A Model for Cooper Pairing in Heavy Fermion Superconductor

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Cooper pair formation in the heavy fermion system is discussed on the basis of a tight-binding model for the Kondo lattice system. The attractive interaction between heavy fermions stems from the coupling with phonons, which arises through the modulations of the transfer to the nearest neighbor site and the single-particle level of the heavy fermion owing to the lattice vibrations. The interaction relevant to the Cooper pair formation is written in the form of the superposition of separable forms with s-, d- and p-like symmetries. A comparison among the transition temperatures for various types of Cooper pairing shows that the singlet pairing is always favorable compared to the triplet one, and that, of singlet pairings, the d-like one is most favorable in the weak coupling case and so is the s-like one in the strong coupling case. The manner in which the d- and s-components mix together below $T_c$ is discussed in the Ginzburg-Landau region, from which it is shown that the possible type of pairing is purely s-like one or d-like one with s-like admixtures, depending whether the highest $T_c$ occurs for s-like or d-like pairing. This implies that the low lying excitations can be nearly gapless for appropriate values of parameters characterizing the model.

§ 1. Introduction

The so-called heavy fermion systems have recently attracted a great deal of attention. Some of them, such as CeCu$_2$Si$_2$, UBe$_{13}$ and UPt$_3$, show superconductivity. It has now become clear that the nature of their superconducting states is very unusual and different from that of well investigated cases of the Cooper pairing such as the simple s-wave BCS state and the ABM or BW state. Indeed, for CeCu$_2$Si$_2$ and UBe$_{13}$, the specific heat at low temperatures shows a power law behavior ($C_V \sim T^n$, $n = 2 \sim 3$) instead of an exponential one in the simple BCS case. It has recently been claimed that this supports the p-wave pairing of the ABM-type. On the other hand, the nuclear relaxation rates of NMR for both compounds show somewhat puzzling behaviors which cannot be explained in the context of ABM-like states. Common features of superconducting states deduced from both types of experiments are considered to be a gapless or nearly-gapless nature of excitations.

While there are the trends of theories that the superconducting state of heavy fermion systems can be understood in the context of triplet pairing analogous to that of $^3$He, possibilities of the singlet pairing have been examined from various points of view. In particular, some of the present authors recently showed that for a model system, in which particles on the same site feel a strong repulsion and those on the neighbour sites feel an appropriate attraction, a nearly gapless s-wave pairing is possible, which is consistent with two kinds of experiments mentioned above at least for CeCu$_2$Si$_2$. The purposes of the present paper are to ask further an origin of the attractive interaction of the model, to extend the model a bit so that all types of interactions concerning nearest neighbour sites are taken into account, and then to examine which type of Cooper pairing, i.e., s, p, d, etc., or their admixture, is the most stable one for a given set of parameters characterizing the extended model.

In §2 we present a model which simulates a Kondo lattice like system of heavy
fermions. Although it might be still controversial how the Fermi liquid nature of heavy fermions stems from original f-electrons, we follow a quasi-particle theory of the Kondo lattice in which coherence among virtual bound states (associated with a singlet bound state of the single Kondo problem) is explicitly taken into account through the d(conduction electron)-f(localized electron) mixing. On this basis, the intra atomic repulsion between heavy fermions and the transfer between nearest neighbour sites (actually the width of the heavy fermion band) are determined by the Kondo temperature as \( t = 4 T_K \) and \( \Lambda = 2 T_K / \pi \). And then, coupling between heavy fermions and phonons arises through mechanism that the transfer and the Fermi level \( \epsilon \) are both modulated by lattice vibrations. Strength of attractive interactions, which are obtained by eliminating the phonon degrees of freedom (its characteristic frequency is much larger than the band width \( 2 \Lambda \)), can be the order of \( \Lambda \) due to the effect of Kondo volume collapse. An importance of the effect of Kondo volume collapse has been emphasized by Razafimandimby, Fulde and Keller on the basis of somewhat different pictures of quasi-particle states of heavy fermions and their coupling with phonons. In this simple model, the effects of the spin-orbit interaction and the paramagnon mediated indirect interaction are not taken into account.

In \( \S 3 \) we discuss the Cooper pairing for a tight-binding model developed in the preceding section. For simplicity, the simple cubic lattice is assumed. Then the interaction between heavy fermions is expressed in terms of the superposition of separable form each of which has appropriate symmetry under rotation of lattice, e.g., s-like, p-like and d-like. So we can examine separately which type of Cooper pairing occurs first. Concretely, we compare the transition temperatures for each pairing. The results are summarized as follows: (i) Triplet pairing is always unfavorable compared to singlet pairing. (ii) Among singlet pairings, d-like pairings are the most favorable ones for the weak coupling limit, and so is s-like pairing if the attractive interaction becomes appropriately strong (~\( \Lambda \)).

Structure of Cooper pairing (mixing of different kind of singlet pairing) and the low lying excitations below the transition temperature are qualitatively discussed in \( \S 4 \). By an analysis of the free energy in the Ginzburg-Landau region, it is shown that possible type of pairing below \( T_c \) is purely s-like one or d-like one with s-like admixtures, depending whether the highest \( T_c \) occurs for s-like or d-like pairing.

\( \S 2. \) A model of heavy fermion system

Of many heavy fermion systems, CeCu_2Si_2 and UBe_13 are considered to be Kondo lattice systems. While there are some attempts to derive their heavy fermion nature from original f-electrons hybridizing with conduction electrons, we follow a quasi-particle theory which is developed by Jichu, Matsuura and Kuroda (JMK) taking explicitly the characteristics of the Kondo lattice into account. According to JMK, the virtual bound states (associated with a singlet bound state of an f-electron and conduction electrons) on rare earth atom sites get coherence through the hybridization with conduction electrons and as a result form an anomalously narrow band around the original Fermi level. Since it is assumed that one rare earth atom supplies one virtual bound state each, the band is half-filled.

According to the results of JMK, we introduce a model Hamiltonian of heavy fermion
system like

\[ H_{\text{fl}} = -\frac{1}{2} \sum_{\langle i, j \rangle} t (c_i^\dagger c_j + \text{h.c.}) + \sum_{i, \sigma} \varepsilon_i c_i^\dagger c_i^\sigma + \sum_i \tilde{\Gamma}_i c_i^\dagger c_i^\sigma, \]

(1)

where \( c_i^\sigma \) is the annihilation operator of heavy fermion on the site \( i \) with spin \( \sigma \), \( \varepsilon \) is the site energy of heavy fermion, the nearest-neighbor (n.n.) transfer \( t \) is given by the relation between the band width \( \Lambda = tz \) (\( z \): number of n.n. sites) and the Kondo temperature, i.e., \( \Lambda = 2T_K/\pi \), and also the intra atomic repulsion \( \tilde{\Gamma}_i \) is related to \( T_K \) as \( \tilde{\Gamma}_i = 4T_K \). A symbol \( \langle i, j \rangle \) means that the summation is taken over n.n. sites.

