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The superconducting mechanism of the heavy-fermion system $CeIn_3$ with three-dimensional properties

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Abstract
On the basis of the three-dimensional Hubbard model, the superconducting (SC) mechanism of $CeIn_3$ under high pressure is investigated by means of third-order perturbation theory with respect to the on-site Coulomb interaction U. Here we propose a d-wave pairing state induced by antiferromagnetic spin fluctuations. The estimated SC transition temperature is lower by one order than that in the two-dimensional system for the same value of U/W (W = bandwidth). This result is consistent with the difference between $CeIn_3$ and $CeRhIn_5$.

1. Introduction

A heavy-fermion compound $CeIn_3$ [1] has been confirmed to exhibit unconventional superconductivity. For instance, in the ^{115}In NQR measurements [2], no coherence peak has been observed in the temperature dependence of $1/T_1$. The superconducting (SC) state appears under pressure P with a critical value $P_c = 2.55$ GPa, and the maximum value of the transition temperature $T_c^{\max} = 0.2$ K. The experimental results [1, 3] suggested that the SC state is related to the antiferromagnetic (AF) phase with the ordering vector $\boldsymbol{Q} = (\pi, \pi, \pi)$ at Ce atoms [3]. The situation strongly suggests that the superconductivity should be connected to 3D AF spin fluctuations.

In this paper, we assume that the $CeIn_3$ system can be described as a Fermi liquid state at low temperatures and study the SC mechanism induced by the wavenumber dependence in the effective interaction between quasi-particles originating from Coulomb interactions among f electrons. The SC state is considered to be realized on the main Fermi surface of Ce 4f electrons [5]. We pursue the possibility of a d-wave pairing state due to AF spin fluctuations near $\boldsymbol{Q} = (\pi, \pi, \pi)$. To describe the heavy fermions, here the 3D Hubbard model is adopted and the effective interaction is evaluated on the basis of third-order perturbation theory (TOPT) in terms of on-site Coulomb interaction [4]. It is concluded that the SC mechanism of $CeIn_3$ is d-wave pairing induced by 3D AF spin fluctuations near $\boldsymbol{Q} = (\pi, \pi, \pi)$.

2. Formulation

The Hubbard Hamiltonian is given by

$$\mathcal{H} = -t_1 \sum_{i,a,\sigma} c^\dagger_{i\sigma} c_{i+a\sigma} + t_2 \sum_{i,b,\sigma} c^\dagger_{i\sigma} c_{i+b\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c_{i\sigma}$ is an annihilation operator for quasi-particles with spin σ at site $\boldsymbol{i}$, $\boldsymbol{a}$ and $\boldsymbol{b}$ are, respectively, the vectors connecting nearest-neighbour and next-nearest-neighbour sites in the simple cubic lattice. The transfer integrals t_1 and t_2 denote nearest-neighbour and next-nearest-neighbour hopping amplitudes, respectively, U is the on-site Coulomb interaction, and $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. Here we consider that the parameters t_1, t_2, and U include a common renormalization factor to construct the heavy fermion. We adjust the dispersion $E_{\boldsymbol{k}}$ so as to reproduce the main Fermi surface of heavy fermions constructed mainly by Ce 4f electrons in the simple cubic structure [5], leading to $E_{\boldsymbol{k}} = -2t_1(\cos k_x + \cos k_y + \cos k_z) + 4t_2(\cos k_x \cos k_y + \cos k_y \cos k_z + \cos k_z \cos k_x)$. As a result, the mass enhancement due to the frequency dependence of the self-energy is included in equation (1). We study mainly the momentum dependence of the effective interactions by means of perturbation theory. Then, we obtain the bare Green function of the quasi-particle as $G_0(k) = 1/[\mathrm{i}\omega_n - (E_k - \mu_0)]$, where k is shorthand notation defined by $k = (\boldsymbol{k}, \omega_n)$, $\boldsymbol{k}$ is the momentum, and $\omega_n = \pi T(2n+1)$ is the fermion Matsubara frequency with temperature T and integer n. Note that the chemical potential μ_0 for the non-interaction case is determined by the electron number n (per site and spin) as $n = \sum_k G_0(k)$, where $\sum_k = (T/N)\sum_{\boldsymbol{k}}\sum_n$ and N is the number of sites. The dressed normal Green function $G(k)$ is given by $G(k) = 1/[\mathrm{i}\omega_n - (E_k - \mu) - \Sigma_n(k)]$, where $\Sigma_n(k)$ is the normal self-energy, given by TOPT with respect to U as

$$\Sigma_n(k) = \sum_{k'} \{U^2 \chi_0(k-k') + U^3[\chi_0^2(k-k') + \phi_0^2(k+k')]\} G_0(k'), \tag{2}$$

with $\chi_0(q) = -\sum_k G_0(k)G_0(q+k)$ and $\phi_0(q) = -\sum_k G_0(k)G_0(q-k)$. Here q is shorthand notation: $q = (\boldsymbol{q}, \nu_n)$, where $\nu_n = 2\pi T n$ is the boson Matsubara frequency. Note that the chemical potential μ, shifted from μ_0, is again determined by the condition $n = \sum_k G(k)$.

