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Study of the anomalously enhanced jump of the specific heat at the superconducting transition point in $CeCoIn_5$

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Abstract

We investigate an anomalously enhanced jump of the electronic specific heat at the superconducting transition point observed in $CeCoIn_5$ within the fluctuation-exchange approximation. The strong antiferromagnetic spin fluctuation leads to strong-coupling superconductivity with a relatively high transition temperature. Simultaneously, the jump of the specific heat becomes large. This tendency also becomes stronger as the antiferromagnetic spin fluctuation becomes stronger.

1. Introduction

Since the superconductivity (SC) in a series of heavy-fermion compounds $CeMIn_5$ (M = Co, Rh, Ir) was discovered, recently [1], a variety of experimental investigations have rapidly proliferated. It is interesting to find features in common with the high-T_c cuprates, and clarify points of difference. In fact, the properties of these compounds are reminiscent of those of the high-T_c cuprates at the following points. These are quasi-two-dimensional materials with layered structure. The symmetry of the SC is that of the $d_{x^2-y^2}$-wave singlet, as indicated by NMR measurements [2] and the thermal conductivity [3]. The temperature dependence of the resistivity follows a power law $\rho - \rho_0 \propto T^n$ with $n = 1$–1.5 at low temperatures. This implies the existence of strong antiferromagnetic spin fluctuation (AFSF). The SC mediated by such AFSF has been vigorously investigated in the high-T_c cuprates, and now the anomalous physical properties in the normal state have been semi-quantitatively discussed within the fluctuation-exchange (FLEX) approximation. On the other hand, a clear difference from the cuprates is the anomalously enhanced jump of the electronic specific heat at the superconducting transition temperature (T_c). The magnitude is the largest for $CeCoIn_5$, which possesses the highest $T_c = 2.3$ K, and $\Delta C/\gamma T_c = 4.5$ [1]. In addition, the normal-state specific heat under a magnetic field sufficient to suppress the SC shows the behaviour $C/T \propto -\ln T$ at low temperatures. This suggests proximity to an antiferromagnetic quantum critical point, and is consistent with NQR experiments [2].

In this paper, we investigate the d-wave SC in $CeCoIn_5$ with use of the FLEX approximation, and semi-quantitatively evaluate the electronic specific heat. The FLEX approximation is useful for taking into account the AFSF in a realistic band structure. For simplicity, we here consider the Hubbard model with a two-dimensional f-band structure, $\xi_k = 2t(\cos(k_x) + \cos(k_y)) - \mu$, and the electron number per spin $n = 0.385$, by following [4], in which the difference between T_c for $CeCoIn_5$ and for $CeIrIn_5$ has been discussed within third-order perturbation theory. This band structure reconstructs the cylindrical Fermi surface with the heaviest cyclotron mass observed in the de Haas–van Alphen measurement [5]. Although, in fact, the situation becomes more complicated due to the hybridization with the conduction band and many f orbitals, this simplification does not change the physical essence, because only one f band near the Fermi level is concerned with the SC in $CeMIn_5$. The effect of the multi-orbitals in this series, which has been discussed by Takimoto *et al* [6], seems to be a minor correction. The order of magnitude of the hopping integral t can be estimated from the band calculation. However, we here consider t as renormalized by the local self-energy part on the basis of the quasi-particle description, which involves the local features, such as the Kondo effect [4]. Thus, t is estimated rather by comparison of T_c with the experimental values, and is of the order of 100 K. We introduce the formalism for the specific heat on the basis of the FLEX approximation in the following section.

2. Formalism and results

In the singlet superconducting state, the one-particle Green's function and the self-energy are 2×2 matrices in Nambu notation:

$$\hat{G}(k) = \begin{pmatrix} \mathcal{G}(k) & \mathcal{F}(k) \\ \mathcal{F}^\dagger(k) & -\mathcal{G}(-k) \end{pmatrix}, \qquad \hat{\Sigma}(k) = \begin{pmatrix} \Sigma_n(k) & \Sigma_a(k) \\ \Sigma_a^\dagger(k) & -\Sigma_n(-k) \end{pmatrix}, \tag{1}$$

where $k = (\boldsymbol{k}, \omega_n)$ and ω_n is a fermion Matsubara frequency. Since the FLEX approximation is a kind of conserving approximation, the self-energy is given by the functional derivative of $\Phi[G]$, and related to the Green's function by the Dyson–Gor'kov equation:

$$\Sigma_n(k) = \frac{1}{2}\frac{\partial \Phi[\hat{G}]}{\partial \mathcal{G}(k)}, \qquad \Sigma_a^\dagger(k) = \frac{\partial \Phi[\hat{G}]}{\partial \mathcal{F}(k)}, \qquad \Sigma_a(k) = \frac{\partial \Phi[\hat{G}]}{\partial \mathcal{F}^\dagger(k)}, \tag{2}$$