Now we observe that the n.n. transfer \( t \) and the site energy \( \varepsilon \) can be modulated by lattice vibrations, and then the fermion-phonon coupling arises through modulations of \( t_{ij} \) and \( \varepsilon_i \). The modulations of \( t_{ij} \) and \( \varepsilon_i \) basically stem from those of \( T_K \), which has strong dependence on pressure or volume of the system (the effect of Kondo volume collapse). Assuming an elastic continuum for lattice, these modulations are written in terms of phonon operators as follows:

\[ t_{ij} = t + \frac{dt}{d|\mathbf{R}_i - \mathbf{R}_j|} \sum_q \left( \frac{\hbar}{2MN\omega_q} \right)^{1/2} \left( \mathbf{\hat{q}} \cdot \mathbf{\hat{R}}_{ij} \right) (e^{i\mathbf{q} \cdot \mathbf{R}_j} - e^{i\mathbf{q} \cdot \mathbf{R}_i})/i \cdot (b_q + b^{\dagger}_q), \]

(2)

\[ \varepsilon_i = \varepsilon + \frac{d\varepsilon}{d\Omega} \sum_q \left( \frac{\hbar}{2MN\omega_q} \right)^{1/2} |q| e^{i\mathbf{q} \cdot \mathbf{R}_i} (b_q + b^{\dagger}_q), \]

(3)

where the \( b_q \)'s are phonon annihilation operators, \( \Omega \) is the volume of Wigner-Seitz cell, \( \mathbf{R}_i = \mathbf{R}_i - \mathbf{R}_j \), \( t_{ij} = t_{ij} \), \( \mathbf{\hat{q}} = q/|q| \), etc., and other notations are usual ones.

Substituting (2) and (3) into (1), we obtain the fermion-phonon interaction as follows:

\[ H_{\text{hf-ph}} = \sum_{\langle i, j \rangle} \sum_q [F^{(1)}_q + \delta_{ij} F^{(2)}_q] c_i^\dagger c_j \varepsilon_i (b_q + b^{\dagger}_q), \]

(4)

where we have used the following abbreviations:

\[ F^{(1)}_q = \frac{dt}{d|\mathbf{R}_i - \mathbf{R}_j|} \sum_q \left( \frac{\hbar}{2MN\omega_q} \right)^{1/2} (e^{i\mathbf{q} \cdot \mathbf{R}_j} - e^{i\mathbf{q} \cdot \mathbf{R}_i})/i \cdot , \]

(5)

\[ F^{(2)}_q = \frac{d\varepsilon}{d\Omega} \sum_q \left( \frac{\hbar}{2MN\omega_q} \right)^{1/2} |q| e^{i\mathbf{q} \cdot \mathbf{R}_i} , \]

(6)

We denote the Hamiltonian, (1), in which \( t_{ij} \) and \( \varepsilon_i \) are replaced by their equilibrium values \( t \) and \( \varepsilon \), by \( H_{\text{fl}}^{(0)} \). This represents a purely heavy fermion part.

It should be noticed that the band width \( 2\Lambda(\sim T_K) \) and the intra atomic repulsion \( \tilde{\Gamma}_i(\sim T_K) \) of heavy fermions are so small compared to \( \omega_D \), the Debye frequency. This means that phonon degrees of freedom can be eliminated to leave us with the instantaneous interactions among fermions. If the heavy fermion-phonon interaction \( H_{\text{hf-ph}} \), (4), is eliminated as usual to the second order perturbation, the indirect interaction among fermions is written in general in the form,

\[ -\sum K_{lm,rs} c^\dagger_l c_m c^\dagger_r c_s \varepsilon_l c^\sigma r, \]

(7)

where \( l \) and \( m \) are the same site or the n.n. sites, and so are \( r \) and \( s \). Of these terms, we restrict the type of interaction to those such that the sites \( (l, m, r, s) \) are selected from one
site or two sites of n.n. This would not be unrealistic considering the fact that wave numbers of the phonons mainly contributing to the indirect interaction are of the order \( k_0 \sim a^{-1} \); \( a \) is the lattice constant), the Debye wave number. Then, the indirect part of the interaction Hamiltonian is written in the following form:

\[
H_{\text{indirect}} = -g_0 \sum_i c_i^\dagger c_i c_i^\dagger c_i - g_1 \sum_{<i,j>} c_i c_j^\dagger c_j^\dagger c_i^\dagger c_i^\dagger c_j - g_2 \sum_{<i,j>} c_i c_j^\dagger (c_i^\dagger c_j - c_j^\dagger c_i) - g_3 \sum_{<ii,i>} \langle c_i^\dagger c_i \rangle \langle c_i^\dagger c_i \rangle^2,
\]

where the coefficients \( g_0, g_1, g_2 \) and \( g_3 \) are given as follows:

\[
g_0 = \frac{1}{2MN} \left( \frac{d\alpha}{d\Omega} \right)^2 \sum_q \frac{q^2}{\omega_q^2},
\]

\[
g_1 = \frac{1}{2MN} \left( \frac{d\alpha}{d\Omega} \right)^2 \sum_q \frac{q^2}{\omega_q^2} \left( q \cdot R_{ij} \right)^2 \frac{1 - e^{i\theta_{ij}}}{\omega_q^2},
\]

\[
g_2 = \frac{1}{2MN} \left( \frac{d\alpha}{d\Omega} \right)^2 \sum_q \frac{q^2}{\omega_q^2} \cos(q \cdot R_{ij}),
\]

\[
g_3 = \frac{1}{2MN} \left( \frac{d\alpha}{d\Omega} \right)^2 \sum_q \frac{q^2}{\omega_q^2} \sin(q \cdot R_{ij}).
\]

In deriving the second equality of Eqs. (9)~(12), we have used the definitions (5) and (6). Now let us estimate the order of magnitude of \( g_0, g_1, g_2 \) and \( g_3 \). For this purpose, we assume a linear dispersion for the phonon spectrum, i.e., \( \omega_q = sq \), since we are interested in the acoustic branch accompanying volume changes. Then, by inspections,

\[
\begin{align*}
g_0 &\sim \frac{1}{M_s^2} \left( \frac{d\alpha}{d\Omega} \right)^2, \\
g_1 &\sim \frac{1}{M_s^2} \left( \frac{3d\alpha}{d\Omega} \right)^2, \\
g_2 &\sim \frac{1}{M_s^2} \left( \frac{d\alpha}{d\Omega} \right)^3
\end{align*}
\]

The derivatives \( dt/d\Omega \) and \( de/d\Omega \) are both reduced to \( dT_k/d\Omega \) in the following way. For \( dt/d\Omega \), on the basis of the relation \( tz = 2T_k/\pi \), the following is straightforwardly derived:

\[
\frac{dt}{d\Omega} = \frac{2}{\pi z} \frac{dT_k}{d\Omega}.
\]

For \( de/d\Omega \), things are more complicated. To express \( de/d\Omega \) in terms of \( dT_k/d\Omega \), we go back to the Anderson model describing the original system of a localized f-electron and conduction electrons. In the "s-d limit", the Kondo temperature \( T_k \) is expressible in terms of \( \epsilon_F \) (the Fermi energy of conduction electrons), \( \epsilon_F \) (the energy level of f-electron), and \( U \) (bare intra atomic Coulomb energy) as follows:

\[
T_k = D \exp \left[ -\frac{1}{V^2} \left( \frac{1}{U + \epsilon_F} + \frac{1}{-\epsilon_F + \epsilon_F} \right) \right].
\]

