Theory on Superconductivity of CeIn$_3$ in Heavy Fermion System

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Heavy fermion compound CeIn$_3$ has been confirmed to exhibit the properties of unconventional superconductivity. For instance, in the $^{115}$In-NQR measurement, no coherence peak has been observed in the temperature dependence of 1/$T_1$. The superconducting (SC) state appears under the pressure $P$ with a critical value $P_c = 2.55$ GPa, and the maximum value of the SC-transition temperature $T_{c,\text{max}} = 0.2$ K. The SC state exists near the antiferromagnetic (AF) phase with the ordering vector $Q = (\pi, \pi, \pi)$ at Ce atoms. The situation strongly suggests that superconductivity should be connected to three-dimensional (3D)-AF spin fluctuations.

In this paper, we assume that the CeIn$_3$ system is given by the Fermi liquid state at low temperatures and study the SC mechanism induced by the wave number dependence in the effective interaction between quasi particles originating from the Coulomb interaction among $f$-electrons. The SC state is considered to be realized on the main Fermi surface of CeIn$_3$, as shown by the Fermi liquid state at low temperatures and study the SC mechanism in 3D CeIn$_3$. The calculation based on TOPT includes also the normal self energy in this study of CeIn$_3$. We treat the wave number dependence originating from the main Fermi surface of CeIn$_3$ and the calculated $T_c$ is reduced by renormalized Fermi energy $E_F$. As a result, we performed a new analysis of CeIn$_3$ in detail on the basis of TOPT. Next, we clarify the suppression of $T_c$ by calculating the dependence of $T_c^{\text{TOPT}}/T_c^{\text{RPA-like}}$ on dimensionality. The change in $T_c$ between 2D and 3D systems applies to that between 2D CeRhIn$_5$ and 3D CeIn$_3$. With regard to CeTIn$_5$ (T=Co, Rh and Ir), Takimoto, Hotta and Ueda$^9$ studied the SC mechanism with a 2D orbital-degenerate Hubbard model. They indicated the appearance of the $d$-wave superconductivity next to the AF magnetic phase in the case where the crystal splitting energy is large. On the other hand, Nishikawa, Ikeda and Yamada$^{11}$ investigated the $d$-wave superconductivity in CeIr$_2$Co$_{1-x}$In$_5$ with the 2D single-band Hubbard model. Here, we apply the single-band model to both CeIn$_3$ and CeRhIn$_5$ due to the following reason. The main Fermi surface of CeIn$_3$ is a single band as shown by the band calculation of Betsuyaku.$^4$ The 3D single band induces the wave number dependence of the AF spin fluctuation, which plays the main role in superconductivity. Both CeIn$_3$ and CeRhIn$_5$ have the same kind of Ce compounds. Therefore, we apply TOPT to the superconductivity in the single band of CeRhIn$_5$ as well as CeIn$_3$. The main difference between the two materials is the dimensionality of the Fermi surface. We clarify the effect of dimensionality on the wave number dependence in the analysis based on TOPT, and moreover, we show the justification of the quasi-2D model in CeRhIn$_5$.

We explain the formulation in the following. The Hubbard Hamiltonian is given by

$$\mathcal{H} = -t_1 \sum_{i,a,\sigma} c^\dagger_{i\sigma} c_{i+a\sigma} + t_2 \sum_{i,b,\sigma} c^\dagger_{i\sigma} c_{i+b\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $c_{i\sigma}$ is an annihilation operator for a quasi particle with spin $\sigma$ at site $i$, $a$ and $i$ are, respectively, the vectors connecting nearest-neighbor and next-nearest-neighbor sites in a simple cubic lattice. Transfer integrals $t_1$ and $t_2$...
$$\phi_0(q) = -\sum_k G_0(k) G_0(q - k).$$  \hspace{1cm} (5)$$

Here, $q$ denotes a short-hand notation $q=(q, \nu_q)$, where $\nu_q=2\pi T n$ is the boson Matsubara frequency. Note that the chemical potential $\mu$, shifted from $\mu_0$, is again determined by the condition $n=\sum_k G(k)$. We show the diagram of the normal self energy in Fig. 1.