$$\hat{G}(k) = [\hat{G}_0(k)^{-1} - \hat{\Sigma}(k)]^{-1}. \tag{3}$$

For G and Σ satisfying these equations, the thermodynamic potential

$$\Omega(T, \mu) = -\sum_k \mathrm{Tr}[\hat{\Sigma}\hat{G} + \ln(-\hat{G}_0^{-1} + \hat{\Sigma})] + \Phi[\hat{G}] \tag{4}$$

is stationary, where $\sum_k = (T/N)\sum_{\boldsymbol{k}}\sum_{\omega_n}$ and N is the number of lattice sites. In the FLEX approximation, the functional $\Phi[G]$ is approximated by

$$\Phi[\hat{G}] = \Phi_2[\hat{G}] + \Phi_s[\hat{G}] + \Phi_c[\hat{G}], \tag{5}$$

$$\Phi_2[\hat{G}] = -\tfrac{1}{2}\sum_k [U^2\chi_s^2], \tag{6}$$

$$\Phi_s[\hat{G}] = \frac{3}{2}\sum_k \left[\ln(1 - U\chi_s) + U\chi_s + \frac{U^2}{2}\chi_s^2\right], \tag{7}$$

$$\Phi_c[\hat{G}] = \frac{1}{2}\sum_k \left[\ln(1 + U\chi_c) - U\chi_c + \frac{U^2}{2}\chi_c^2\right], \tag{8}$$

$$\chi_s(q) = -\sum_k [\mathcal{G}(k+q)\mathcal{G}(k) + \mathcal{F}^\dagger(k+q)\mathcal{F}(k)], \tag{9}$$

$$\chi_c(q) = -\sum_k [\mathcal{G}(k+q)\mathcal{G}(k) - \mathcal{F}^\dagger(k+q)\mathcal{F}(k)], \tag{10}$$

where $q = (\boldsymbol{q}, \nu_n)$ and ν_n is a boson Matsubara frequency. Thus, by evaluating equation (2), we obtain a series of self-consistent equations: equation (3) and

$$\Sigma_n(k) = \sum_{k'} V_{eff}(k-k')\mathcal{G}(k'), \tag{11}$$

$$\Sigma_a^\dagger(k) = \sum_{k'} V_{sing}(k-k')\mathcal{F}^\dagger(k'), \tag{12}$$

with

$$V_{eff}(q) = U^2\left[\frac{3}{2}\frac{\chi_s(q)}{1-U\chi_s(q)} + \frac{1}{2}\frac{\chi_c(q)}{1+U\chi_c(q)} - \frac{1}{2}(\chi_s(q)+\chi_c(q))\right], \tag{13}$$

$$V_{sing}(q) = U^2\left[\frac{3}{2}\frac{\chi_s(q)}{1-U\chi_s(q)} - \frac{1}{2}\frac{\chi_c(q)}{1+U\chi_c(q)} - \frac{1}{2}(\chi_s(q)-\chi_c(q))\right]. \tag{14}$$

In this case, the entropy $S = -(\partial\Omega/\partial T)_\mu$ is given by the explicit derivative of $\Omega(T, \mu)$ with respect to T, since its implicit derivative, through the self-energy, vanishes in the stationary solutions $\hat{G}$ and $\hat{\Sigma}$ [7]. Thus, we obtain the entropy

$$S = -\frac{\partial}{\partial T}\left[\frac{T}{N}\sum_{\boldsymbol{k}}\sum_{\omega_n} \mathrm{Tr}\ln\hat{G}(k)\right]. \tag{15}$$

After the analytic continuation on the real axis, in the normal state

$$S = 2\frac{1}{2\pi\mathrm{i}T}\frac{1}{N}\sum_{\boldsymbol{k}}\int \mathrm{d}\epsilon\,\epsilon\left(-\frac{\partial f}{\partial\epsilon}\right)[\ln\mathcal{G}_n^R - \ln\mathcal{G}_n^A], \tag{16}$$

and in the superconducting state

$$S = \frac{1}{2\pi\mathrm{i}T}\frac{1}{N}\sum_{\boldsymbol{k}}\int \mathrm{d}\epsilon\,\epsilon\left(-\frac{\partial f}{\partial\epsilon}\right)[\ln G_{sc}^R - \ln G_{sc}^A], \tag{17}$$

where $G_{sc}^{R,A} = [\omega_\pm^2 Z^2 - \bar{\xi}_{\boldsymbol{k}}^2 - \Sigma_a^2]^{-1}$ with $\bar{\xi}_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} + \chi$ and $\Sigma_n(\boldsymbol{k}, \pm\omega) = \pm\omega(1-Z) + \chi$.