* The symbol \( U \) in this section is not to be confused with the same symbol in the following sections indicating an effective repulsion between heavy fermions on the same site.
where notations are usual ones.\textsuperscript{22) If we assume a nearly symmetric case, i.e., $E_f - \varepsilon_F \approx -U/2$, the $\Omega$-derivative of (15) is essentially given by
\begin{equation}
\frac{dT_k}{d\Omega} \approx T_k \frac{U}{V^2 \rho} \frac{1}{2 \varepsilon_F} \frac{d\varepsilon_F}{d\Omega},
\end{equation}
where we have used $D^{-1}dD/d\Omega \sim \rho^{-1}dp/d\Omega \sim \varepsilon_F^{-1}d\varepsilon_F/d\Omega$, $U \gg V^2 \rho$, and the fact that $U$ and $E_f$ are almost $\Omega$-independent. A bare coupling between f-electrons and phonons is the second type of (4) with coupling (6); but in the present case $d\varepsilon/d\Omega$ in (6) should be read as $d\varepsilon_F/d\Omega$. In the spirit of the quasi-particle theory of JMK, this bare coupling $d\varepsilon_F/d\Omega$ is renormalized by the wave function renormalization factor $1/\tilde{\chi}$ in the sense of the Fermi liquid theory\textsuperscript{18)} and then is transformed to the coupling $d\varepsilon/d\Omega$ between heavy fermions and phonons:
\begin{equation}
\frac{d\varepsilon}{d\Omega} = \frac{1}{\tilde{\chi}} \frac{d\varepsilon_F}{d\Omega},
\end{equation}
where the renormalization factor is $1/\tilde{\chi} = 4T_k/\pi^2 V^2 \rho$. Then, from Eqs. (16) and (17), $d\varepsilon/d\Omega$ is expressed in terms of $dT_k/d\Omega$ as
\begin{equation}
\frac{d\varepsilon}{d\Omega} \approx \frac{8}{\pi^2} \frac{\varepsilon_F}{U} \frac{dT_k}{d\Omega}.
\end{equation}
By Eqs. (14) and (18), relations (13) are reduced to
\begin{equation}
\begin{align*}
g_0, g_2 &= \frac{T_k^2}{M^2} \left( \frac{8}{\pi^2} \frac{\varepsilon_F}{U} \right)^2 \eta^2, \\
g_1 &= \frac{T_k^2}{M^2} \left( \frac{6}{\pi^2} \right)^2 \eta^2, \\
g_3 &= \frac{T_k^2}{M^2} \left( \frac{6}{\pi^2} \right)^2 \left( \frac{8}{\pi^2} \frac{\varepsilon_F}{U} \right) \eta^2,
\end{align*}
\end{equation}
where $\eta$ is defined by
\begin{equation}
\eta = -\frac{Q}{T_k} \frac{dT_k}{d\Omega}.
\end{equation}
The value of $\eta$ amounts to considerably large (the effect of Kondo volume collapse), e.g. for CeCu$_2$Si$_2$, $\eta \approx 20-80$,\textsuperscript{17,21}) as has been pointed out by Razafimandimby et al. The ratio $\varepsilon_F/U$ is in general of order unity. These imply that the parameters $g_0, g_1, g_2$ and $g_3$ could be comparable to the band width $2\Lambda(=4T_k/\pi)$ even if $T_k \ll M^2$. Indeed, $g_1$ and $g_3$ are estimated as follows. If we take $T_k \approx 10K$, $M^2 \sim 10^4K$, $z=6$ (simple cubic), and $\varepsilon_F \sim U$, then from (19) we find
\begin{equation}
g_1 \sim \frac{1}{\pi} g_3 \sim \frac{T_k^2}{M^2} \frac{\eta^2}{\pi^2} = \frac{4T_k}{4\pi} \frac{1}{M^2} \frac{T_k}{\pi^2} \eta^2 \sim \frac{1}{2\pi} \times 10^{-3} \eta^2 \Lambda.
\end{equation}
The right-hand side of (21) can be of order $\Lambda$, if $\eta$ is large as mentioned above.

If the phonon spectrum were truly linear, i.e., $\omega_q = sq$, in the whole region of $q$-space (as we assumed above), the coefficient $g_2$, (11), would vanish because $\Sigma(q^2/\omega_q^2) \times \cos(q \cdot R_{ij}) = s^2 \Sigma \cos(q \cdot R_{ij}) = 0$. If the dispersion of the phonon spectrum is taken into account, $g_2$ does not vanish, but is expected to be much smaller than $g_0, g_1$ and $g_3$.\textsuperscript{19)
§ 3. Comparison of transition temperatures for different kinds of Cooper pairing

A model Hamiltonian developed in the preceding section consists of $H_{\text{indirect}}^{(1)}$, (1), and $H_{\text{indirect}}^{(8)}$. If the terms of the type $c_{k\sigma}^+ c_{-k\sigma} c_{-k'\sigma} c_{k'\sigma}$ are retained in the interaction part, it is expressed in terms of the Fourier transformed quantities as follows:

$$
H = \sum_{k\sigma} \xi_k c_{k\sigma} c_{k\sigma} + \frac{1}{N} \sum_{k'} [(t_{k'k} - g_0) - 2g_1 \gamma_{k+k'} - 2g_2 \gamma_{k-k'} - 2g_3 (\gamma_k + \gamma_{k'})] c_{k\sigma}^+ c_{-k\sigma}^+ c_{-k'\sigma} c_{k'\sigma},
$$

(22)

where $c_{k0} = N^{-1/2} \sum_i e^{ik\cdot R} c_{i\sigma}$, etc., $\gamma_q = \sum_s e^{iq\cdot R_s}$, and single particle energy $\xi_k$ includes the chemical potential (appropriately defined) so that $\xi_k$ vanishes at the Fermi level. For half-filled bands (such as the Kondo lattice system), $\xi_k$ is given by

$$
\xi_k = -t \gamma_k.
$$

(23)

For clear presentation, hereafter we assume the simple cubic for the lattice structure. Then $\gamma_k$ takes the form

$$
\gamma_k = 2(\cos k_x a + \cos k_y a + \cos k_z a).
$$

(24)

(a is the lattice constant.) It is easy to see that $\gamma_{k\pm k'}$ is expressible in the separable form. Indeed, simple rearrangements give us

$$
\gamma_{k\pm k'} = \frac{1}{6} (\gamma_k \gamma_{k'} + \gamma_k \gamma_{k'} + \xi_k \xi_{k'}),
$$

$$
+ 2(\sin k_x a \sin k_x a + \sin k_y a \sin k_y a + \sin k_z a \sin k_z a),
$$

(25)

where $\eta$ and $\xi$ are defined as follows:

$$
\eta_k = \sqrt{6} (\cos k_x a - \cos k_y a),
$$

(26a)

$$
\xi_k = \sqrt{2} (\cos k_x a + \cos k_y a - 2 \cos k_z a).
$$

(26b)

Each term appearing in (25) has a separable form and factors in different terms are orthogonal to each other and normalized in the sense,

$$
\frac{1}{N} \sum_k \gamma_k \eta_k = 0, \quad \text{etc.,} \quad \frac{1}{N} \sum_k \gamma_k^2 = \frac{1}{N} \sum_k \eta_k^2 = \frac{1}{N} \sum_k \xi_k^2 = 6,
$$

$$
\frac{1}{N} \sum_k \sin^2 k_x a = \frac{1}{2}, \quad \text{etc.}
$$

(27)

The symmetry of $\gamma_k$, $(\eta_k, \xi_k)$, and $\sin k_z a$ ($a = x, y, z$) under lattice rotation is s-like, d$y$-like and p-like, respectively.

For the moment we discuss separately (a) singlet and (b) triplet pairings.

