mp \frac{\tilde{J}}{2} \langle J_z \rangle, \\ \sigma_{iz} &= \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} [a_{\mathbf{k}'\uparrow}^\dagger a_{\mathbf{k}\uparrow} - a_{\mathbf{k}'\downarrow}^\dagger a_{\mathbf{k}\downarrow}], \\ \sigma_{i\pm} &= \frac{2}{N} \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} a_{\mathbf{k}'\alpha}^\dagger a_{\mathbf{k}-\alpha}, \\ J_\pm &= J_x \pm iJ_y. \quad (4) \end{aligned}$$

In the expressions for  $\bar{\varepsilon}$  and  $\sigma_{i\pm}$  in (4), the upper and lower signs are chosen when  $\alpha$  expresses the up and down spin states, respectively. For the ferromagnetic order,  $\langle \sigma_z \rangle$  and  $\langle J_z \rangle$  are independent of the site  $i$ . The constant term has been neglected in (3).

From this mean-field Hamiltonian (3), we derive the equation for  $\langle \sigma_z \rangle$ ,

$$\begin{aligned} \langle \sigma_{iz} \rangle &= \langle \sigma_z \rangle \equiv \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_i} \langle a_{\mathbf{k}'\uparrow}^\dagger a_{\mathbf{k}\uparrow} - a_{\mathbf{k}'\downarrow}^\dagger a_{\mathbf{k}\downarrow} \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k}} [f(\bar{\varepsilon}_{\mathbf{k}\uparrow}) - f(\bar{\varepsilon}_{\mathbf{k}\downarrow})] \\ &= \frac{\tilde{J} \langle J_z \rangle}{N} \sum_{\mathbf{k}} \frac{f(\bar{\varepsilon}_{\mathbf{k}\uparrow}) - f(\bar{\varepsilon}_{\mathbf{k}\downarrow})}{\bar{\varepsilon}_{\mathbf{k}\downarrow} - \bar{\varepsilon}_{\mathbf{k}\uparrow}}. \quad (5) \end{aligned}$$

In the last line we have drawn the factor  $\tilde{J} \langle J_z \rangle$  by using (4). The summation appearing in (5) can be approximated as the  $q=0$  component of the paramagnetic susceptibility of the conduction electron in the unit of  $(g\mu_B)^2$ , since the correction due to  $\langle J_z \rangle$  is of the order  $\tilde{J}\rho_F \langle J_z \rangle / N \ll 1$ , where  $\rho_F$  is the density of states at the Fermi surface. Thus we write (5) as

$$\langle \sigma_{iz} \rangle = 2\tilde{J} \langle J_z \rangle \chi^c(q=0) = 2\tilde{J} \langle J_z \rangle \sum_j \chi_{ij}^c. \quad (6)$$

The equation for  $\langle J_z \rangle$  is written as

$$\begin{aligned} \langle J_z \rangle &\equiv \frac{1}{Z} \sum_{n'} e^{-\beta E_n'} \langle n' | J_z | n' \rangle \\ &= \frac{\tilde{J} \langle \sigma_z \rangle}{\sqrt{(D-d)^2 + (\tilde{J} \langle \sigma_z \rangle)^2}} \frac{e^{-\beta E_1'} - e^{-\beta E_2'}}{e^{-\beta E_1'} + e^{-\beta E_2'} + e^{-\beta E_3'}}, \quad (7) \end{aligned}$$

where  $|n'\rangle$  represents the  $n'$ th crystalline field state for  $H_{\text{crystal}}^{\text{MF}}$  in (3) and its eigenenergy  $E_n'$  is given by

$$\begin{aligned} E_1' &= \frac{1}{2} [D + d - \sqrt{(D-d)^2 + (\tilde{J} \langle \sigma_z \rangle)^2}], \\ E_2' &= \frac{1}{2} [D + d + \sqrt{(D-d)^2 + (\tilde{J} \langle \sigma_z \rangle)^2}], \\ E_3' &= D + d. \quad (8) \end{aligned}$$

Equations (6) and (7) determine  $T_M$  and the magnetization. In solving (6) and (7) we replace  $\sum_j \chi_{ij}^c$  with  $\sum_{j(\neq i)} \chi_{ij}^c$  in (6) so as to avoid the same-site contribution. This manipulation, which modifies a simple mean-field approximation, is required to guarantee the consistency with the analysis for the conduction electron susceptibility.<sup>13</sup> Akai and Ishii<sup>14</sup> calculated  $\chi_{ij}^c$  in the second order perturbation of  $\tilde{J}$  and showed that  $\chi_{ii}^{c(2)} \ll \chi_{ij}^{c(2)}$  ( $i \neq j$ ) in this order. However, in the mean-field or RPA susceptibility the same-site contribution is included as if it were given by the operation  $j \rightarrow i$  in  $\chi_{ij}^c$ . To correct this fault in RPA, the susceptibility for  $f$  electrons should be given by

