Nonmagnetic impurity resonance states as a test of superconducting pairing symmetry in CeCoIn5

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We theoretically study the effect of a nonmagnetic impurity in heavy fermion superconductor CeCoIn5 within a coherent three-dimensional Anderson lattice model and the T-matrix approximation approach. By considering two known possible pairing symmetry candidates $d_{x^2-y^2}$ and $d_{xy}$, we find that although both total density of states exhibit a similar V-shaped gap-like feature, only $d_{x^2-y^2}$-wave pairing symmetry gives rise to robust intragap impurity resonance states reflected by the resonance peaks near the Fermi energy in the local density of states. These features can be readily probed by scanning tunneling microscopy experiments, and are proposed to shed light on the pairing symmetry and provide hints on the microscopic mechanism of unconventional superconductivity in the Ce-based heavy fermion superconductors.

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Recently, the interplay of antiferromagnetic (AF) order and unconventional superconductivity in Ce-based heavy fermion superconductors CeMIn5 (M = Co, Rh, Ir) have been intensively studied. For instance, CeCoIn5 is a superconductor with the highest transition temperature $T_c \approx 2.3K$ whereas CeRhIn5 orders antiferromagnetically below $T_N \approx 3.7K$. On the other hand, superconductivity is observed in the latter compound by application of pressure whereas unconventional superconductivity in CeCoIn5 emerges in close proximity to an AF quantum critical point as in the cuprates and pnictides superconductors. Moreover, neutron scattering experiments indicate strong AF quasielastic excitations at wavevectors $Q=(\frac{1}{2}, \frac{1}{2})$ and equivalent positions in the paramagnetic regime. When entering the superconducting state, the magnetic excitations spectra by inelastic neutron scattering show the appearance of a sharp spin resonance. These finding underline the analogy to the cuprate high-temperature superconductors and the new iron superconductors, where AF spin fluctuations may actually mediate unconventional superconductivity.

So far, the superconducting pairing symmetry in CeCoIn5 has been discussed from both experimental and theoretical sides, it has not yet been determined unambiguously. Soon after the discovery of CeCoIn5 material, its Fermi surface (FS) has been studied in detail by quantum oscillation, which consists of nearly cylindrical one and small ellipsoidal ones. The cylindrical sheets reflect quasi-two-dimensional (2D) character, by analogy with cuprates. Then the pairing state in CeCoIn5 has been widely believed to be unconventional with d-wave symmetry.

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vertical line node, and should be observed for the whole set of momenta \( Q = (\frac{\pi}{4}, 0) \) with \( 0 \leq x \leq \frac{1}{2} \). However, this explanation of the resonance in CeCoIn\(_5\) disagrees with the experiments where the neutron scattering resonance is only found at \( Q = (\frac{\pi}{4}, 0) \) [30–32]. In Ref. 33 the authors argued that the absence of strong resonances at other momenta may due to the facts that the quasi-2D FS was not a perfect cylindrical as evidences by the existence of three different dHvA orbits, that gap parameter generally varied along the z axis, and that 3D FS should also had contributions[33]. Thus they proposed a potential candidate-the "magnon" scenario for spin resonance in 3D superconductor in CeCoIn\(_5\), which didn’t require a \( d_{x^2−y^2} \) gap.

Since most of the experimental evidence for d-wave pairing symmetry is indirect, further theoretical and direct experimental work such as ARPES measurements and phase sensitive experiments is still needed and necessary to identify the order parameter in CeCoIn\(_5\). In this paper, we propose to use local electronic structure around a single nonmagnetic impurity to probe the pairing symmetry in CeCoIn\(_5\) superconductor, since such properties have proved to be successful in identifying the unconventional pairing states of different classes of superconductors[34–42]. Within a coherent 3D Anderson lattice model and the T-matrix approximation approach, we theoretically calculate the local density of states in the unitary limit of impurity scattering, and find that although both total density of states exhibit a similar V-shaped gaplike feature, the impurity induced intragap resonance state only occurs when the pairing symmetry is of \( d_{x^2−y^2} \), similar to the case of d-wave cuprate superconductor. Our prediction can be directly measured by scanning tunneling microscopy experiments in heavy fermion superconductor CeCoIn\(_5\).