(a) Singlet pairing: As usual, we obtain a gap equation from (22) in the form
where $E_k \equiv (\xi_k^2 + |\Delta_k|^2)^{1/2}$ is the quasi-particle energy in the superconducting state. The interaction $V_{k,k'}^{\text{singlet}}$ is separated into s-like and d-like parts,

$$V_{k,k'}^{\text{singlet}} = V_{k,k'}^s + V_{k,k'}^d,$$

where

$$V_{k,k'}^s = U - 2g_3(\gamma_k + \gamma_{k'}) - \frac{1}{3}g_5\eta_k\eta_{k'},$$
$$V_{k,k'}^d = -\frac{1}{3}g_5(\eta_k\eta_{k'} + \xi_k\xi_{k'}).$$

Here $U$ and $g_5$ have been defined as $U = \tilde{U}_c - g_0$ and $g_5 = g_2 + g_1$, respectively.\textsuperscript{1)} To solve the gap equation (28), we assume a general form for $\Delta_k$ like

$$\Delta_k = \Delta_1 + \Delta_2 \gamma_k + \Delta_3 \eta_k + \Delta_4 \xi_k,$$

where the coefficients $\Delta_1 \sim \Delta_4$ are complex numbers in general. Since each term of (30) is orthogonal among them in the sense (27), the gap equation (28) is separated into four coupled algebraic equations:

$$\Delta_1 = -\frac{1}{N} \sum_k (-U + 2g_3 \gamma_k) \frac{\Delta_k}{2E_k} \text{th} \frac{E_k}{2T},$$
$$\Delta_2 = \frac{1}{N} \sum_k (2g_3 + 3g_5 \gamma_k) \frac{\Delta_k}{2E_k} \text{th} \frac{E_k}{2T},$$
$$\Delta_3 = \frac{1}{N} \sum_k \frac{1}{3} g_5 \eta_k \frac{\Delta_k}{2E_k} \text{th} \frac{E_k}{2T},$$
$$\Delta_4 = \frac{1}{N} \sum_k \frac{1}{3} g_5 \xi_k \frac{\Delta_k}{2E_k} \text{th} \frac{E_k}{2T}.$$

Equations determining the transition temperature $T_c(\equiv 1/\beta_c)$ are obtained from Eqs. (31a) ~ (31d) putting $E_k \sim \xi_k$ in them, and are decoupled into two classes, s-like part and d-like part:

For s-pairing,

$$\begin{bmatrix}
1 + U\Phi_1(\beta_c) & -2g_3\Phi_2(\beta_c) \\
-2g_3\Phi_2(\beta_c) & 1 - \frac{1}{3}g_5\Phi_3(\beta_c)
\end{bmatrix} \begin{bmatrix}
\Delta_1 \\
\Delta_2
\end{bmatrix} = 0,$$

for d-pairing,

$$\left[ \frac{1}{g_5} - \frac{1}{3} \Phi_d(\beta_c) \right] \Delta_{4,\xi} = 0,$$

where the $\Phi$’s are defined as

\textsuperscript{1)} If we put $V_{k,k'}^s$ and $g_5$ equal to zero, we obtain a model discussed in Ref. 19.)
Triplet pairing: For simplicity, we discuss only the case of the equal spin pairing (ESP). It is sufficient at least for discussing the transition temperature. Then the procedures from (28) to (31d) to obtain the gap equation can be transcribed to this case. Corresponding to Eqs. (30) and (31a)～(31d), we obtain the gap parameter as

$$\Delta_k = \Delta_{yx} \sin k_x a + \Delta_{yy} \sin k_y a + \Delta_{zz} \sin k_z a,$$

which has a p-like character, and the gap equation as

$$\Delta_{pa} = 4 g_t \frac{1}{N} \sum_k \sin k_x a \frac{\Delta_k}{2E_k} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k}, \quad (a=x, y, z)$$

where $g_t = g_2 - g_1$. Equation determining the transition temperature $T_c (=1/\beta_c)$ is then given in the form

$$\left[ \frac{1}{g_t} - 4 \Phi_p(\beta_c) \right] \Delta_{pa} = 0, \quad (a=x, y, z)$$

where $\Phi_p$ is defined as

$$\Phi_p(\beta) = \frac{1}{N} \sum_k \sin^2 k_x a \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k}.$$

Now let us proceed to the comparison among the $\beta_c$'s, the solutions of Eqs. (32), (33) and (37). The (inverse) transition temperature $\beta_c$ of each type of pairing depends on the value of parameters $g_s, g_t, g_3$ and $U$. While in general it may be needed for the comparison between the $\beta_c$'s to solve their gap equations numerically (we shall do this later), it can be performed analytically for the limiting cases (i) $\beta_c \sim \infty$, and (ii) $\beta_c \sim 0$.

(i) $\beta_c \sim \infty$ (weak coupling limit): The asymptotic forms of the $\Phi$'s, Eqs. (34a～c) and (38), for $\beta \gg 1/t$ are given in Appendix A by Eqs. (A'5), (A'6), (A'12) and (A'14), respectively. The transition temperature for the s-pairing is obtained from Eq. (32) by putting a determinant of matrix coefficient equal to zero:

$$\frac{1}{g_s} = \frac{1}{3} \Phi_s(\beta_s) \left[ 1 - \frac{4 g_s^2 \Phi_s(\beta_s)}{1 + U \Phi_s(\beta_s)} \Phi_s(\beta_s) \right]^{-1}.$$  

Using Eqs. (A·5) and (A·6), this takes the form

$$\frac{1}{g_s} = \frac{1}{3 t} \left( 1 - \frac{4 g_s^2}{t U} \right)^{-1} - \frac{1}{t} O(1/\ln \beta_s t),$$

which means that a condition of $g_s$ and $g_3$ for the s-pairing to occur is (assuming that $U$...
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is given independently)

$$g_s > 3t - \frac{12g_3^2}{U}.$$ \hspace{1cm} (41)

Notice that if $g_s > \sqrt{tU}/2$, the s-pairing is possible even if $g_s < 0$ for which neither d nor p-pairing is possible. If the attractive interactions $g_s$ and $g_3$ are so weak that the condition (41) does not hold, the first occurring pairing is not an s-like one; that is, there is a threshold for $g_s$ and $g_3$. The transition temperatures for d-pairing and p-pairing are obtained from Eqs. (33) and (37), using Eqs. (A-12) and (A-14), in the forms

$$\frac{1}{g_s} \sim \frac{2138}{6t} \ln \beta_s t$$ \hspace{1cm} (42)

and

$$\frac{1}{g_1} \sim \frac{1}{3t} \ln \beta_{p_1} t,$$ \hspace{1cm} (43)

respectively. Since numerical factor of (42) is larger than that of (43) and $g_1(=g_3-g_1)$ is always smaller than $g_s(=g_2+g_1)$, the d-pairing is favorable compared to the p-pairing (i.e., $\beta_d > \beta_p$) in the present case, i.e., in the weak coupling case.

(ii) $\beta_c \sim 0$ (strong coupling limit): The asymptotic forms of the $\Phi$'s, Eqs. (34a~c) and (38), are given up to $O(\beta^3)$ in Appendix B. Using Eqs. (B·5) and (B·6), relation (39) determining the transition temperature of an s-like pairing is reduced to (up to $O(\beta^3)$)

$$\frac{1}{g_s} \sim \frac{\beta_s}{2} \left[1 + \frac{3}{2} \beta_s^2 \left(g_3^2 - \frac{5}{6} t^2 \right) \right].$$ \hspace{1cm} (44)

The corresponding equations for d-like and p-like pairings are obtained from Eqs. (33) and (37), using Eqs. (B·7) and (B·8), in the forms

$$\frac{1}{g_s} \sim \frac{\beta_s}{2} \left(1 - \frac{1}{4} \beta_s^2 t^2 \right)$$ \hspace{1cm} (45)

and

$$\frac{1}{g_1} \sim \frac{\beta_2}{2} \left(1 - \frac{5}{12} \beta_2^2 t^2 \right),$$ \hspace{1cm} (46)

respectively. From comparison among the terms of $O(\beta)$ in (44)~(46), one can see that the singlet (s-like or d-like) pairing is favorable compared to the triplet (p-like) pairing (i.e., $\beta_p > \beta_s, \beta_d$), because $g_1(=g_3-g_1)$ is smaller than $g_s(=g_2+g_1)$. Difference of the stability between the s-like and the d-like pairings stems from the terms of $O(\beta^3)$: If $g_3 > \sqrt{2/3} t$, the s-like pairing is stable compared to the d-like one; and vice versa. As discussed in §2, $g_3$ can be comparable to $t$, so that in the strong coupling case the s-like pairing can be the most stable one.