$$\chi_{\mu\mu}(\mathbf{q}, \omega) = \frac{\chi_{\mu\mu}^V(\omega)}{1 - \tilde{J}^2 \chi_{\mu\mu}^V(\omega) \bar{\chi}^c(\mathbf{q})}, \quad (9)$$

with

$$\bar{\chi}^c(\mathbf{q}) = \chi^c(\mathbf{q}) - \frac{1}{N} \sum_{\mathbf{q}'} \chi^c(\mathbf{q}'), \quad (10)$$

where  $\chi_{\mu\nu}^V(\omega)$  is the Van Vleck susceptibility

$$\chi_{\mu\nu}^V(\omega+i\eta) = \frac{1}{Z} \sum_{m,n} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{E_n - E_m + \omega + i\eta} \langle n | J_\mu | m \rangle \langle m | J_\nu | n \rangle, \quad (11)$$

and  $\chi^c(\mathbf{q})$  is the conduction electron susceptibility. For the free electron band,  $\chi^c(\mathbf{q})$  is expressed as

$$\chi^c(\mathbf{q}) = \frac{\rho_F}{4N} f\left(\frac{q}{2k_F}\right), \quad (12)$$

where  $f(x)$  is the Lindhard function,

$$f(x) = 1 + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right|. \quad (13)$$

The summation in (10) is taken over the first Brillouin zone, which is approximated by the integral over the sphere with the same volume to give  $1.84(\rho_F/4N)$ .

With (10) for  $q=0$ , we calculate (6) as

$$\langle \sigma_z \rangle = 0.08 \frac{\tilde{J} \rho_F}{N} \langle J_z \rangle. \quad (14)$$

Substituting (14) into (7), we derive a self-consistent equation for  $\langle J_z \rangle$ , which is expressed as

$$\langle J_z \rangle = \frac{0.08V \langle J_z \rangle}{K} \times \frac{e^{[(1+d'-K)/2t]} - e^{-[(1+d'+K)/2t]}}{e^{-[(1+d'-K)/2t]} + e^{-[(1+d'+K)/2t]} + e^{-[(1+d')/t]}}, \quad (15)$$

where

$$K = \sqrt{(1-d')^2 + (0.08V \langle J_z \rangle)^2}, \quad (16)$$

$$t = \frac{T}{D}, \quad d' = \frac{d}{D}, \quad V = \frac{\tilde{J}^2 \rho_F}{ND}.$$

This equation has no solution for  $\langle J_z \rangle$  when  $V < V_M = 12.5(1-d')$ . When  $V > V_M$ , by solving (15) we obtain  $\langle J_z \rangle$  as a function of  $t$ . Furthermore, by linearizing (15) we can obtain  $T_M$  as a function of  $V$ . The result will be discussed in Sec. IV together with the result of  $T_c$ .

In the presence of the magnetic order, the RPA susceptibility tensor for  $f$  electrons  $\hat{\chi}$  has off-diagonal components because both the Van Vleck susceptibility tensor and the conduction electron susceptibility tensor have off-diagonal elements. Therefore, we have to modify somewhat the RPA susceptibility for  $f$  electrons in (9). Since ferromagnetic order occurs in parallel with the  $z$  axis below  $T_M$ ,  $\chi_{xy}^V$  becomes finite. On the other hand, the change of the conduction electron susceptibility by the effect of the magnetic order is small compared with the change of the Van Vleck susceptibility, so that it is neglected. Therefore, in the presence of the magnetic order we express the RPA susceptibility tensor for  $f$  electrons as

$$\hat{\chi}(\mathbf{q}, \omega) = \hat{\chi}^V(\omega) \cdot [1 - \tilde{J}^2 \hat{\chi}^V(\omega) \overline{\chi^c(\mathbf{q})}]^{-1}, \quad (17)$$

where  $\hat{\chi}^V(\omega)$  is the Van Vleck susceptibility tensor which has an  $xy$  component as well as diagonal components. The

$zz$  component is defined for  $J_z - \langle J_z \rangle$  in place of  $J_z$  in (11). The  $xy$  component of (17) is expressed as

$$\chi_{xy} = \chi_{xy}^V [(1 - \tilde{J}^2 \chi_{xx}^V \overline{\chi^c}) (1 - \tilde{J}^2 \chi_{yy}^V \overline{\chi^c}) - \tilde{J}^4 \chi_{xy}^V \chi_{yx}^V (\overline{\chi^c})^2]^{-1}. \quad (18)$$

$\hat{\chi}(0,0)$  is calculated for the present system represented by (3). Its nonvanishing elements are shown in Figs. 1(a) and 1(b) for  $d'=0.1$  and  $0.5$ , respectively. The divergence of  $\chi_{zz}$  at  $T_M$  indicates the appearance of the spontaneous magnetization parallel to the  $z$  axis. These diagonal elements decrease with increase of  $d'$ , especially below  $T_M$ . On the other hand,  $\chi_{xy}$  vanishes for  $\omega=0$ .