According to band structure calculations[30–32,41,42], CeCoIn\(_5\) comprises several \( f \)-bands and conduction bands which are hybridized in a complex manner. Due to a large spin-orbit coupling the Ce-4f electron states are split into upper \( j=7/2 \) and lower \( j=5/2 \) states, the latter one is further split into three crystalline electric field (CEF) Kramers doublet states. Because CEF splitting energy is much bigger than the heavy quasiparticle band width (about 4 meV), we can restrict to the lowest CEF doublet which has an effective pseudo-spin 1/2. Thus we here consider a 3D coherent Anderson lattice model which could reproduce the result of band calculations, realize real FS, and is also technically manageable for a T-matrix calculation in the superconducting states. In fact, this has been done previously for CeCoIn\(_5\)[43], and the resulting hybridized quasiparticle energy dispersion can be read as:

\[
E_{k±} = \frac{1}{2} (\varepsilon_k^f + E_k^f) ± \sqrt{(E_k^f − \varepsilon_k^f)^2 + 4V_k^2} \tag{1}
\]

where \( \varepsilon_k^f \) and \( E_k^f \) are the effective \( f \)-band and the conduction band dispersions, respectively, and \( V_k \) is the effective hybridization strength, which is renormalized by the on-site \( f − f \) Coulomb repulsion. The detailed \( \varepsilon_k^f, E_k^f \) and \( V_k \) as well as the parameters are defined as in Ref. 43, and the resulting FS is shown in Fig. 1. Note that band \( E_{k−} \) reproduces the above FS and is denoted as the \( \beta \)-band in the de Hass van Alphen experiments[30–32]. While band \( E_{k+} \) remains above the Fermi energy, and thus has no contribution to the FS topological structure. Therefore, the novel low energy electronic state properties of CeCoIn\(_5\) mainly originate from the band \( E_{k−} \).

In the superconducting state, the bare Green’s function within the Nambu space is given by

\[
\hat{G}_0^{-1}(\mathbf{k}, i\omega_n) = i\omega_n \mathbf{1} - \begin{pmatrix}
E_{k+} & \Delta_k & 0 & 0 \\
\Delta_k & -E_{k+} & 0 & 0 \\
0 & 0 & E_{k−} & \Delta_k \\
0 & 0 & \Delta_k & -E_{k−}
\end{pmatrix} \tag{2}
\]

where \( \omega_n = (2n + 1)\pi T \) is the Matsubara frequency for fermions. The superconducting gap function is described by \( \Delta_k \). Then the corresponding bare real-space Green’s function can be obtained from the Fourier transform as

\[
\hat{G}_0(i, j; i\omega_n) = \frac{1}{N} \sum_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}_{ij}} \hat{G}_0(\mathbf{k}, i\omega_n), \tag{3}
\]

where \( \mathbf{R}_{ij} = \mathbf{R}_i − \mathbf{R}_j \) with \( \mathbf{R}_i \) being lattice vector and \( N \) is the number of lattice sites. In the presence of a single-site nonmagnetic impurity of strength \( U_0 \) located at the origin \( r_i = 0 \), the site dependent Green’s function in term of the T-matrix approach can be obtained as

\[
\hat{G}(i, j; i\omega_n) = \hat{G}_0(i, j; i\omega_n) + \hat{G}_0(i, 0; i\omega_n) \hat{T}(i\omega_n) \hat{G}_0(0, j; i\omega_n), \tag{4}
\]

where

\[
\hat{T}(i\omega_n) = \frac{\hat{U}_0}{1 - \hat{G}_0(0, 0; i\omega_n)\hat{U}_0} \tag{5}
\]
and the potential scattering matrix takes the following structure:

$$
\hat{U}_0 = \begin{pmatrix}
U_0 & 0 & V & 0 \\
0 & -U_0 & 0 & -V \\
V & 0 & U_0 & 0 \\
0 & -V & 0 & -U_0
\end{pmatrix}
$$

(6)

where $U_0$ and $V$ are the strength of the intra- and interband scattering potential.

