Nearly Gapless Singlet-Pairing in Pure System of Heavy Fermion Superconductor

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Cooper pairing in heavy fermion system, in which the interaction on the same site is repulsive and that between the neighbour sites is attractive, is discussed. The conclusion is that a nearly gapless s-wave pairing is possible, which is consistent with existing experiments of heavy fermion superconductors.

Heavy fermion superconductors, recently found in compounds with f-electrons (such as CeCu$_2$Si$_2$ and UBe$_13$), have attracted much attention.$^{1-6}$ One of the recent issues is concerning the type of Cooper pairing; singlet (even parity) or triplet (odd parity) type? Although a nature of heavy fermion itself has not been completely clarified from a theoretical point of view, it is likely from experimental evidences that heavy fermions behave as a fermi liquid with very small Fermi energy of order $T_K$. There was an attempt to explain, along this line, heavy fermion superconductors within the singlet BCS scheme.$^1$ Since the motion of heavy fermion is slower than those of light-electrons and ions, the Coulomb interaction between heavy fermions is screened instantaneously by rapid motions of the latter; so that the interaction potential in $k$-space between heavy fermions is given by $V_k=4\pi\varepsilon^2/k^2\varepsilon(k,0)>0$, where $\varepsilon(k,0)$ is the static dielectric constant. The reason why the triplet case is considered to be a likely possibility seems to be that $V_k$ is positive for the whole regions of $k$-space. Indeed, several theorists have recently claimed that the triplet pairing is the most likely possibility.$^{8,9}$ However, the present authors recently pointed out that $s$-wave pairing is still possible owing to the spatial correlations among particles, at least in principle, even if $V_k$ is always positive.$^{10}$

The experimental results concerning the above issues are also very controversial. For CeCu$_2$Si$_2$, Assmus et al.$^6$ claimed that the Landau parameter $R_0^e$ is positive which is in favour of singlet pairing. On the other hand, Ott et al.$^6$ recently showed that the low temperature specific heat of UBe$_{13}$ exhibits $T^4$-dependence, which is in favour of the $p$-wave superconductivity of ABM-type. Moreover, Kitaoka et al.$^{11}$ recently found an unusual nuclear relaxation for CeCu$_2$Si$_2$ which cannot be understood by neither $s$-wave scheme of simple BCS-type nor $p$-wave scheme of ABM-type.

The purpose of this paper is to point out that a singlet-pairing with nearly gapless excitations is possible for a model in which the interaction between fermions on the same site is strongly repulsive while that on the neighbour sites is appropriately attractive, and that consequences of this model are consistent with existing experiments of heavy fermion superconductors. In particular, a puzzling behavior of nuclear relaxation of CeCu$_2$Si$_2$ found by Kitaoka et al.$^{11}$ is qualitatively explained by this model.

On the basis of a quasi-particle theory of Kondo lattice,$^{10,12}$ we simulate a heavy fermion system as a half-filled band of fermions with a Hamiltonian

$$
H = -\frac{1}{2} \sum_{\langle i,j \rangle} t(a_i a_j + h. c.) - \mu \sum_i n_i \\
+ \sum_i (U n_i n_{i+1} - \frac{1}{2} \sum_{\langle i,j \rangle} g n_{i} n_{j}) \tag{1}
$$

where $i$ and $j$ are in the nearest-neighbour (n. n.) sites, $\mu$ is the chemical potential, the repulsive interaction $U>0$ is related to the band width $(2\Lambda)$ as $U \sim 2\pi \Lambda$, and the attractive interaction $-g<0$ is assumed to stem from the electron-phonon interaction. A requirement that $V_k>0$ is expressed in this case as $V_k=U - \gamma g > 0$, where $\gamma_k=\sum_{\langle i,j \rangle} \exp[ik \cdot (R_i-R_j)]$.