### III. ELIASHBERG EQUATIONS

As mentioned in the previous section, when  $V > V_M$ , magnetic order appears. On the other hand, as discussed in [I], for  $V < V_M$  superconductivity can occur at a finite  $T_c$  although magnetic order does not appear. Therefore, when  $V > V_M$ , we are very interested in the relation between superconductivity and magnetic order. We discuss the possibility of the superconductivity for this case. We start by setting up the Eliashberg equations in the presence of the magnetic order, following the theory for the superconductivity suffering the time-reversal breaking interaction<sup>15</sup> and in the magnetic materials.<sup>16-18</sup>

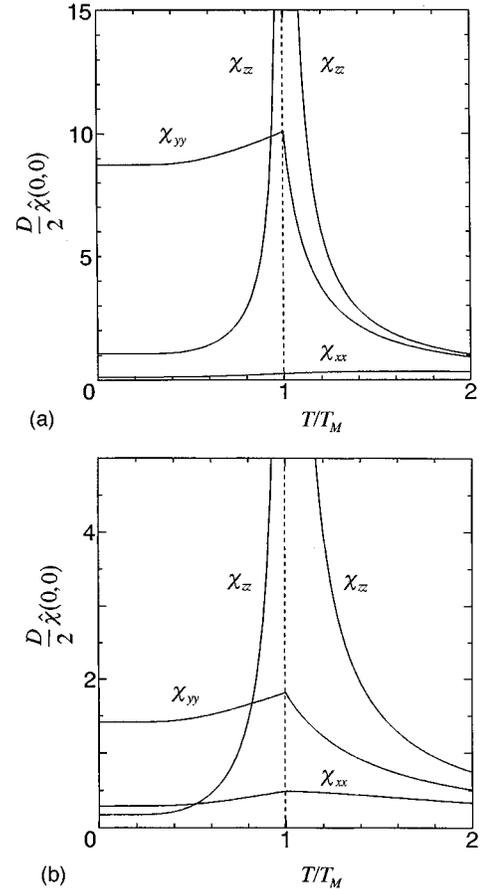


FIG. 1. Three diagonal elements of the RPA susceptibility tensor  $\hat{\chi}(0,0)$  as a function of  $T$  normalized by  $T_M$  for  $V=15$ . The results for  $d'=0.1$  and  $d'=0.5$  are shown in (a) and (b), respectively.

We introduce a four-component Nambu field and its conjugate<sup>15</sup> as

$$\hat{\psi}_{\mathbf{k}} = \begin{pmatrix} a_{\mathbf{k}\uparrow} \\ a_{\mathbf{k}\downarrow} \\ a_{-\mathbf{k}\downarrow}^\dagger \\ a_{-\mathbf{k}\uparrow}^\dagger \end{pmatrix}, \quad (19)$$

and

$$\hat{\psi}_{\mathbf{k}}^\dagger = (a_{\mathbf{k}\uparrow}^\dagger, a_{\mathbf{k}\downarrow}^\dagger, a_{-\mathbf{k}\uparrow}, a_{-\mathbf{k}\downarrow}). \quad (20)$$

The one electron Green's function in the matrix form is defined by

$$\hat{G}(\mathbf{k}, \tau) = -\langle T_\tau \hat{\psi}_{\mathbf{k}}(\tau) \hat{\psi}_{\mathbf{k}}^\dagger \rangle, \quad (21)$$

and its Fourier transform  $\hat{G}(\mathbf{k}, i\omega_n)$  is linked with the unperturbed Green's function  $\hat{G}_0(\mathbf{k}, i\omega_n)$  by the Dyson equation

$$\hat{G}^{-1}(\mathbf{k}, i\omega_n) = \hat{G}_0^{-1}(\mathbf{k}, i\omega_n) - \hat{\Sigma}(\mathbf{k}, i\omega_n), \quad (22)$$

where  $\omega_n = (2n+1)\pi/\beta$  and  $\hat{\Sigma}(\mathbf{k}, i\omega_n)$  represents the self-energy due to the  $s$ - $f$  exchange interaction.  $\hat{G}_0$  is given<sup>18</sup> by

$$\hat{G}_0^{-1}(\mathbf{k}, i\omega_n) = i\omega_n \mathbf{1} - \epsilon_{\mathbf{k}} \boldsymbol{\rho}_3 + E_z \mathbf{1} \boldsymbol{\sigma}_3, \quad (23)$$