An effective pairing interaction $V$ between quasi particles is evaluated using TOPT. Although the origin of superconductivity is investigated by total terms in $V$, in order to analyze the role of $V$ in detail, it is convenient to divide it into two parts as

$$V(k, k') = V_{\text{RPA}}(k, k') + V_{\text{vertex}}(k, k'),$$  \hspace{1cm} (6)$$

where $V_{\text{RPA}}$ represents the terms obtained by the random phase approximation (RPA) and $V_{\text{vertex}}$ indicates the third-order vertex correction terms. The RPA-like term reflects the nature of simple spin fluctuations, while the third-order vertex correction terms originate from the electron correlation other than the spin fluctuations. For singlet pairing, $V_{\text{RPA}}$ and $V_{\text{vertex}}$ are given by

$$V_{\text{RPA}}(k, k') = U + U^2 \chi_0(k-k') + 2U^3 \chi_0^2(k-k'),$$  \hspace{1cm} (7)$$

$$V_{\text{vertex}}(k, k') = 2U^3 \text{Re} \sum_{k''} G_0(k+k''-k') \left( \chi_0(k+k'') - \phi_0(k+k'') \right) G_0(k'').$$  \hspace{1cm} (8)$$

We show the diagrams for singlet pairing in Fig. 2.

An anomalous self-energy $\Sigma_a$ is expressed using $F(k')$ and an anomalous Green’s function $F(k)$ as $\Sigma_a(k) = -\Sigma_b V(k, k') F(k')$. At $T=T_c$, the linearized Eliashberg equation including $\Sigma_a$ and $F(k)$ is reduced to the eigenvalue equation,

$$\lambda \Sigma_a^{\dagger}(k) = -\sum_{k'} V(k, k') \left[ G(k') \right]^2 \Sigma_a(k').$$  \hspace{1cm} (9)$$

When the eigenvalue $\lambda$ becomes unity, the SC state is realized and $T_c$ is obtained. We solve the equation on the assumption that $\Sigma_a^{\dagger}$ has singlet or triplet pairing symmetry. We divide the first Brillouin zone into $64\times 64 \times 64$ momentum meshes and take $N_f=512$ for Matsubara frequency $\omega_n$. The bandwidth $W$ is a necessary range of $\omega_n$ for reliable calculations. The range is covered with the condition: $|W| < \pi T N_f$. To satisfy the condition, we calculate in the region with $T > 0.0037$.

As a result, the dominant symmetries are $d_{x^2-y^2}$ and $d_{3z^2-r^2}$-wave pairings, which are degenerate due to the space symmetry of the cubic system. In Fig. 4, we show the wave number dependence of the anomalous self-energy $\Sigma^A(q, \omega_n = \pi T)$ for $d_{x^2-y^2}$-wave pairing. On the other hand, we did not obtain stable solution in the present calculations for other pairing symmetries such as $d_{xy}$-wave.

We explain in detail the mechanism of the $d$-wave pairing, which indicates $d_{z^2}$ or $d_{3z^2-r^2}$-wave pairing. To describe the main large-volume Fermi surface (see Fig. 3), we choose a parameter set as $t_2 = -0.2$ and $n=0.45$, near the half-filling $n=0.5$. The main Fermi surface with a nesting property enhances the bare suspen-
tibility \( \chi_0(\mathbf{q}, \omega_n) \), due to the feature of 3D-AF spin fluctuations near \( Q=(\pi, \pi, \pi) \), as shown in Fig. 3. The AF spin fluctuation originating from the RPA-like term provides an advantageous contribution to the eigenvalue \( \lambda \) for the \( d \)-wave pairing, as shown in Fig. 5. In the case including only the RPA-like terms, \( \lambda \) always increase with increasing \( U \). However, it is significantly suppressed for a large \( U \) value when all terms in TOPT are taken into account, since the vertex correction terms suppress the \( d \)-wave superconductivity.

Next, we show the \( U \) dependence of \( T_c \) in Fig. 6. Here, it is emphasized that the evaluated \( T_c \) in the unit of \( t_1 \) is consistent with the experimental SC-transition temperature \( T_c=0.2 \) K in the value \( T_c \sim 0.003 \). We estimated the renormalized \( T_c \) with the electron effective mass \( m^* \) obtained by the experiment of dHvA. The details of the estimation are as the follows. The renormalized bandwidth \( W \) is given as \( zW_0 \) with the renormalization factor \( z \). As another relation, \( W \) is given as \( W=12t_1 \) from the \( t_2=-0.2 \). Here, \( W_0 \) is a bare bandwidth. The renormalization factor is defined by \( z=m_0/m^* \) and \( m_0 \) is the bare electron mass. Dispersion \( E_k \) of eq. (2) at \( Q=Q_0 \) is a bare bandwidth. The relation of \( W \) is \( 12t_1=zW_0 \). The bare bandwidth \( W_0 \) is \( 0.1 \) Ry=1.58 \( \times 10^4 \) K in the band calculation. \( z \) is obtained as \( z=1/16 \) using the cyclotron mass of dHvA. From the relation, the renormalized \( t_1 \) is obtained as \( t_1=0.819 \times 10^2 \) K. By means of \( t_1 \), the calculated value \( T_c \sim 0.003(t_1) \) at \( U \sim 9.0 \) corresponds to \( T_c=0.246 \) K, which is near the experimental SC-transition temperature \( T_c=0.2 \) K. Thus, the present calculation for \( T_c \) well explains the possibility of the \( d \)-wave pairing state in CeIn. Because the calculated \( T_c \) on the basis of TOPT is near the experimental SC-transition temperature, we consider that the system has a strong electron correlation \( U \sim 90 \), which is larger than the value of the bandwidth.