To see the intermediate behavior of the transition temperature vs coupling constants ($g_s$, $g_1$, $g_3$ and $U$), it is needed to solve numerically Eqs. (33), (37) and (39). Figure 1 gives $\Phi_a/3$, (34c), $4\Phi_p$, (38), and the right-hand side of (39) as a function of $\beta$ for several values of $g_s$ and $U$. From this one can find $T_c$ of each pairing corresponding to the couplings $g_s$ and $g_3$. ($U$ is fixed to $2\pi A = 12\pi t$.) For $g_3 < 2t$, the s-like pairing is favorable only for
gs ≥ 3t (strong coupling), while for gs > 2t the region of gs where the s-like pairing is favorable prevails rapidly; for gs > √U/2 = √3πt, in particular, the s-like pairing is always the most favorable one.

The above discussion, based on the model Hamiltonian (23), is summarized as follows: (i) The triplet pairing is always unfavorable compared to the singlet one. (ii) Of the singlet pairings, the d-like one is most favorable in the weak coupling case, and so is the s-like one in the strong coupling case.

Of course, we have not taken into account an indirect interaction due to the paramagnon exchange which is expected to stabilize the triplet pairings and to suppress the singlet ones. So, there still remains a possibility that the triplet p-pairing is the most stable one. However, we believe this may be an unlikely possibility, since g3 is much smaller than g1 ~ Tk (band width of heavy fermions), numerical factor of (43) is smaller than that of (42), and strength of the paramagnon corrections to gs (~ t) and gi (~ t) are at most 1/8 · 3/4 · Tk/2 ~ 9/16 · t.14

§ 4. Properties below the transition temperature

In this section we briefly discuss qualitative properties of the Cooper pairing and low lying excitations below the transition temperature. According to the results of the

---

Fig. 1. (a) Curves D, P and S present tΦd/3, 4tΦs, and the right-hand side of Eq. (39) times t, respectively, as a function of t/Tc. The value of U is fixed to the theoretical one, i.e., U = 2πA = 12πt.18 The numbers attached to curves S are those of gs/t. An abscissa corresponding to the value of an ordinate, t/gs or t/gi, gives the transition temperature for each pairing. (cf. Eqs. (33), (39) and (37).)

(b) The right-hand side of Eq. (39) times t as a function of t/Tc for several values of gs. The numbers attached to the curves denote the values of gs/t.
preceding section, we restrict discussion to the case of the singlet pairings.

It appears at first sight that Cooper pairing below $T_c$ is always an admixture of s-like and d-like components since the gap equations (31a)~(31d) become coupled whatever type of pairing shows instability at $T_c$. However, it can be seen by inspections of Eqs. (31a)~(31d) that the solutions $\Delta_k$, consisting of pure (s or d) component like $\Delta_s + \Delta_d \eta_k$ and $\Delta_d \xi_k$, are still possible below $T_c$. (Notice the properties analogous to (27).) To see what kind of Cooper pairing, pure or mixed, is realized below $T_c$, it is needed to examine the free energy. We do this in the Ginzburg-Landau region following Leggett.23

The free energy is expressed in terms of the gap parameter $\Delta_k$ and the pair amplitude $F_k=\langle c_k, c_{-k} \rangle = (\Delta_k/2\xi_k) \cdot \text{th}(\beta E_k/2)$ like

$$ F[\Delta_k; T] = F_0(T) + 2\sum_k \Delta_k d F_k^* + \sum_{k,k'} F_k^* V_{k,k'} F_{k'}, $$

(cf., Eqs.(5.49) or (5.82) of Ref. 23), where $V_{k,k'}$ stands for $V_{k,k'}^{\text{singlet}}$, (29). We expand $F_k$ in powers of $\Delta_k$:

$$ F_k = \Delta_k \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} + \frac{\Delta_k |\Delta_k|^2}{2d(\xi_k^2)} \frac{d}{d(\xi_k^2)} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} + O(\Delta^4). $$

Substituting this into (47) and performing the integration concerning $\Delta_k$, we have

$$ F[\Delta_k; T] = F_0(T) + \sum_k \left[ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} - \frac{3}{2} |\Delta_k|^4 \frac{d}{d(\xi_k^2)} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \right] $$

$$ + \sum_{k,k'} \left\{ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \Delta_k V_{k,k'} \Delta_k^* \left[ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} + \frac{\Delta_k |\Delta_k|^2}{2d(\xi_k^2)} \frac{d}{d(\xi_k^2)} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \right] + \text{c.c.} \right\}. $$

Using Eqs. (29a) and (29b) for $V_{k,k'}$ and (30) for $\Delta_k$ and performing the $k, k'$-sum in (49), after tedious calculations we find the form of the free energy up to terms of order $\Delta^4$ as follows:

$$ F[\Delta_k; T] = F_0(T) + \Phi_1 (1 + U \Phi_1) |\Delta_s|^2 + \Phi_1 (1 - \frac{g_3}{3} \Phi_1) |\Delta_d|^2 - 2g_3 \Phi_1 \Phi_1 (\Delta_s^* \Delta_s + \text{c.c.}) $$

$$ + \Phi_2 \left( \frac{3}{2} + 2U \Phi_1 \right) \chi_1 |\Delta_s|^2 + \left( \frac{3}{2} - \frac{2}{3} g_3 \Phi_1 \right) \chi_1 |\Delta_d|^4 + \left( \frac{3}{2} - \frac{2}{3} g_3 \Phi_1 \right) \chi_1 (|\Delta_s|^4 + |\Delta_d|^4) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_2 (2|\Delta_s|^2 |\Delta_d|^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_3 (2|\Delta_s|^2 |\Delta_d|^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_4 (2|\Delta_s|^2 + |\Delta_d|^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_5 (2|\Delta_s|^2 + |\Delta_d|^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2 + (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_6 (2|\Delta_s|^2 + |\Delta_d|^2 - (\Delta_s^* \Delta_s + \text{c.c.})^2 - (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ + \left( \frac{3}{2} + U \Phi_1 - \frac{g_3}{3} \Phi_1 \right) \chi_7 (2|\Delta_s|^2 + |\Delta_d|^2 - (\Delta_s^* \Delta_s + \text{c.c.})^2 - (\Delta_s^* \Delta_s + \text{c.c.})^2) $$

$$ \cdot \left[ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} - \frac{3}{2} |\Delta_k|^4 \frac{d}{d(\xi_k^2)} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \right]$$

$$ + \left[ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \Delta_k V_{k,k'} \Delta_k^* \left[ \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} + \frac{\Delta_k |\Delta_k|^2}{2d(\xi_k^2)} \frac{d}{d(\xi_k^2)} \frac{\text{th} \frac{1}{2} \beta \xi_k}{2 \xi_k} \right] + \text{c.c.} \right\}. $$