where  $\boldsymbol{\rho}_i$  ( $i=1,2,3$ ) and  $\boldsymbol{\sigma}_i$  ( $i=1,2,3$ ) are the Pauli matrices in the electron-hole space and in the spin space, respectively. The spin-dependent mean-field energy is represented by the last term of (23), where  $E_z = (\tilde{J}/2)\langle J_z \rangle$  by (4). In [I] we have proved that the Migdal theorem holds for the present system, so that the conduction electron self-energy  $\hat{\Sigma}$  is given by the process in which two bare vertices are connected by  $\hat{G}$  and  $\hat{\chi}$  as

$$\begin{aligned} \hat{\Sigma}(\mathbf{k}, i\omega_n) &= \left(\frac{\tilde{J}}{2}\right)^2 \frac{1}{N\beta} \sum_{\mathbf{k}', n'} \sum_{\mu, \nu=x,y,z} \hat{\alpha}_\mu \hat{G}(\mathbf{k}', i\omega_{n'}) \\ &\quad \times \chi_{\mu\nu}(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'}) \hat{\alpha}_\nu, \end{aligned} \quad (24)$$

where  $\hat{\alpha}_x = \boldsymbol{\rho}_3 \boldsymbol{\sigma}_1$ ,  $\hat{\alpha}_y = \boldsymbol{\rho}_3 \boldsymbol{\sigma}_2$ , and  $\hat{\alpha}_z = \mathbf{1} \boldsymbol{\sigma}_3$ . This expression is the extension of the one given in [I] by including the off-diagonal components of the RPA susceptibility for  $f$  electrons, which appear in the presence of the magnetic order.

Next we set up the Eliashberg equations. Paying attention to the effect of the off-diagonal components of  $\hat{\chi}$  in (24), we put the self-energy in a form

$$\begin{aligned} \hat{\Sigma}(\mathbf{k}, i\omega_n) &= [1 - Z(\mathbf{k}, i\omega_n)] i\omega_n \mathbf{1} + [\tilde{\epsilon}(\mathbf{k}, \omega_n) - \epsilon_{\mathbf{k}}] \boldsymbol{\rho}_3 \\ &\quad + [E_z - \tilde{E}_z(\mathbf{k}, i\omega_n)] \mathbf{1} \boldsymbol{\sigma}_3 - Y(\mathbf{k}, i\omega_n) \boldsymbol{\rho}_3 \boldsymbol{\sigma}_3 \\ &\quad - \sum_{\gamma=s,x,y,z} \Delta_\gamma(\mathbf{k}, i\omega_n) \boldsymbol{\rho}_\gamma, \end{aligned} \quad (25)$$

where  $\boldsymbol{\rho}_\gamma$  ( $\gamma=s,x,y,z$ ) are defined as

$$\boldsymbol{\rho}_s = \boldsymbol{\rho}_1 \boldsymbol{\sigma}_3, \quad \boldsymbol{\rho}_x = -\boldsymbol{\rho}_2 \boldsymbol{\sigma}_2, \quad \boldsymbol{\rho}_y = \boldsymbol{\rho}_1 \boldsymbol{\sigma}_1, \quad \boldsymbol{\rho}_z = \boldsymbol{\rho}_1 \mathbf{1}. \quad (26)$$

The first term in the right-hand side of (25) represents the spin-independent self-energy part of the conduction electrons and the second term the correction of the energy of the conduction electrons. The third term corresponds to the correc-

tion of the Zeeman energy. The fourth term is the spin-dependent self-energy part and the last term the anomalous part of the self-energy  $\hat{\Sigma}$ . As we studied in [I], when the magnetic order is absent,  $\hat{\Sigma}$  consists of the first, second, and last terms in (25). Equation (22) with (23) and (25) turns to

$$\begin{aligned} \hat{G}^{-1}(\mathbf{k}, i\omega_n) &= i\omega_n Z(\mathbf{k}, i\omega_n) \mathbf{1} - \tilde{\epsilon}(\mathbf{k}, i\omega_n) \boldsymbol{\rho}_3 + \tilde{E}_z(\mathbf{k}, i\omega_n) \mathbf{1} \boldsymbol{\sigma}_3 \\ &\quad + Y(\mathbf{k}, i\omega_n) \boldsymbol{\rho}_3 \boldsymbol{\sigma}_3 + \sum_{\gamma=s,x,y,z} \Delta_\gamma(\mathbf{k}, i\omega_n) \boldsymbol{\rho}_\gamma. \end{aligned} \quad (27)$$

Then, it turns out that  $\hat{G}$  is spanned by the same bases as  $\hat{G}^{-1}$  in (27).