An effective pairing interaction V between quasi-particles is evaluated by TOPT. Although the origin of the superconductivity is investigated via total terms in V, in order to analyse the role of V in detail, it is convenient to divide it into two parts: $V(k,k') = V_{\mathrm{RPA}}(k,k') + V_{\mathrm{vertex}}(k,k')$, where V_{RPA} represents the terms obtained from the random phase approximation (RPA) and V_{vertex} indicates the third-order vertex correction terms. The RPA-like term reflects the nature of the simple spin fluctuations, while the third-order vertex correction terms originate from the electron correlations other than the spin fluctuations. For the singlet pairing, V_{RPA} and V_{vertex} are given by

$$V_{\mathrm{RPA}}(k,k') = U + U^2\chi_0(k-k) + 2U^3\chi_0^2(k-k'), \tag{3}$$

$$V_{\mathrm{vertex}}(k,k') = 2U^3\,\mathrm{Re}\sum_{k''} G_0(k+k''-k')[\chi_0(k+k'') - \phi_0(k+k'')]G_0(k''). \tag{4}$$

An anomalous self-energy Σ_a is expressed by using $V(k,k')$ and an anomalous Green function $F(k)$ as $\Sigma_a(k) = -\Sigma_{k'} V(k,k')F(k')$. At $T = T_c$, the linearized Eliashberg equation including Σ_a and $F(k)$ is reduced to the eigenvalue equation $\lambda\Sigma_a^\dagger(k) = -\sum_{k'} V(k,k')|G(k')|^2\Sigma_a^\dagger(k')$. When the eigenvalue λ 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. For the calculations, we divide the first Brillouin zone into $64 \times 64 \times 64$ meshes and the cut-off for the frequency sum is set as $N_f = 512$.

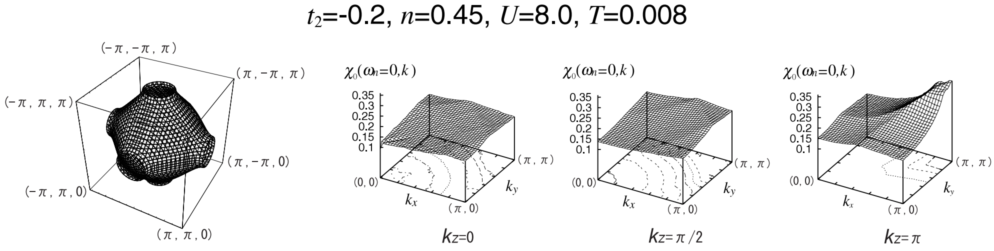

Figure 1. The Fermi surface in a quarter of the first Brillouin zone and the bare susceptibility $\chi_0(\boldsymbol{q}, \nu_n = 0)$.

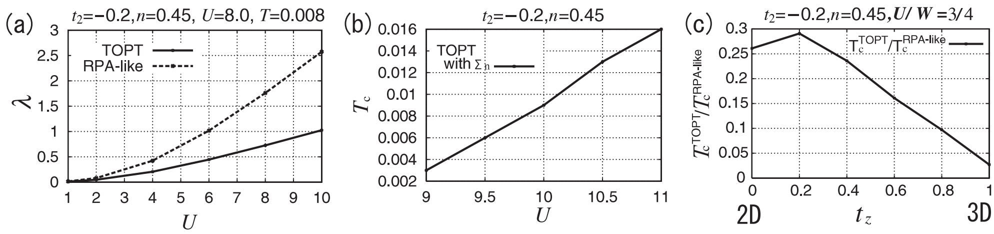

Figure 2. (a) The U-dependence of λ obtained from TOPT and RPA-like terms. (b) The U-dependence of T_c obtained from TOPT. (c) The change in $T_c^{\mathrm{TOPT}}/T_c^{\mathrm{RPA}}$ in going between 2D and 3D systems.

3. Results

The dominant symmetries are $d_{x^2-y^2}$- and $d_{3z^2-r^2}$-wave ones, which are degenerate due to the space symmetry of the cubic system. On the other hand, we do not obtain stable solutions for other pairing symmetries such as the d_{xy}-wave one.