Furthermore, it is quite instructive to consider the comparison between 2D and 3D cases. We investigate the effect of dimensionality on the constant strength of the substantial electron correlation. Here, the strength of the substantial electron correlation means the value of \( U \) in comparison with the bandwidth. Thus, \( U/W \) keeps a constant value in the change from 2D to 3D systems. For the same value of \( U/W \sim 3/4 \) \( (t_2=-0.2, n=0.45, W^{3D} \sim 12t_1 \text{ and } W^{2D} \sim 8t_1) \), we obtain \( T_c^{3D} \sim 0.042 \) in a 2D square lattice and \( T_c^{3D} \sim 0.0067 \) in a 3D simple cubic lattice. Namely, \( T_c \) for the 3D system is lower by about one order than that for the 2D system. This is consistent with the experimental findings that \( T_c^{3D} \sim 0.2 \) K for CeIn (3D system) and \( T_c^{2D} \sim 2.1 \) K for CeRhIn \( 5 \) (quasi-2D system). We show in Fig. 7 the change in \( T_c^{TOPT}/T_c^{RPA} \) between 2D and 3D systems obtained by the present calculation using the dispersion

\[
E_k = -2t_1(\cos k_x + \cos k_y + t_z \cos k_z) + 4t_2(\cos k_x \cos k_y + t_z \cos k_y \cos k_z + t_z \cos k_z \cos k_x).
\]

Here, the hopping integrals \( t_1 \) and \( t_2 \) in the c-axis direction are multiplied by \( t_z \). Namely, the dispersion relations with \( t_z=0 \) and 1 correspond to those for the 2D square and 3D simple cubic lattices, respectively. As a result, the suppression of \( T_c \) by the vertex correction is stronger.
in the 3D system than in the 2D system. By including the suppression on the basis of TOPT, the difference in $T_c$ becomes one order between 2D and 3D systems. In addition to this, the decrease in $T_c$ is slight with the increase in the 3D characteristic in the region near the quasi-2D system. Actually, in the range that $t_z$ is small ($t_z = 0 \sim 0.4$), the change in $T_c$ by TOPT is small under the condition that $U/W$ is constant (see the inset of Fig. 3). Therefore, the $T_c$ calculated on the basis of the 2D model is appropriate for CeRhIn$_5$, even if the band structure of CeRhIn$_5$ possesses a weak 3D characteristic.

Here, we explain the different suppression depending on dimensionality in the analysis of TOPT. We consider the wave number dependence of $\chi_0$ on the $k_x-k_y$ plane perpendicular to the $k_z$-axis, as shown in Fig. 3. In the quasi-2D system with AF spin fluctuations, the same prominent peaks exist near $Q=(\pi, \pi)$ on planes at all $k_z$. In the 3D system, $\chi_0$ has prominent peaks around $Q=(\pi, \pi)$ on planes only near $k_z=\pi$. On the other hand, the complex wave number dependence spreads on planes at all $k_z$, as shown in Fig. 3. In the present calculation including the suppression of $T_c$ by the third-order vertex correction, $T_c$ in the 3D cubic systems is lower by one order than that in the 2D square system for the same value of $U/W$, in good agreement with the experimental results for 2D and 3D Ce-based heavy fermion superconductors, CeRhIn$_5$ and CeIn$_3$. It has been pointed out by means of FLEX that the superconductivity induced by AF spin fluctuations is suppressed in the 3D system compared with that in the 2D system$^{7,8}$ but here we stress that the difference is obtained also by means of TOPT including the vertex correction in this paper. Moreover, we found that the suppression of $T_c$ by the vertex correction is stronger in the 3D system than in the 2D system for the same value of $U/W$. A part of this paper is contained in the proceeding of ASR2002.$^{15}$ The authors thank Dr. H. Ikeda, Professo T. Hotta and Professor H. Harima for valuable discussions.
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