In the paramagnetic phase  $\hat{\chi}$  is diagonal. Hence, in the right-hand side of (24), the off-diagonal parts of  $\chi_{\mu\mu} \hat{\alpha}_\mu \hat{G} \hat{\alpha}_\mu$  in the  $4 \times 4$  matrix representation make the Eliashberg equations separate from each other for  $\Delta_\gamma$  ( $\gamma=s,x,y,z$ ) when (25) is inserted in the left-hand side of (24). This is the situation studied in [I]. However, in the presence of the magnetic order,  $\hat{\chi}$  turns off-diagonal and also the spin-dependent terms  $\tilde{E}_z \mathbf{1} \boldsymbol{\sigma}_3$  and  $Y \boldsymbol{\rho}_3 \boldsymbol{\sigma}_3$  appear in (25). For the present CF,  $\chi_{xy}$  mixes  $\Delta_s$  and  $\Delta_z$  in the Eliashberg equations. Furthermore, the presence of the spin-dependent terms  $\tilde{E}_z \mathbf{1} \boldsymbol{\sigma}_3$  and  $Y \boldsymbol{\rho}_3 \boldsymbol{\sigma}_3$ , although these are diagonal, connects  $\Delta_x$  with  $\Delta_y$  and also  $\Delta_s$  with  $\Delta_z$ . This is because the spin-dependent diagonal elements of  $\hat{\Sigma}$  or  $\hat{G}^{-1}$  affect the weight of the anomalous terms of  $\hat{G}$ . Then, for the set of nonvanishing  $\Delta_s$  and  $\Delta_z$ , we express the anomalous part of  $\hat{G}$  with the bases  $\boldsymbol{\rho}_s$  and  $\boldsymbol{\rho}_z$  given in (26). In the same way, for the set of nonvanishing  $\Delta_x$  and  $\Delta_y$  we extend it by  $\boldsymbol{\rho}_x$  and  $\boldsymbol{\rho}_y$ . These expressions for  $\hat{G}$  and Eq. (25) are inserted in (24) to set up the Eliashberg equations for the set of  $\Delta_x$  and  $\Delta_y$  ( $\Delta_s$  and  $\Delta_z$ ) as well as for  $Z$ ,  $\tilde{\epsilon}$ ,  $\tilde{E}_z$ , and  $Y$ . The kernels are given by the following combinations of  $\chi_{\mu\nu}$ :

$$\begin{aligned} X_s &= \chi_{xx} + \chi_{yy} + \chi_{zz}, \\ X_x &= \chi_{xx} - \chi_{yy} - \chi_{zz}, \\ X_y &= -\chi_{xx} + \chi_{yy} - \chi_{zz}, \\ X_z &= -\chi_{xx} - \chi_{yy} + \chi_{zz}, \\ X_{xy} &= i(\chi_{xy} - \chi_{yx}). \end{aligned} \quad (28)$$

To solve these Eliashberg equations, we proceed to replace the  $\mathbf{k}'$  sum by

$$\sum_{\mathbf{k}'} \rightarrow \rho_F \int \frac{d\Omega}{4\pi} \int_{-\infty}^{\infty} d\epsilon_{\mathbf{k}'}, \quad (29)$$

where  $d\Omega$  represents the differential solid angle on the Fermi surface. Then, one finds that the integration over  $\epsilon_{\mathbf{k}'}$  sweeps off all the correction represented by  $\tilde{\epsilon}(\mathbf{k}, i\omega_n)$ ,  $\tilde{E}_z(\mathbf{k}, i\omega_n)$  and  $Y(\mathbf{k}, i\omega_n)$ . Therefore, neglecting the terms disappearing by the procedure of (29), we write down the sets of Eliashberg equations: (i) for  $\Delta_x$  and  $\Delta_y$

$$\begin{aligned}
& [1 - Z(\mathbf{k}, i\omega_n)] i\omega_n \\
&= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} X_s(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \cdot i\omega_{n'} Z' \\
&\quad \times \left( \frac{1}{D_1} + \frac{1}{D_2} \right), \quad (30)
\end{aligned}$$

$$\begin{aligned}
\Delta_x(\mathbf{k}, i\omega_n) &= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} X_x(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \times \left[ \Delta'_x \left( \frac{1}{D_1} + \frac{1}{D_2} \right) + \Delta'_y \left( \frac{1}{D_1} - \frac{1}{D_2} \right) \right], \quad (31)
\end{aligned}$$

$$\begin{aligned}
\Delta_y(\mathbf{k}, i\omega_n) &= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} X_y(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \times \left[ \Delta'_x \left( \frac{1}{D_1} - \frac{1}{D_2} \right) + \Delta'_y \left( \frac{1}{D_1} + \frac{1}{D_2} \right) \right], \quad (32)
\end{aligned}$$

where  $\Delta'_x \equiv \Delta_x(\mathbf{k}', i\omega_{n'})$ ;  $\Delta'_y$  and  $Z'$  are defined by the same way.  $D_1$  and  $D_2$  stand for

$$D_{1,2} = (i\omega_{n'} Z')^2 - (\varepsilon_{\mathbf{k}'} \mp E_z)^2 - (\Delta'_x \pm \Delta'_y)^2. \quad (33)$$