To take the $s$-wave Cooper pairing correlations into account, we introduce gap parameters $\Delta$ and $\Delta'$:

$$
\Delta = U \langle a_i a_i \rangle \quad \text{and} \quad \Delta' = -g \langle a_i a_i \rangle \tag{2}
$$

From the point of view that heavy fermion systems are "Brinkman-Rice" Fermi liquid,$^{13,14}$ $U \sim 4\Lambda$. 

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where $\Delta'$ is independent of a choice of a pair of n.n. sites $(i, j)$ owing to the s-wave character of the Cooper pair. Using (2), an effective Hamiltonian in the mean field approximation is given by

$$H_0 = \sum_{k} \xi_k a_k^\dagger a_k + \sum_{k} [\Delta_k a_k a_{-k}^\dagger + h.c.], \quad (3)$$

where $\xi_k = -t(\gamma_k - \gamma_0) - \mu$, and $\Delta_k = \Delta + \gamma_k \Delta'$. Now introduce a parameter $x$ defined by $x \equiv \gamma_0 - \mu / t$. This is exactly equal to zero, if all the transfers between n.n. site are the same and the band is half-filled, as is the case for Hamiltonian (1). However, for the actual system (such as CeCu$_2$Si$_2$), there is anisotropy in the n.n. transfer as well as in the attractive interaction $-g$ between n.n. site. So, we parametrize these effects by $x$, leaving the form of Hamiltonian (2) unchanged. Then $k$-dependent gap parameter $\Delta_k$ is written as $\Delta_k = \Delta + x \Delta' / t^\prime \xi_k$.

As usual, an excitation spectrum of Hamiltonian (3) is given by

$$E_k = \sqrt{1 + \Delta'^2 / t^\prime 2} \xi_k^2 + \Delta^2, \quad (4)$$

where

$$\xi_k = \xi_k - \frac{\Delta + x \Delta'}{t^\prime (1 + \Delta'^2 / t^\prime 2}},$$

and

$$\Delta_k = \frac{\Delta + x \Delta'}{1 + t^\prime / \xi_k^2}. \quad (5)$$

The pair wave function is also given by usual formula $\langle a_k^\dagger a_{-k} \rangle = \Delta_k / 2E_k$. Substituting this relation into (2), we obtain self-consistent equations for $\Delta$ and $\Delta'$ as follows:

$$\begin{align*}
\Delta &= -U \frac{1}{Nz} \sum_k \Delta + x \Delta' - \frac{\Delta^2}{t^\prime} \xi_k \text{th} E_k / 2T, \\
\Delta' &= g \frac{1}{2z} \sum_k \gamma_k \Delta + x \Delta' - \frac{\Delta'^2}{t^\prime} \xi_k \text{th} E_k / 2T, \quad (6)
\end{align*}$$

where $z$ is the number of nearest-neighbour.

Equation (6) is reduced to the following:

$$\Delta + x \Delta' = \Delta' \frac{x + U \sum_k \xi_k / 2E_k \text{th} E_k / 2T}{1 + U \sum_k \xi_k / 2E_k \text{th} E_k / 2T}. \quad (7)$$

It is rather complicated to solve Eqs. (7) and (8) self-consistently. So hereafter we investigate the following cases: Case (a), $x=0$; Case (b), $|x|<1$; Case (c), $|x|<1$ and $U>|\Delta|$.

**Case (a):** From Eq. (8), one can see that the excitation is gapless, i.e., $\Delta_g = 0$ and $E_k = (1 + \Delta'^2 / t^2)^{1/2} \xi_k$. Substituting these into Eq. (7), we have an equation determining $\Delta'$ as follows:

$$\begin{align*}
\Delta' \left[ 1 - \frac{g}{2z} \frac{1}{Nz} \sum_k \xi_k^2 \right] = \frac{1}{1 + \Delta'^2 / t^2} \frac{\text{th} E_k / 2T}{E_k / 2T},
\end{align*}$$

which has non-trivial solution for $g>2Nt^2z / \Sigma \xi_k^2 = g_c$. It should be remarked that there is a threshold value of $g_c$ for Eq. (9) to have a solution $\Delta'>0$. If constant density of states is assumed, $g_c$ is estimated as $4t'^2 \lambda / (\lambda + U / 2\lambda)$, which satisfies the condition $V_k>0$. From Eq. (9), $\Delta'$ ($T=0$), the transition temperature $T_c$, and the ratio $\Delta\sqrt{C_n(T_c)}$ of specific heat jump at $T_c$ to normal specific heat at $T_c$, etc., are given by usual procedures.

