Microscopic study of noncentrosymmetric heavy fermion superconductors CeRhSi$_3$ and CeIrSi$_3$

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Abstract. We study the upper critical fields $H_{c2}$ along the $c$-axis in the noncentrosymmetric heavy fermion superconductors CeRhSi$_3$ and CeIrSi$_3$ by solving the Eliashberg equations. It is demonstrated that when the spin-orbit interaction due to the lack of inversion symmetry is sufficiently strong the Pauli limiting fields are extremely large and the upper critical fields are determined by the orbital limiting fields. From microscopic calculations taking into account the strong antiferromagnetic spin fluctuations, we show that $H_{c2}$ is much enhanced as the system approaches the quantum critical point.

1. Introduction
In the past few years, superconductors without an inversion center have attracted much interest. A number of compounds, such as CePt$_3$Si[1], CeRhSi$_3$[2, 3], CeIrSi$_3$[4, 5], UIr[6], Li$_2$Pd$_3$B and Li$_2$Pt$_3$B[7], were discovered and have been studied extensively. In such compounds, the lack of inversion symmetry leads to strong anisotropic spin-orbit interactions which can materially affect the superconducting states as well as the normal states[8, 9]. From microscopic studies of the pairing symmetries of the superconductivities in CePt$_3$Si[13], CeRhSi$_3$ and CeIrSi$_3$[14], extended $s + p$ wave states can be stabilized though their detailed gap structures are different. Systems under applied magnetic fields are also examined by several authors. It is reported that the Pauli limiting fields are largely enhanced by the spin-orbit interaction[10] and there can exist a novel superconducting state called the herical vortex state[11]. These phenomena are considered to be remarkable in the presence of the strong electron correlations[9] which are a central issue in the heavy electron systems.

Recently, the heat capacity in CeIrSi$_3$[15] and the upper critical fields in both compounds[16, 17] were measured under high pressures. The jumps in the heat capacity at $T_c$ up to 5.7 were reported and the maximum $H_{c2}$ was estimated to be over 30T, which is the highest value among the upper critical fields for heavy fermion superconductors ever discovered. The above results strongly suggest that the two compounds are strong coupling superconductors.

Motivated by these experiments, in this study, we will investigate the strong coupling effects due to antiferromagnetic(AF) spin fluctuations in CeRhSi$_3$ and CeIrSi$_3$. To make a comparison with the experiments, we employ the microscopic band structure and phenomenologically take into account the large spin fluctuations near the quantum critical point[18]. By solving the
Eliashberg equations, we calculate $H_{c2}$ for both Pauli and orbital limiting cases to figure out which is dominant.

2. Model and calculation

We focus on the low energy quasiparticles which are formed through hybridizations with conduction electrons and describe them by the following effective Hamiltonian,

$$
H = H_t + H_s + H_{SF},
$$

$$
H_t + H_s = \sum_k c_k^\dagger \varepsilon(k)c_k + \sum_k c_k^\dagger \alpha \mathbf{L}_{ji}(k) \cdot \sigma c_k,
$$

$$
H_{SF} = -\sum_q g^2 \chi(q) \mathbf{S}_q \cdot \mathbf{S}_{-q},
$$

where $c_k = (c_{k\uparrow}, c_{k\downarrow})^T$ is the annihilation operator of the Kramers doublet and $S_q^i = \sum_k c_{k+q}^\dagger \sigma^i/2 c_k$. The first, second and third terms respectively represent the kinetic term, the spin-orbit interaction due to the lack of inversion symmetry including the Zeeman splitting, and the electron-electron interactions through spin fluctuations. For CeRhSi$_3$ and CeIrSi$_3$ which have body centered tetragonal lattice structures, the dispersion relation and the spin-orbit interaction are given by $\varepsilon(k) = -2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_z \cos k_y - 8t_3 \cos(k_x/2) \cos(k_y/2) \cos k_z - \mu$ and $\alpha \mathbf{L}_{ji}(k) = (\alpha \sin k_y, -\alpha \sin k_x, -\mu B)$.

The parameters are fixed as $(t_1, t_2, t_3, n, \alpha) = (1.0, 0.475, 0.3, 1.05, 0.5)$ by taking $t_1$ as the energy unit. The Fermi surface determined by these parameters is in qualitative agreement with the band calculation results and can reproduce the peak structures of the susceptibility observed by the neutron scattering experiments [14, 19, 20]. To describe the strong spin fluctuations, we phenomenologically introduce the effective interaction between quasiparticles [18],

$$
\chi(i\nu_n, q) = \sum_a \frac{\chi_0 \xi^2}{1 + \xi^2(q - Q_a)^2 + |\nu_n|/(\Gamma_0 \xi^{-2})},
$$

$$
\xi(T) = \frac{\xi}{\sqrt{T + \theta}}.
$$

where $\chi_0$ and $\Gamma_0$ are respectively the susceptibility and the energy scale of spin fluctuations without strong correlations. These are renormalized through the coherence length $\xi(T)$ as the system approaches the quantum critical point. The temperature dependence of $\xi(T)$, eq.(5), is characteristic of AF fluctuations and $\theta$ is considered to decrease monotonically as the applied pressure approaches the critical value for the AF order [21, 22]. Equation (5) is also consistent with the recent NMR experiment for CeIrSi$_3$ [12]. The propagating vectors are $Q_1 = (0.43\pi, 0.5\pi)$ and its equivalents by the lattice symmetry according to the neutron scattering experiments [20]. In this study, we fix the parameters in $\chi$ as $\Gamma_0 = 3.6$ and $\xi = 0.4647$. The former is a little smaller than the Fermi energy and the latter leads to $\xi(T = 0.001, \theta = 0.002) \approx 8 \times $ (lattice constant) $\approx 30\AA$, assuming the lattice constant in the $xy$ plane equals $4\AA$ which is an approximate value of the experimentally measured ones [3, 5].