The local density of states (LDOS) which is proportional to the local differential tunneling conductance measured by STM can be expressed as:

$$
\rho(i, \omega) = -\frac{1}{\pi} \text{Im} \text{Tr} [\hat{G}(i, i; \omega_n \rightarrow \omega + i0^+)]
$$

(7)

The above scheme is sufficiently general to capture the essential properties of the single impurity scattering in a two-band superconductor. For the present case, the FS crossing originates only from band $E_{k_x}$ as discussed above, while band $E_{k_z}$ contributes little to the density of states (DOS) near Fermi energy. Therefore, it will be reasonable to carry out the following calculations to only consider the impurity scattering effect in intraband $E_{k_x}$, and ignore the scattering from band $E_{k_z}$ and the interband impurity scattering (i.e., $V = 0$).

Before investigating the effect of the single impurity scattering, we need to firstly look into the properties of DOS. Notice that the corrugated FS of CeCoIn$_5$ is characterized by three-dimensionality and is not a perfect cylindrical alone the (0 0 1) line, following the method applied in Ref. 44 we firstly restrict to the $ab$ plane by averaging over the momenta in the $k_z$ direction, and analyze the DOS and local electronic structure induced by a nonmagnetic impurity for each slice of the FS at a particular $k_z$, and then by averaging over the individual DOS and LDOS of each $k_z$ slice to obtain the final total DOS and LDOS along the (001) direction.

The considered pairing symmetry includes two possible candidates as discussed above, namely $d_{x^2-y^2}$ gap symmetry with

$$
\Delta_k = \Delta_0 (\cos k_x - \cos k_y)/2
$$

(8)

and $d_{xy}$ gap symmetry with

$$
\Delta_k = \Delta_0 (\sin k_x \sin k_y).
$$

(9)

The magnitude of the d-wave gap parameter $\Delta_0$ should in principle be determined self-consistently, but for sake of allowing for an analytic calculation, it is reasonable to assume its value is known. And also for the convenience of comparison, we assume the value $\Delta_0$ is the same for different $k_z$ layer and for both two pairing symmetries.

We now turn to analyze the FS topological structure and the gap function in the first Brillouin zone for individual $k_z$. The upper panels of Fig. 2 represent the FS evolution with the $d_{x^2-y^2}$ gap function, where the node lines cut the FS (red solid line) at any value of $k_z$. While in the lower panels, the properties of the nodal structure is completely different. For small values $k_z < 0.6\pi$ the gap function with $d_{xy}$ symmetry has no node points on the FS, but changes sign across two neighboring FS arc. With increasing $k_z$ to about $0.6\pi$ value the inner FS appears and gives rise to the nodal structure as seen in Fig. 2e. As $k_z$ gradually increases and approaches $\pi$ in Fig. 2f, a new FS topological structure occurs, then the node line keeps away from the FS and the node points on the FS again disappear.

The effect of the nodal structure on the FS can be clearly reflected by the calculated DOS which is proportional to the differential tunneling conductance tested by Tunneling experiment. In Fig. 3, the DOS for the normal state (black solid line), superconducting state with $d_{x^2-y^2}$ (red dashed line) and $d_{xy}$ (blue dotted line) gap symmetry are plotted for different cut of the FS at $k_z = 0, 0.6\pi, \pi$. For the $d_{xy}$ pairing symmetry, a V-shaped DOS only at $k_z = 0.6\pi$ as shown in Fig. 3b is exhibited reflecting the existence of nodal structure, while in other values of $k_z$ the DOS is characterized by a U-shaped feature due to the nodeless gap structure and is very similar to the case of conventional s-wave superconductors. While for the $d_{x^2-y^2}$ case, the DOS always behaves to be V-shaped character at all value of $k_z$ because of the sign change within each FS arc. We also find that the DOS in normal state at small values of $k_z$ is rather smaller near the Fermi energy compared to the case of larger $k_z \ll [0.6\pi, \pi]$.