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\[ +\left(\frac{3}{2} - \frac{g_s}{3} \Phi_\tau - \frac{g_s}{3} \Phi_\delta\right)\chi_{\tau\alpha}[2|\Delta_\tau|^2(|\Delta_\tau|^2 + |\Delta_\delta|^2) + (\Delta_\tau^* \Delta_\tau + c.c.)^2 + (\Delta_\tau \Delta_\delta + c.c.)^2] + \left(\frac{3}{2} - \frac{2}{3} g_s \Phi_\delta\right)\chi_{\delta\tau}[2|\Delta_\delta|^2|\Delta_\delta|^2 + (\Delta_\delta^* \Delta_\delta + c.c.)^2] - 2g_s[(\Phi_\tau_\chi_1 + 3 \Phi_\tau_\chi_3)|\Delta_\tau|^2 + (3 \Phi_\tau_\chi_3 + \Phi_\chi_1 \chi_3)|\Delta_\delta|^2 + (\Phi_\tau_\chi_3 + \Phi_\tau \chi_2)|\Delta_\delta|^2 + (\Phi_\tau \chi_2 + \Phi_\chi_1 \chi_2)|\Delta_\tau|^2] - 2g_s(\Phi_\tau_\chi_3 + \Phi_\chi_1 \chi_2)(\Delta_\tau^* \Delta_\tau + c.c.)(\Delta_\tau^* \Delta_\delta + c.c.) + 2g_s(\Phi_\tau_\chi_3 + \Phi_\chi_1 \chi_2)(|\Delta_\tau|^2(\Delta_\tau^* \Delta_\tau + c.c.) + (\Delta_\delta^* \Delta_\delta + c.c.)(\Delta_\tau^* \Delta_\delta + c.c.))] + 2g_s \Phi_\delta[|\Delta_\delta|^2(\Delta_\tau^* \Delta_\tau + c.c.) + (\Delta_\delta^* \Delta_\delta + c.c.)(\Delta_\tau^* \Delta_\delta + c.c.)], \tag{50} \]

where the \( \chi \)'s are defined as follows:

\[
\chi_\tau = \frac{1}{N} \sum_k \eta_k^2 Q_k, \quad \chi_\delta = \frac{1}{N} \sum_k \gamma_k^2 Q_k = \frac{1}{N} \sum_k \xi_k^2 Q_k, \\
\chi_{\tau\tau} = \frac{1}{N} \sum_k \gamma_k^4 Q_k, \quad \chi_{\tau\delta} = \frac{1}{N} \sum_k \gamma_k^2 \eta_k^2 Q_k = \frac{1}{N} \sum_k \gamma_k^2 \xi_k^2 Q_k, \\
\chi_{\delta\delta} = \frac{1}{N} \sum_k \eta_k^4 Q_k = \frac{1}{N} \sum_k \xi_k^4 Q_k, \quad \chi_{\tau\tau} = \frac{1}{N} \sum_k \eta_k^2 \gamma_k Q_k, \\
\chi_{\tau\tau} = \frac{1}{N} \sum_k \gamma_k^2 \xi_k Q_k; \quad Q_k = \frac{d}{d(\xi_k^2)} \cdot [\text{th}(\beta \xi_k)/2] / 2 \xi_k < 0. \tag{51} \]

The equations determining the transition temperature is obtained from the quadratic terms of (50), and are nothing but Eqs. (32) and (33). The quartic terms determine the relative magnitudes of the parameters \( \Delta_1, \Delta_\tau, \Delta_\delta \) and \( \Delta_\tau \) below \( T_c \).

Since there are no terms like \( (s\text{-like } \Delta)^3 \cdot (d\text{-like } \Delta)^* \) in (50), if it is an s-like pairing that shows instability at \( T_c \) there are no admixtures of d-like components at least near \( T_c \). (See §5E of Ref. 23.) This is consistent with the results by Anderson and Morel who examined in detail the problem concerning the relative mixing of spherical harmonics with different angular momentum for the zero-temperature case of an isotropic Fermi liquid.24J

If \( \Delta_1 \) and \( \Delta_\tau \) were zero below \( T_c \) at which d-like pairings occur, the free energy (50) would reduce to

\[
F[\Delta_\tau, \Delta_\delta; T] = F_0(T) + \Phi_\delta \left(1 - \frac{g_s}{3} \Phi_\delta\right)(|\Delta_\tau|^2 + |\Delta_\delta|^2) + \left(\frac{3}{2} - \frac{2}{3} g_s \Phi_\delta\right)\chi_{\tau\alpha}[|\Delta_\tau|^3 + |\Delta_\delta|^3] + \chi_{\tau\tau}[2|\Delta_\tau|^2|\Delta_\delta|^2 + (\Delta_\tau^* \Delta_\delta + c.c.)^2]. \tag{52} \]

Considering the inequality \( \chi_{\tau\delta} < \chi_{\tau\tau} < 0 \), by an elementary algebra the solution which minimizes (52) is shown to satisfy

\(^*\) The reason why such terms vanish is that \( (1/N) \sum_k \gamma_k Q_k = (1/N) \sum_k \xi_k Q_k \) and \( (1/N) \sum_k \gamma_k Q_k \) vanish at all.
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\[ \frac{\Delta_t}{\Delta_s} = \pm i \quad \text{or} \quad \Delta_s \Delta_t + \text{c.c.} = 0 , \]  

(53)

that is, the gap parameter of the purely d-like pairing below \( T_c \) (if it were possible) takes the form like

\[ \Delta_t^d = \Delta(\eta \pm i \xi) . \]  

(54)

In this case, however, s-like components inevitably mix to Eq. (54). To illustrate this, let us take the gap as \( \Delta_h = \Delta_h^d + \Delta_t + \Delta_t \gamma \). If \( \Delta_t \) and \( \Delta_t \gamma \) are finite, they will give positive contribution to the free energy (50) up to the quadratic terms like \(|\Delta_t|^2\), \(|\Delta_t \gamma|^2\) and \((\Delta_t^* \Delta_t + \text{c.c.})\). On the other hand, there exist linear terms in \( \Delta_t \) and \( \Delta_t \gamma \); indeed, the last term of (50) has such form

\[ - \chi_{\pi i} \left[ \left( \frac{g_+}{3} \right) \Phi_t g_\Phi \Phi_t (\Delta_t^* \Delta_t + \text{c.c.}) + 2 g_4 \Phi_t (\Delta_t^* \Delta_t + \text{c.c.}) \right] |\Delta_t|^2 , \]  

(55)

where the terms proportional to \((\Delta_t^* \Delta_t + \text{c.c.})\) have been omitted due to Eq. (53). By a suitable choice of \( \Delta_t \) and \( \Delta_t \gamma \), the linear term (55) can always dominate the quadratic terms; therefore, by adding the admixture of s-like components, the free energy can be decreased. However, the ratio \( \Delta_t / \Delta \) or \( \Delta_t / \Delta \gamma \) is at most of order \((T_c - T) / T_c\).