To describe the quasiparticles in the strong coupling regime, we introduce the normal selfenergy up to the first order in $g^2 \chi_0$ which is given by,

$$
\Sigma_{s_1s_2}(k) = \frac{T}{N} \sum_{k'} g^2 \chi(k - k') C^0_{s_1s_2}(k') \delta_{s_1s_2},
$$

where $C^0$ is the Green’s function for noninteracting quasiparticles. Here we have introduced the notation $k = (i\omega_n, k)$. 


Figure 1. Temperature dependence of the upper critical fields for the extended s-wave state. The dotted line with open circles represents the Pauli limiting field for \( \theta = 0.005 \) and the others the orbital limiting fields for several \( \theta \).

We study the transition temperatures under applied fields by solving the Eliashberg equations for the superconducting gap \( \Delta \) with the paring interaction \( V \) which is evaluated at the lowest order in \( g^2 \chi_0 \),

\[
\Delta_{\alpha\alpha'}(i\omega_n, \mathbf{k}; \mathbf{R}) = -\frac{T}{N} \sum_{k',\beta\beta'} V_{\alpha\alpha',\beta\beta'}(k, k') G_{\beta\gamma}(i\omega_n, k') + \Pi_{\beta\gamma\gamma'}(-i\omega_n, -k') \Delta_{\gamma\gamma'}(i\omega_n, k'; \mathbf{R}),
\]

and \( \Pi(\mathbf{R}) = -i\nabla_{\mathbf{R}} + 2eA(\mathbf{R}) \) with \( \nabla_{\mathbf{R}} \times A(\mathbf{R}) = (0, 0, H) \). For the calculations of orbital fields, only the \( N = 0 \) Landau level is considered, which would be reasonable for orbital limiting cases. It will be shown in the following that the situation in the present study is the case.

3. Results

By solving eq. (7), we find that the \( A_1 \) symmetric superconducting state is most stable among the five irreducible representations of point group \( C_{4v} \), which is consistent with the previous study[14]. The \( A_1 \) symmetric order parameter is in the form of \( \Delta(i\omega_n, \mathbf{k}) = [\Delta_s(i\omega_n)d_0(\mathbf{k}) + \Delta_t(i\omega_n)d(\mathbf{k}) \cdot \sigma]i\sigma_2 \) with \( d_0 = \cos(2k_z) \), \( d = \cos(2k_z)L_0 \). In our model, however, the amplitude of the triplet part \( \Delta_t \) is so small (\( \propto 0.01\Delta_s \)) that we will neglect it from now on.

Figure 1 shows upper critical fields as functions of temperature for several \( \theta \). To represent calculated results in the unit of kelvin and tesla, we use the values; (lattice constant)=4\( \text{Å} \) and \( t_1 = 110K \). The latter is obtained by identifying the calculated maximum transition temperature \( T_c = 0.01175 \) as 1.3K which is the averaged value of maximum \( T_c \) for CeRhSi\(_3\)[2] and CeIrSi\(_3\)[4].

The dotted line with open circles corresponds to the Pauli limiting field for \( \theta = 0.005 \) and the other lines to the orbital limiting fields for several \( \theta \). In the present parameters, transition temperatures are typically \( T_c \approx 0.001 \) and thus the spin-orbit coupling constant is very large compared to \( T_c \) (\( \alpha = 0.5 \approx 50T_c \)), leading to the Pauli limiting fields largely exceeding the orbital limiting fields. From this result, we can conclude that when \( \alpha \) is sufficiently large \( \alpha \gg T_c \), the upper critical fields are determined by the orbital limiting fields. It could be asserted that this generally holds true for the noncentrosymmetric superconductors[10]. In Fig. 1, we can also see that the orbital limiting fields are enhanced as \( \theta \) is decreased. \( H_{c2}(T) \) curves have downward curvatures and the values at low temperature limit may reach 25T, which could explain the experimentally observed huge values. The important point is that, through the temperature dependence of \( \xi(T) \), the spin fluctuations are much more enhanced as the temperature is lowered,
resulting in increase in $H_{c2}$ at low $T$. This behavior is significant especially for small $\theta$, because $\xi(T) \propto 1/\sqrt{T}$ at low temperatures for tiny $\theta \ll T_c$ while $\xi(T) \propto 1/\sqrt{\theta}$ for large $\theta \gg T_c$.

The above mentioned results which are consistent to the experiments\cite{16, 17} could confirm that the superconductivity in CeRhSi$_3$ and CeIrSi$_3$ is mediated by the antiferromagnetic strong spin fluctuations.

4. Summary

We have studied the strong coupling effects on the upper critical fields in CeRhSi$_3$ and CeIrSi$_3$. The Fermi surface is adjusted so as to be consistent with the band calculation results, and the electron-electron interaction is phenomenologically introduced in accordance with the neutron scattering experiments and the NMR experiments. Solving the Eliashberg equations, we have found that the Pauli limiting fields are much larger than the orbital ones. The orbital limiting fields are enhanced through decreasing $\theta$, the parameter which indicates how close the system is to the quantum critical point. The maximum value of calculated $H_{c2}$ is about 30T which is comparable to the experimental values, and this could confirm that the superconductivities in CeRhSi$_3$ and CeIrSi$_3$ are mediated by the strong spin fluctuations.

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