(ii) For  $\Delta_s$  and  $\Delta_z$

$$\begin{aligned}
[1 - Z(\mathbf{k}, i\omega_n)] i\omega_n &= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} X_s(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \times \left[ i\omega_{n'} Z' \left( \frac{1}{D_3} + \frac{1}{D_4} \right) \right. \\
&\quad \left. + E_z \left( \frac{1}{D_3} - \frac{1}{D_4} \right) \right], \quad (34)
\end{aligned}$$

$$\begin{aligned}
\Delta_s(\mathbf{k}, i\omega_n) &= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} \left[ (X_s - X_{xy})(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \right. \\
&\quad \times \frac{\Delta'_s + \Delta'_z}{D_3} + (X_s + X_{xy})(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \left. \times \frac{\Delta'_s - \Delta'_z}{D_4} \right], \quad (35)
\end{aligned}$$

$$\begin{aligned}
\Delta_z(\mathbf{k}, i\omega_n) &= \frac{\tilde{J}^2}{8N\beta} \sum_{\mathbf{k}', n'} \left[ (X_z + X_{xy})(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \right. \\
&\quad \times \frac{\Delta'_s + \Delta'_z}{D_3} + (X_z - X_{xy})(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \left. \times \frac{\Delta'_s - \Delta'_z}{D_4} \right], \quad (36)
\end{aligned}$$

where

$$D_{3,4} = (i\omega_{n'} Z' \pm E_z)^2 - \varepsilon_{\mathbf{k}'}^2 - (\Delta'_s \pm \Delta'_z)^2. \quad (37)$$

To know which of the two sets (i)  $\Delta_x$  and  $\Delta_y$  and (ii)  $\Delta_s$  and  $\Delta_z$  does appear as superconducting order, we calculate  $T_c$  for each set in the next section.

#### IV. SUPERCONDUCTING TRANSITION TEMPERATURE

We investigate  $T_c$  above and below the magnetic ordering temperature  $T_M$  on the basis of the study in the preceding section. We linearize the Eliashberg equations by deleting  $\Delta_\gamma$  in (33) and (37). Here, we give the result of the ferromagnetic transition temperature  $T_M$  obtained by solving the linearized equation (15) in Figs. 2(a) and 2(b) for  $d'=0.1$  and 0.5, respectively.

First, above  $T_M$ , no spin polarization exists so that  $E_z=0$ , by which  $D_1=D_2$  holds in (33) and  $D_3=D_4$  in (37). Furthermore,  $\hat{\chi}$  is diagonal. The situation is the same as that studied in [I]. The coupled Eliashberg equations (31) and (32) for  $\Delta_x$  and  $\Delta_y$  separate and coincide each other with Eq. (26) in [I], which is written for  $\gamma=x, y$  as

$$\begin{aligned}
\Delta_\gamma(\mathbf{k}, i\omega_n) &= \frac{\tilde{J}^2}{4N\beta} \sum_{\mathbf{k}', n'} X_\gamma(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \\
&\quad \times \frac{\Delta_\gamma(\mathbf{k}', i\omega_{n'})}{[Z(\mathbf{k}', i\omega_{n'}) i\omega_{n'}]^2 - \varepsilon_{\mathbf{k}'}^2}. \quad (38)
\end{aligned}$$

The same things hold for (35) and (36) with respect to  $\Delta_s$  and  $\Delta_z$ . Equations (30) and (34) for  $Z$  coincide each other and

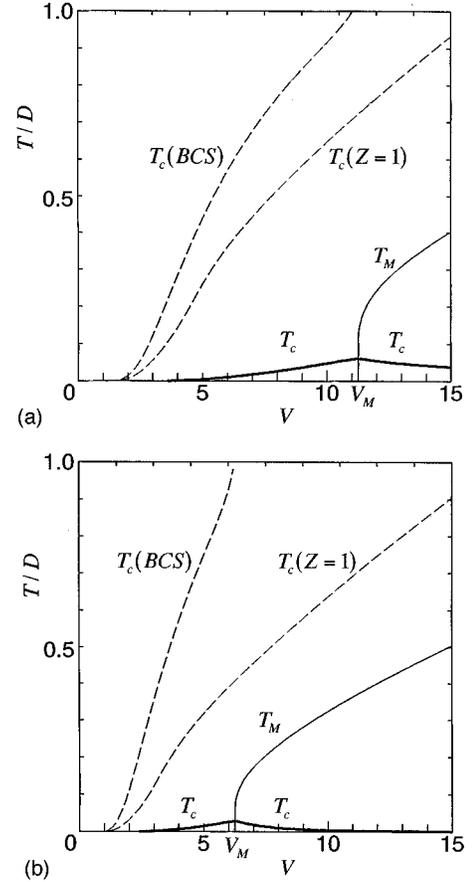


FIG. 2. The superconducting transition temperature  $T_c$  (heavy solid line) and the magnetic transition temperature  $T_M$  (solid line) as a function of  $V$  for (a)  $d'=0.1$  and (b)  $d'=0.5$ .  $V_M$ , above which  $T_M$  becomes finite, decreases with  $d'$ .  $T_c$  below  $V_M$  is the result obtained in [I]. The dashed lines represent the results for  $T_c$  by the BCS approximation and by the approximation of setting  $Z=1$  in Eq. (38).