We now proceed to analyze the response of the local electronic structure to the single nonmagnetic impurity scattering in the superconducting state of CeCoIn$_5$. In Fig. 4 we plot the LDOS of quasiparticles on the im-
purity’s nearest neighboring site for different FS cuts at $k_z = 0, 0.6\pi, \pi$ considering the impurity scattering strength in the unitary limit $U_0 = 100t$. The LDOS at $U_0 = 0$ (black solid line) which is equivalent to DOS in the clean system, shows two coherent peaks with different spectral weight due to the particle-hole asymmetry near the gap edges and other van Hove singularity peaks originated from the particular FS topological structure at different value of $k_z$.

For the superconducting state with $d_{x^2−y^2}$ pairing symmetry as shown in the upper panels of Fig. 4a-4c, we find that impurity induced resonance states near the Fermi energy occurs denoted by the resonance peaks (red dashed line), which is the result of the sign change within each FS arc due to the node line cutting the FS, and is similar to what happens in unconventional cuprate superconductors. At the same time, the superconducting coherent peaks are heavily suppressed. We also notice that the spectral weight of the resonance peak strongly depends on the special FS topological feature and therein the nodal structure. The impurity induced intragap resonance peak only occurs at $k_z = 0$ to $k_z = \pi$ due to the special nodal structure on the FS as shown in Fig. 2a-2c, the spectral weight of the resonance peak is thus correspondingly enhanced. While for the $d_{xy}$ pairing symmetry case, we find that the impurity induced intragap resonance peak only occurs at $k_z = 0.6\pi$ as shown in Fig. 4e, while at other value of $k_z$ disappears and is replaced by resonance peaks near the gap edges. This is consistent with the aforementioned nodal structure and DOS.

Since the observable local electronic structure in CeCoIn$_5$ is of the three-dimensional (3D) feature and should be an average over the FS slices at different $k_z$, we have to consider the calculated DOS and LDOS averaged in the (001) direction. In this case, we plot the averaged DOS and LDOS for the superconducting states with $d_{x^2−y^2}$ pairing symmetry and $d_{xy}$ pairing symmetry in Fig. 5. We find that although both total DOS exhibits a similar V-shaped gaplike feature, only the $d_{x^2−y^2}$-wave pairing symmetry gives rise to robust im-
purity resonance states reflected by a zero energy resonance peak in LDOS. Our result confirms the recent experimental results where such pairing breaking effect by impurities has been indirectly measured in CeCoIn$_5$ after doping hole or electron. We propose that these features can be directly measured by scanning tunneling microscopy (STM) experiments, and then shed light on the pairing symmetry and pairing mechanism in CeCoIn$_5$ and other Ce-based heavy fermion superconductors, since they have the similar HoCoGa$_5$-type electronic structure.

In conclusion, by applying the T-matrix approximation approach we have studied the effect of a single nonmagnetic impurity in CeCoIn$_5$ superconductor within a coherent Anderson lattice model which can reproduce the real 3D FS topological feature. We have found that, considering two types of pairing symmetry $d_{x^2-y^2}$ and $d_{xy}$, only $d_{x^2-y^2}$ pairing gives rise to robust intragap impurity induced resonance state near the Fermi energy in the unitary limit of impurity scattering, though both pairing gap in the superconducting state indicate the similar V-shaped feature of DOS. Based on these results, we propose to use STM experiment to test the local electronic structure around nonmagnetic impurities so as to identify the pairing symmetry and provide hints on the microscopic mechanism of unconventional superconductivity in the Ce-based heavy fermion superconductors.

After completing the present work, we are aware of the recent high-resolution STM experiment on the CeCoIn$_5$ superconductor, where due to the cleaving procedure which could cut the surface at different $k_z$ points, the STM spectrum is available for different $k_z$ plane. After analyzing $k_z$ plane measured in above experiment and its FS topology, we find it is basically located in the $k_z \subseteq [0.6r, \pi]$ as shown in Figs. 2b-2c and Figs. 2e-2f, and impurity-induced intragap bound states experimentally probed indeed confirm our theoretical predictions as seen in Figs. 4b-4c for the $d_{x^2-y^2}$ pairing state.

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