The most favourable pairing symmetry is $\mathrm{d}_{x^2-y^2}$ wave as expected. Figure 1(a) illustrates the maximum of the anomalous self-energy $\Sigma_a(\boldsymbol{k}, \pi T)$ as a function of T/T_c for $U/t = 4.0$, 4.5, and 5.0. We can see that the SC becomes strong-coupling type as U/t and $\chi_s(Q)$ becomes larger. In this case, the entropy S is evaluated as in figure 1(b). The convex behaviour from high temperatures, which is not shown, originates from the mass enhancement for the AFSF. On the other hand, the too small entropy below $T/t = 0.005$ may be due to the formation of a pseudogap for the AFSF, or numerical errors. With use of polynomial fitting of the entropy in the vicinity of T_c, we obtain the specific heat C and the enhanced jump of the specific heat $\Delta C/\gamma T_c$ in figure 1(c). As U/t becomes larger, T_c and $\Delta C/\gamma T_c$ also become larger, but are saturated in time. In this case, at $U/t = 5.0$, $T_c/t = 0.017$ and $\Delta C/\gamma T_c = 4.6$. The increase of C/T in the normal state at lower temperatures can be considered as reflecting the proximity of $-\ln T$, which is predicted by the SCR theory in the two-dimensional AFSF. Furthermore, if we set $T_c = 0.017t$ as 2.3 K, C/T just above T_c corresponds to $\sim$200 mJ mol^{-1} K^{-2} (290 mJ mol^{-1} K^{-2} for the experimental data). Thus, the curious behaviour of the specific heat of $CeCoIn_5$ can be almost explained by the quasi-two-dimensional AFSF. In addition, from comparison with the high-T_c cuprates, we can say that this system shows strong AFSF,

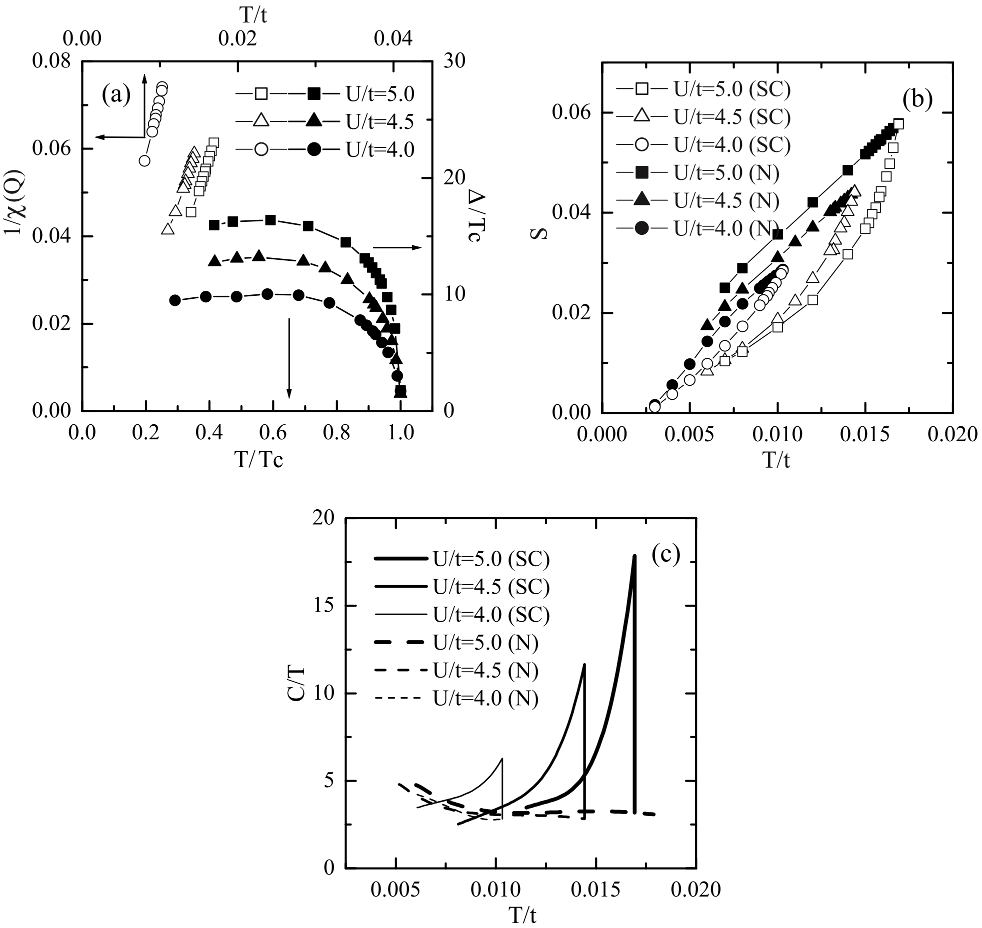

Figure 1. (a) $1/\chi(Q)$ as a function of T/t and $\Delta/T_c = \Sigma_a^{max}(\boldsymbol{k}, \pi T)/T_c$ as a function of T/T_c. (b) The entropy S and (c) the specific heat C for the normal and the SC states. As U/t becomes larger, the SC becomes strong-coupling type, and the jump of C/T at T_c is also enhanced.

but does not show remarkable SC fluctuation. We think that this is related to the dimensionality of this system. Establishing this is a problem for the future.

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