From (23), (24) and (30), the excitation energy \( E_h \) is in general written as follows:

\[ E_h = \sqrt{1 + |\Delta_t|^2 / t^2} \cdot \sqrt{\bar{\xi}_s^2 + \bar{\Delta}_s^2} , \]  

(56)

where

\[ \bar{\xi}_s = \frac{\xi_s - \text{Re}(\Delta_t^* \Delta_h / t)}{\sqrt{1 + |\Delta_t|^2 / t^2}} , \]  

(57a)

\[ \bar{\Delta}_s = \sqrt{\left\{ |\Delta_h|^2 + \frac{1}{2} [ |\Delta_t|^2 |\Delta_t|^2 - \text{Re}(\Delta_t^* \Delta_h)^2 ] / t^2 \right\} / (1 + |\Delta_t|^2 / t^2)} \]  

(57b)

and

\[ \bar{\Delta}_h = \Delta_t + \Delta_t \eta \xi + \Delta_t \xi \xi . \]  

(57c)

The excitation spectrum (56) has the same structure as that previously discussed in Ref. 19. (See Eqs. (4) and (5) of Ref. 19) in which only the gap parameters \( \Delta_t \) and \( \Delta_t \gamma \), denoted by \( \Delta + \xi \Delta' \) and \( \Delta' \), respectively, appeared.)

The above discussions show that two kinds of pairing are possible below the transition temperature; (1) purely s-like pairing, or (2) d-like pairing with admixtures of s-components. According to the discussion in §3, case (1) is realized for the interaction parameter \( g_3 > t \). In this case, from (31a), the relation between \( \Delta_t \) and \( \Delta_t \gamma \) is given like

\[ \Delta_t = \frac{1}{N} \sum_k (U - 2 g_3 \gamma_k) \gamma_k \frac{\text{th} \frac{1}{2} \beta E_k}{2 E_k} \Delta_t \]  

\[ 1 + \frac{1}{N} \sum_k (U - 2 g_3 \gamma_k) \frac{\text{th} \frac{1}{2} \beta E_k}{2 E_k} \]  

(58)
The summations over $k$ in (58) are estimated as follows:

$$\frac{1}{N} \sum_k (U - 2g_\lambda \gamma_k) \frac{\beta E_k}{2E_k} \sim U \frac{\Delta_s}{t} \left( \frac{\Delta_s}{A} \right) \frac{g_3}{2t^2} \frac{\Lambda}{t} \approx \frac{3g_3}{t},$$

$$\frac{1}{N} \sum_k (U - 2g_\lambda \gamma_k) \frac{\beta E_k}{2E_k} \sim \frac{U}{2A \ln (\Delta_s / T)} \left( \frac{\Delta_s}{t} \right) \frac{g_3}{t} \frac{\Lambda}{T} \approx \pi \ln \left( \frac{6t}{\Delta_s / T} \right),$$

where we have assumed $\Delta_s \approx t$, $\Delta_s \ll \Lambda$, $U \approx 2\pi A$, and $\Lambda = 6t$, and have used the abbreviation $(\Delta_s, T)$ which denotes the larger one of $\Delta_s$ and $T$. So, the excitation (56) (with $\Delta_s$ and $\Delta_t$ taken to be zero) has no nearly gapless nature, in contrast to the results of Ref. 19. (But see the following section.) If $g_\lambda < t$, case (2) is realized. In this case, near $T_c$ the gap consists almost of d-components and as $T$ decreases s-like admixtures grow. Unless the transition temperatures for d-pairing and s-pairing are very close, the relative amplitude of s-like components is expected to be small and grow only in the temperature region $T \ll T_c$. Since the gap (54) of d-like character has point like nodes at the Fermi surface in the $(1, 1, 1)$ and equivalent directions, the excitation (56) may show the nearly gapless nature. Indeed, until the s-like component $\Delta_s$ grows well the specific heat and the nuclear relaxation rate would show the ABM-like behaviors; as $\Delta_s$ grows, unusual behaviors are expected. In particular, the nuclear relaxation rate $1/T_1$ may show bump discovered by Kitaoka et al. for CeCu$_2$Si$_2$. Such problems certainly deserve more investigations, which we shall do in a future publication.

§ 5. Concluding remarks

We would like to comment on couple of points which we have implicitly by-passed in the preceding sections.

First, we have discussed the properties of the superconducting state assuming the simple cubic lattice. The results of §3, i.e., the transition temperature for various types of pairings, would not be changed qualitatively even if other types of lattice structures were adopted; neither would the results of §4 on the possible types of mixing of s-pairings and d-pairings below $T_c$. However, whether the excitation energy of a purely d-like pairing is gapless or not might depend on the lattice structure. This problem seems to deserve more investigations.

Second, we have neglected the renormalization effect on various quantities of heavy fermions due to the interaction with phonons. This effect is expressed symbolically in the way that dimensionless coupling constant $IV(0)$ (relevant to the Cooper pair formation) is renormalized to $\Gamma(1+\lambda)^{-2}N(0)(1+\lambda)=\Gamma N(0)(1+\lambda)^{-1}$, where $\lambda$ denotes a dimensionless coupling constant of the particle-phonon interaction. However, since dimensionless coupling constants $g_s/\lambda$, $g_\varepsilon/\lambda$ and $g_t/\lambda$ of the present model are at most of order unity, qualitative results of the preceding sections would not be changed if such effect were taken into account.

Third, the bare density of states of normal heavy fermions might take the pseudo-gap.

*) The gap parameter (54) has a counterpart in the general theory of d-wave pairing in an isotropic Fermi liquid discussed by Mermin. The structure of (54) corresponds to that in Region II of Mermin. (See Eq. (20) of Ref. 25.)
structure, which has been proposed by Bredl et al.\textsuperscript{24} to explain the temperature dependence of the specific heat of CeCu$_2$Si$_2$, and was also included implicitly in JMK.\textsuperscript{20}

Indeed, along JMK such structure is obtained for the density states of heavy fermions, if the conduction electron band reflecting the lattice symmetry is used. Moreover, recent experiment on the nuclear relaxation above $T_c$ for CeCu$_2$Si$_2$\textsuperscript{9} was claimed to suggest an existence of structural phase transition which may cause the pseudo-gap structure of the density of states. Such structure is favorable for the occurrence of the s-like pairing which is relevant to the interaction $-\frac{1}{3} g_s \gamma_s \gamma_v$, and results in a nearly gapless excitation spectrum as that of Ref. 19).

Finally, the effect of scattering by nonmagnetic impurities is certainly crucial for the occurrence of superconductivity in the present system whose band structure is very anisotropic. For such systems, quantitative results by the conventional treatments\textsuperscript{27} of its effect are to be considerably modified. Future work on this problem is planned.

Appendix A

In this appendix, we present calculations of asymptotic forms for $\beta t > 1$ of $\Phi_1(\beta)$, $\Phi_2(\beta)$, $\Phi_3(\beta)$, and $\Phi_4(\beta)$.

From the definition (34a), $\Phi_1(\beta)$ can be written as

$$
\Phi_1(\beta) = \int_{-\infty}^{\infty} d\xi \rho(\xi) \frac{\text{th} \frac{1}{2} \beta \xi}{2 \xi},
$$

where $\rho(\xi)$ denotes the density of states. Taking the $\beta$-derivative of (A-1) and performing the partial integration of $\xi$, we have

$$
\frac{d\Phi_1(\beta)}{d\beta} = -\frac{1}{2\beta} \int_{-\infty}^{\infty} d\xi \frac{d\rho}{d\xi} \text{th} \frac{1}{2} \beta \xi .
$$

Then, since $\Phi_1(0) = 0$,

$$
\Phi_1(\beta) = \frac{1}{2} \int_0^t d\lambda \frac{1}{\lambda} \int_{-\infty}^{\infty} d\xi \left( -\frac{d\rho}{d\xi} \right) \text{th} \frac{1}{2} \lambda \xi .
$$

So,

$$
\lim_{\beta \to \infty} \Phi_1(\beta) \approx \frac{1}{2} \int_0^t d\lambda \frac{1}{\lambda} \int_{-\infty}^{\infty} d\xi \left( -\frac{d\rho}{d\xi} \right) \text{sgn} \xi \approx \rho(0) \ln \beta t .
$$