**Case (b):** From Eq. (8), we obtain

$$\Delta + x \Delta' = \frac{x \Delta'}{1 + c_1 \ln \frac{c_2 A}{\max(x \Delta', T)}} < \Delta', \quad (10)$$

where $c_1$ and $c_2$ are numerical constants of order unity. On the accuracy that $O(x^2)$ is neglected compared to unity, Eq. (7) is reduced to Eq. (9); i.e., the equation determining $\Delta'$ is essentially the same with that of Case (a). Since the gap parameter $\Delta'$ at $T=0$ is in general the same order with the transition temperature $T_c$, a minimum excitation energy $\omega_0 = \Delta_0 (1 + \Delta'^2 / t^2)^{1/2}$ at $T=0$ (see Eq. (5)) is much smaller than $T_c$. So we call this case nearly gapless.

**Case (c):** From Eq. (8), we obtain

$$\Delta + x \Delta' = \frac{x \Delta'}{1 + s_1 \ln \frac{s_2 A}{\max(x \Delta', T)}} < \Delta', \quad (11)$$

where $s_1$ and $s_2$ are numerical constants of order unity. As far as the quantities of order $(\Lambda / U)(t / \Lambda)^2$ and $(\Lambda / U \ln (U / \Lambda'))^2$ can be neglected compared to unity, Eq. (7) is reduced to Eq. (9)); i.e., the equation determining $\Delta'$ is again essentially the same as that of Case (a). The near-
ly gapless nature also holds for this case. Actual heavy fermion superconductors are likely to be near this case, since $U \sim 2k_\text{F} \Delta^{10}$ or $U \sim 4A^{4,13}$.

A density of states $N_s(E)$ for low-lying excitations given by Eqs. (4) and (5) is as follows:

$$N_s(E) = \begin{cases} \frac{N_n}{\sqrt{1 + \Delta'^2/\ell^2}} \sqrt{E^2 - \Delta'^2(1 + \Delta'^2/\ell^2)} & \text{for } E > \omega_0, \\ 0 & \text{otherwise,} \end{cases}$$

(12)

where $N_n$ is the density of states in the normal state. This leads to an unusual thermodynamic behaviour at low temperature different from that of a simple $s$-wave BCS superconductor. As far as $T > (\omega_0/2)$, exponential specific heat would never be observed (even if $T \ll \omega_0$). This is consistent with the results on the low temperature specific heat of CeCu$_2$Si$_2$ and UBe$_{13}$.\(^6\)

Nuclear relaxation rate: A ratio of the nuclear relaxation rate at superconducting- and normal states is expressed in the form

$$\frac{T_{1n}}{T_{1s}} = 2 \int_0^\infty \frac{dE}{E} \frac{N_s(E)}{N_n} E^2 + (1 - \Delta'^2/\ell^2) \Delta' \left( -\frac{df}{dE} \right),$$

(13)