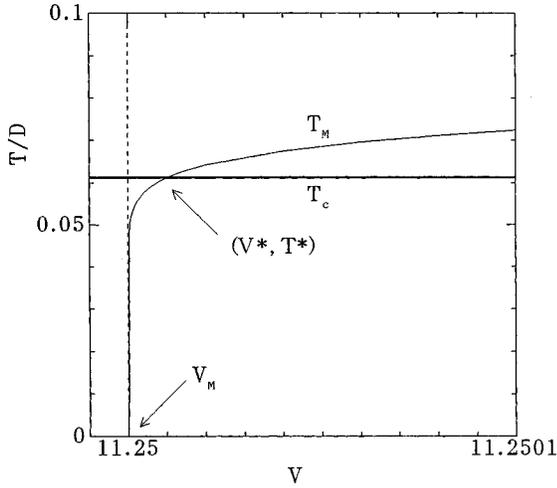


FIG. 3. Magnification of the very vicinity of  $V_M$  in Fig. 2(a).

turns to Eq. (25) in [I], which is written

$$[1 - Z(\mathbf{k}, i\omega_n)]i\omega_n = \frac{\tilde{J}^2}{4N\beta} \sum_{\mathbf{k}', n'} X_s(\mathbf{k} - \mathbf{k}', i\omega_n - i\omega_{n'}) \times \frac{Z(\mathbf{k}', i\omega_{n'})i\omega_{n'}}{[Z(\mathbf{k}', i\omega_{n'})i\omega_{n'}]^2 - \varepsilon_{\mathbf{k}'}}. \quad (39)$$

As discussed in [I], assuming the free electron band for the conduction electrons, we solve separately these sets of the Eliashberg equations for  $\Delta_\gamma$  ( $\gamma = s, x, y, z$ ) and  $Z$  to find the highest  $T_c$ . We calculate (38) and (39) completely following the procedure made in [I], so that its description should be omitted. After the calculation, we have found  $T_c$  above  $T_M$  in the very narrow region of  $V$  above  $V_M$ , where  $T_M$  starts with infinite slope from  $V_M$ . This narrow region of Fig. 2(a) is magnified in Fig. 3, where  $T_c$  is smoothly extended from the region  $V < V_M$  up to the point crossing with the curve of  $T_M$ . The coordinate of this crossing point is denoted by  $(V^*, T^*)$ . In Fig. 3, one finds  $(V^* - V_M)/V_M = 9.8 \times 10^{-7}$ . For  $V > V^*$ ,  $T_M$  lies far above  $T^*$  and we can no more find  $T_c$  above  $T_M$ . This denies the naive expectation made in the Introduction. To know the reason why  $T_c$  does not lie above  $T_M$  in this region, we have solved Eq. (38) by the BCS approximation in which the self-energy correction is neglected, namely  $Z(i\omega_n) = 1$  and the kernel is replaced by the static value  $X_\gamma(i\omega_n - i\omega_{n'}) = X_\gamma(0)$  at  $T = 0$  with the introduction of the cutoff energy  $D$  equal to the CF energy in (2). By this approximation we certainly find  $T_c$  for  $\Delta_x$  above  $T_M$ . As discussed in [I] in detail, this superconducting state is of  $l = 1$ , triplet  $S_x = 0$ . The obtained result for  $T_c$  is shown in Figs. 2(a) and 2(b). We also show the result obtained by setting  $Z = 1$  in (38) but no other approximations are introduced, which is denoted by  $Z = 1$  in Figs. 2(a) and 2(b). The fact that a finite  $T_c$  appears for  $V > V^*$  only by these approximations manifests a crucial role of the depairing effect due to the self-energy correction.