For the simple cubic lattice, $\rho(0)$ has been calculated numerically as\textsuperscript{38}

$$
\rho(0) = 0.1427 \frac{1}{t} .
$$

Substituting this into (A-3), we obtain

$$
\lim_{\beta \to \infty} \Phi_1(\beta) \approx 0.1427 \frac{1}{t} \ln \beta t .
$$

The result of numerical calculation for the asymptotic form of $\Phi_2(\beta)$ is
From the definition (38), $\Phi_\nu(\beta)$ is calculated as follows:

$$
\Phi_\nu(\beta) = \int_{-\infty}^{\infty} d\xi \frac{1}{N} \sum \delta (\xi - 2t (\cos k_x a + \cos k_y a + \cos k_z a)) \sin^2 k_x a \left( \text{th} \frac{1}{2} \beta \xi \right) = \int_{-\infty}^{\infty} d\xi \frac{1}{2\beta} \frac{1}{\beta} \int_{-\infty}^{\infty} ds e^{-ist} \left( \frac{a}{2\pi} \int_{-\infty}^{\infty} dx \sin^2 k_x a e^{2ist \cos k_y a} \right) x \left( \frac{a}{2\pi} \int_{-\infty}^{\infty} dy e^{2ist \cos k_z a} \right)$$

Similarly, the density of states $\rho(\xi)$ is written as

$$
\rho(\xi) = \frac{1}{N} \sum \delta (\xi - 2t (\cos k_x a + \cos k_y a + \cos k_z a)) = \frac{1}{2\pi} \int_{-\infty}^{\infty} du e^{-ist} J_0(u).$$

Define a function $I(\xi)$ by

$$
I(\xi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} du e^{-ist} J_0(1) J_0(u).$$

By a straightforward calculation, the following relation is shown to hold:

$$
\frac{dI(\xi)}{d\xi} = -\frac{\xi}{2t^2} \rho(\xi).$$

Taking $\beta$-derivative of this relation, and using (A·10), after integrating by parts concerning $\xi$, we obtain

$$
\frac{d\Phi_\nu(\beta)}{d\beta} = \frac{1}{\beta} \frac{1}{2t^2} \int_{-\infty}^{\infty} d\xi \rho(\xi) \xi \text{th} \frac{1}{2} \beta \xi.$$

From the definition (34b), $\Phi_\nu(\beta)$ is equal to a coefficient of $1/\beta$ in (A·11). Then, substituting (A·6) into this, we obtain

$$
\frac{d\Phi_\nu(\beta)}{d\beta} = \frac{1}{12\beta} \Phi_\nu(\beta).$$

Since $\Phi_\nu(0) = 0$,

$$
\Phi_\nu(\beta) = \frac{1}{12} \int_0^\beta d\lambda \frac{1}{\lambda} \Phi_\nu(\lambda).$$

So, using (A·6), we obtain
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\[
\lim_{\beta \to \infty} \Phi_\beta(\beta) \approx \frac{1}{12} \int d\lambda \frac{1}{\lambda} \Phi_\lambda(\infty) \approx \frac{1}{12t} \ln \beta t.
\]  

(A·12)

From the definitions (34a–c) and (38), one can see the following relation holds:

\[
2 \Phi_\alpha(\beta) + \Phi_\beta(\beta) = \frac{36}{N_x} \sum \cos^2 k_x a \frac{\sinh \frac{1}{2} \beta \xi_k}{2 \xi_k} = 36 (\Phi_1(\beta) - \Phi_\alpha(\beta)).
\]

So,

\[
\Phi_\beta(\beta) = 18 [\Phi_1(\beta) - \Phi_\alpha(\beta)] - \frac{1}{2} \Phi_\beta(\beta).
\]  

(A·13)

If we substitute the asymptotic forms of \(\Phi_1\), \(\Phi_\alpha\) and \(\Phi_\beta\) (Eqs. (A·5), (A·12) and (A·6)), we obtain the asymptotic form of \(\Phi_\beta(\beta)\) as

\[
\lim_{\beta \to \infty} \Phi_\beta(\beta) \approx 18 \left( 0.1427 \frac{1}{t} - \frac{1}{12} \frac{1}{t} \right) \ln \beta t = 1.069 \frac{1}{t} \ln \beta t.
\]  

(A·14)

Appendix B

In this appendix, calculations of \(\Phi_1(\beta)\), \(\Phi_\beta(\beta)\), \(\Phi_\delta(\beta)\) and \(\Phi_\delta(\beta)\) to \(O(\beta^3)\) are presented.

From the definition (34a), \(\Phi_1\) is expanded up to \(O(\beta^3)\) as

\[
\Phi_1(\beta) \approx \frac{1}{N_x} \sum \frac{1}{2 \xi_k} \frac{\beta \xi_k}{2} \left( 1 - \frac{1}{12} \beta^2 \xi_k^2 \right) = \frac{\beta}{4} \frac{1}{N_x} \sum \left( 1 - \frac{\beta^2}{12} \xi_k^2 \right).
\]  

(B·1)

Similarly, for \(\Phi_\beta\), \(\Phi_\delta\) and \(\Phi_\delta\) (Eqs. (34b), (34c) and (38), respectively), the following are obtained:

\[
\begin{align*}
\Phi_\beta(\beta) &\approx 3 \beta \frac{1}{N_x} \sum (\cos^2 k_x a + 2 \cos k_x a \cos k_x a) \left( 1 - \frac{\beta^2}{12} \xi_k^2 \right), \\
\Phi_\delta(\beta) &\approx 3 \beta \frac{1}{N_x} \sum (\cos^2 k_x a - \cos k_x a \cos k_x a) \left( 1 - \frac{\beta^2}{12} \xi_k^2 \right), \\
\Phi_\delta(\beta) &\approx \frac{\beta}{4} \frac{1}{N_x} \sum \sin^2 k_x a \left( 1 - \frac{\beta^2}{12} \xi_k^2 \right).
\end{align*}
\]  

(B·2) \hspace{1cm} (B·3) \hspace{1cm} (B·4)

Since \(\xi_k\) is given by (24) and (25), the \(k\)-sum in Eqs. (B·1)–(B·4) are elementary performed:

\[
\begin{align*}
\Phi_1(\beta) &\approx \frac{\beta}{4} \left( 1 - \frac{1}{2} \beta^2 t^2 \right), \\
\Phi_\beta(\beta) &\approx \frac{3 \beta}{2} \left( 1 - \frac{5}{4} \beta^2 t^2 \right), \\
\Phi_\delta(\beta) &\approx \frac{3 \beta}{2} \left( 1 - \frac{1}{4} \beta^2 t^2 \right), \\
\Phi_\delta(\beta) &\approx \frac{\beta}{8} \left( 1 - \frac{5}{12} \beta^2 t^2 \right).
\end{align*}
\]  

(B·5) \hspace{1cm} (B·6) \hspace{1cm} (B·7) \hspace{1cm} (B·8)
References

13) C. M. Varma, April 1984 Preprint.
23) A. J. Leggett, Rev. Mod. Phys. 47 (1975), 331, §5E.
28) T. Morita and T. Horiguchi, Table of the Lattice Green’s Function for the Cubic Lattices (1971), Tohoku University.

Note added in proof: After we submitted the present paper, we received a preprint from F. Ohkawa and H. Fukuyama who treated a similar model to ours but in a different way. (J. Phys. Soc. Jpn., to be published.)