where $f$ is the Fermi function. If the density of states (12) is used in (13), an integral in (13) diverges logarithmically. But in a real system, the singularity in the density of states $N_s(E)$ is smeared out somewhat owing to the anisotropy of $\Delta_k$ (which cannot be taken into account only through the parameter $x$). The results for $T_{1n}/T_{1s}$ depend in detail on this anisotropy. A peculiar temperature dependence of $T_{1n}/T_{1s}$ stems from the nearly gapless nature of the excitations. Let us denote an integrand in (13) by $P^2(x) (-df/dE)$. A qualitative behaviour of $P^2(x)$ is such that it has rather sharp peak around $x \sim \omega_0/\ell$, and approaches $1/(1 + \Delta'^2/\ell^2)$ as $x$ increases. For $T$ very near $T_c$ such that $T_c \Delta_0 > \Delta'^2$, $T_{1n}/T_{1s}$ is expected to exceed unity as in the usual BCS case.\(^4\) However, this region is limited in very narrow temperature region below $T_c$ (roughly speaking, $(1 - T/T_c) \ll \Delta(T=0)/\Delta'(T=0)$). For the temperatures, $\Delta_0 < T < T_c(1 - [\Delta_0(T=0)/\Delta'(T=0)]^2)$, $T_{1n}/T_{1s}$ decreases rather rapidly as $\Delta'$ grows (so, $P^2(x)$ for $x > \omega_0/\ell$ decreases to $1/(1 + \Delta'^2/\ell^2)$). As $T$ approaches $\omega_0$ (where $\Delta'$ has only weak $T$-dependence), $T_{1n}/T_{1s}$ increases again because a flat part of $P^2(x) \approx 1/\ell$ for $x > \omega_0/\ell$ goes away from the region where the remaining factor $(-df/dE)$ in (13) has appreciable value. Finally for $T < \omega_0$, $T_{1n}/T_{1s}$ decreases again as $\exp(-\omega_0/T)$, which should be compared to $\exp(-\Delta_{\text{BCS}}/T)$ in the simple BCS case.\(^4\)

A behaviour of $T_{1n}/T_{1s}$ for $T \gg \omega_0$ coincides qualitatively with anomalous temperature dependence of $1/T$ observed in CeCu$_2$Si$_2$ by Kitaoka et al.\(^11\)

To make this scenario quantitative, we present a model calculation of $T_{1n}/T_{1s}$ on the basis of the model form of $P(x) = 0$ for $x < 2\omega_0/3\ell$, $P(x) = (3\ell/2)(1 + \Delta'^2/\ell^2)^{-1/2} \approx 2\omega_0/3\ell$ for $2\omega_0/3\ell < x < 2\omega_0/\ell$, $P(x) = (T/14\omega_0)(1 + \Delta'^2/\ell^2)^{-1/2} (29\omega_0/\ell - x)$ for $2\omega_0/\ell < x < 3\omega_0/\ell$, and $P(x) = 1/(1 + \Delta'^2/\ell^2)$ for $3\omega_0/\ell < x$. The results are presented in Fig. 1 together with experimental results by Kitaoka et al.\(^11\)

Qualitative agreement between theory and experiment is fairly good, if the parameters are taken as appropriate values.

![Fig. 1. log$_{10}(T_{1n}/T_{1s})$ vs $T_c/T$. The solid circles with bar are the experimental results by Kitaoka et al.\(^11\) Solid lines (I), (II) and (III) show the results calculated by BCS singlet, ABM triplet models for $l=1$, $m=1$ and $l=1$, $m=0$, respectively.\(^11\) Solid lines (IV) and (V) are the results of the present theory, in which it is assumed that $\Delta'/\ell = 2.0 (1 - T/T_c)^{1/2}$, and $\Delta + x\Delta'/\ell' = 1/10$ for (IV) and 1/20 for (V), respectively. Symbols $\check{V}$ and $\triangleleft$ indicate the position of minimum and of maximum, respectively.](https://academic.oup.com/ptp/article-abstract/72/3/652/1907743/1907743)
Detailed calculations on the specific heat, the nuclear relaxation rate, the upper critical field, the effect of nonmagnetic impurities, etc., will be published elsewhere.

In conclusion, the equal-spin pairing, say \( p \)-wave, is also always possible (i.e., \( g_c = 0 \)) for the systems described by Hamiltonian (1), because the repulsive interaction does not work due to the Pauli principle. Nevertheless, in this case, \( 1/T \) shows no anomalous behaviour such as NMR experiment by Kitaoka et al.\(^1\)

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9) C. M. Varma, April 1984 Preprint.
14) See, for example, P. G. de Gennes, \textit{Superconductivity of Metals and Alloys} (Benjamin, New York, 1966), §4.