We explain in detail the mechanism of the d-wave pairing, which indicates $d_{x^2-y^2}$- or $d_{3z^2-r^2}$-wave pairing. To describe the main large-volume Fermi surface [5] (see figure 1), we choose the parameter set $t_2 = -0.2$ and $n = 0.45$, near the half-filling $n = 0.5$. The main Fermi surface with nesting properties enhances the bare susceptibility $\chi_0(\boldsymbol{q}, \nu_n)$, due to the feature of 3D AF spin fluctuations near $\boldsymbol{Q} = (\pi, \pi, \pi)$, as shown in figure 1. The AF spin fluctuations originating from the RPA-like term, which provides an advantageous contribution to the eigenvalue λ for the d-wave pairing, are shown in figure 2(a). In the case including only the RPA-like terms, λ always becomes large with increasing U, but it is significantly suppressed for large values of U 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 figure 2(b). Here it is emphasized that T_c evaluated in units of t_1 is consistent with the value $T_c^{\max}/E_F = 0.004$–0.0067 estimated from $T_c^{\max} = 0.2$ K and the Fermi energy $T_F = 30$–50 K. E_F is estimated from the T-dependence of the resistivity [6]. Thus, the present calculation for T_c explains well the possibility of a d-wave pairing state in $CeIn_3$.

Furthermore, it is quite instructive to consider the comparison between two-dimensional (2D) and 3D cases. For the same value of $U/W \sim 3/4$ ($t_2 = -0.2$, $n = 0.45$, $W^{\mathrm{3D}} \sim 12t_1$, and $W^{\mathrm{2D}} \sim 8t_1$), we obtain $T_c^{\mathrm{2D}} = 0.042$ in the 2D square lattice and $T_c^{\mathrm{3D}} = 0.004$ in the 3D simple cubic lattice. That is, T_c for the 3D system is lower by one order than that for the 2D system. This is consistent with the experimental fact that $T_c^{3D} \approx 0.2$ K for $CeIn_3$ (a 3D system) and $T_c^{\mathrm{2D}} \approx 2.1$ K for $CeRhIn_5$ (a quasi-2D system) [7]. We show in figure 2(c) the change in $T_c^{\rm TOPT}/T_c^{\rm RPA}$ in going between 2D and 3D systems obtained by the present calculation using the dispersion $E_{\boldsymbol{k}} = -2t_1(\cos k_x + \cos k_y + t_z \cos k_z) + 4t_2(\cos k_x \cos k_y + t_z \cos k_y \cos k_z + t_z \cos k_z \cos k_x)$. Here the hopping integrals t_1 and t_2 in the direction of the c-axis are multiplied by t_z. That is, the dispersion relations with $t_z = 0$ and 1 correspond to those for the 2D square and 3D simple cubic lattices, respectively. In the result, the suppression of T_c by the vertex corrections is stronger in 3D than in 2D systems.

4. Summary

We have evaluated T_c by using TOPT based on the 3D Hubbard model. It is concluded that the SC mechanism of $CeIn_3$ is $d_{x^2-y^2}$-wave (or $d_{3z^2-r^2}$-wave) pairing, mainly induced by 3D AF spin fluctuations near $\boldsymbol{Q} = (\pi, \pi, \pi)$. In the present calculation including the suppression of T_c by the third-order vertex corrections, T_c in the 3D cubic system 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 the 2D and 3D Ce-based heavy-fermion superconductors $CeRhIn_5$ and $CeIn_3$. It has been pointed out, using FLEX, that superconductivity induced by AF spin fluctuations is suppressed in the 3D system compared with that in the 2D system [8], but here we stress that the difference is confirmed also by using TOPT including the vertex corrections in this paper. Moreover, we have found that the suppression of T_c by the vertex corrections is stronger in the 3D system than in the 2D system for the same value of U/W.

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References

[1] Mathur N D *et al* 1998 *Nature* **394** 39
[2] Kawasaki S *et al* 2002 *Phys. Rev.* B **66** 054521
[3] Morin P J *et al* 1988 *Low. Temp. Phys.* **70** 377
[4] Hotta T 1994 *J. Phys. Soc. Japan* **63** 4126
Jujo T *et al* 1999 *J. Phys. Soc. Japan* **68** 1331
[5] Betsuyaku K 1999 *Thesis* Osaka University
[6] Knebel G *et al* 2002 *Phys. Rev.* B **65** 024425
[7] Hegger H *et al* 2000 *Phys. Rev. Lett.* **84** 4986
[8] Arita R *et al* 1999 *Phys. Rev.* B **60** 14585
Takimoto T and Moriya T 2002 *Phys. Rev.* B **66** 134516