Next we investigate  $T_c$  below  $T_M$  for  $V > V^*$ . In this case, as we have noticed,  $E_z \neq 0$  and  $\chi_{xy} \neq 0$ . As for the set of  $\Delta_x$  and  $\Delta_y$ , they couple each other due to  $D_1 \neq D_2$  through (31) and (32). However, the integration over  $\varepsilon_{\mathbf{k}'}$  in (29) sweeps away the difference between  $D_1$  and  $D_2$  to decouple (31) and

(32), and these equations become equivalent to (38) with  $\gamma = x, y$ . On the other hand, Eq. (30) for the normal self-energy part turns to (39). We have solved (38) and (39) to find  $T_c$  by the same procedure as done in [I]. As the result of it, in contrast with the case  $T > T_M$ , we obtain a finite  $T_c$  for  $\Delta_x$ , which is shown in Figs. 2(a) and 2(b) by the heavy solid line. It is a characteristic that  $T_c$  decreases with increase in  $V$  or  $T_M$ . This is because the RPA susceptibility or the pairing interaction decreases with increase of  $V$ . As for the CF anisotropy, it is found by comparing Figs. 1(a) and 1(b) that  $T_M$  increases and  $T_c$  decreases with increasing  $d'$ . This is due to the behavior of the susceptibility shown in Fig. 1, where the increase of  $d'$  brings the decrease of the diagonal components of  $\hat{\chi}$  below  $T_M$ . As mentioned before, the state represented by  $\Delta_x$  is of  $l = 1$  and triplet  $S_x = 1$ .

For the set of  $\Delta_s$  and  $\Delta_z$ , they couple each other by the presence of  $E_z$  and  $\chi_{xy}$  through (35) and (36). In this case, the effect of  $E_z$  does not disappear by the operation (29) since  $D_3$  and  $D_4$  in (37) contain  $E_z$  in a way different from  $D_1$  and  $D_2$  in (33). Moreover,  $X_{xy}$  exists. We have tried to find  $T_c$  for the set of the coupled Eqs. (34), (35) and (36) by numerical calculation. However, no solution has been found. In the paramagnetic phase as studied in [I], reflecting that  $\chi_{xx}$  is the smallest of all the components of the RPA susceptibility tensor as shown in Fig. 1, neither  $\Delta_s$  nor  $\Delta_z$  appears. On the other hand, in the ferromagnetic phase,  $\chi_{zz}$  can be the smallest of all the components of the RPA susceptibility tensor as in the case shown in Fig. 1(b), so that  $|X_z|$  in (28) can be the largest among  $X_x$ ,  $X_y$ , and  $X_z$ . However, even in this case, the coupling of  $\Delta_z$  with  $\Delta_s$  described above makes the state with  $\Delta_z$  impossible.

## V. CONCLUSION AND DISCUSSION

Following our previous paper, we have studied the possibility of the superconductivity mediated by the virtual excitation of the CF singlet ground state in the case where the ferromagnetic order exists. Contrary to the expectation given in Sec. I, the superconductivity does not appear, except for the very vicinity of  $V_M$ , above the ferromagnetic Curie temperature  $T_M$ , where the Van Vleck susceptibility is highly enhanced and so is the pairing force. This is due to the depairing effect which is also enhanced near  $T_M$ . If it were not the case, substances which show magnetic order would show the superconductivity above their  $T_M$ . On the other hand, in the very narrow region above  $V_M$ ,  $T_c$  certainly appears above  $T_M$ . In this region,  $T_c$  is expressed by the line smoothly extended from  $V < V_M$  up to the point crossing with  $T_M$ . Since  $T_M$  starts with infinite slope from  $V_M$ , and slightly turns right, the crossing point of  $T_M$  with  $T_c$  lies in the very vicinity of  $V_M$ . After all, for  $V > V_M$ , except for this narrow region, we have found the superconducting transition temperature below  $T_M$ . Owing to the effect of the magnetic order, the Eliashberg equations suffer modification. However, it turns out that, for the free electron band, the realized superconducting state is the same state appearing in the paramagnetic phase for a much weaker interaction.

Competition or coexistence of superconductivity with magnetic order has been a classic problem attracting great interest. Especially, since the 1970s, many studies were made extensively, stimulated by the discovery of supercon-

ductors in magnetic materials, which are clearly reviewed and discussed by Vonsovsky *et al.*<sup>18</sup> However in comparison with these studies, a distinct point of the present theory is that we deal with the superconductor in which the virtual excitation of the CF singlet ground state induces the superconductivity and, at the same time, it also induces the magnetism. This is in contrast with the case in which superconductivity and magnetism come from different sources.

In the present model, superconductivity is shown to appear for  $V > V^*$  in the ferromagnetic order. In this respect we are interested in heavy fermion systems such as URu<sub>2</sub>Si<sub>2</sub> and UPt<sub>2</sub> for which the possibility of the CF singlet ground state is sometimes discussed<sup>19</sup> and superconducting transition is

found in the antiferromagnetic (AF) ordering phase.<sup>20</sup> To shed some light on understanding of these heavy fermion systems, although our model assumes the localized  $f$  electronic states as a limit of small  $s$ - $f$  hybridization, we are now extending the study to the case of the AF order, which will be reported elsewhere.

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