Local electronic structures around impurities in superconductors without an inversion center

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Abstract.

Motivated by recent discoveries of noncentrosymmetric superconductors, we investigate theoretically the impurity resonance states considering the spin-orbit coupling interaction. Due to the nodal structure of gap function originating from the interference between spin-triplet and spin-singlet components of the superconducting order parameters, we find that a single nonmagnetic impurity induced resonance states appear in the local density of state. In addition, we analyze the evolution of the local density of states for coexisting isotropic s-wave and p-wave superconducting states, and compare with that of anisotropic s-wave and p-wave symmetries of the superconducting gap. We propose that the scanning tunneling microscopy can shed light on the particular structure of the superconducting gap in noncentrosymmetric superconductors.

1. Introduction

Recent discoveries of superconductivity in noncentrosymmetric materials such as $\text{CePt}_3\text{Si}$[1], $\text{CeRhSi}_3$[2], $\text{Li}(\text{Pd}_{1-x}\text{Pt}_x)3$[3] have raised an interest in theoretical investigation of superconductivity. Among interesting questions the most important one concerns the underlying symmetry of the superconducting order parameter. Due to lack of inversion symmetry, there is a nonzero potential gradient $\nabla V$ averaged in the unit cell, which results in the anisotropic spin-orbit interaction. Its general form can be determined by a group theoretical argument[4], and leads to many interesting properties[5, 6, 7, 8, 9, 10, 11]. For example, there is a mixing of the spin-singlet and spin-triplet superconducting states. In $\text{CePt}_3\text{Si}$ the pairing symmetry has been studied theoretically[6, 7, 8, 9, 10, 12] and it is believed that the $s+p$-wave superconducting state may be realized. Frigeri et al.[8] pointed out that the spin-orbit interaction could determine the direction of the $d$-vector as $|\vec{d}|/|\vec{l}|$ ($l$ is the vector of the Rashba spin-orbit coupling) for which the highest transition temperature was obtained. The experimental studies of the temperature dependencies of the spin-lattice relaxation[13], the magnetic penetration depth[14], and the thermal conductivity measurements[15] are also consistent with this conjecture.

It is known that the non-magnetic as well as the magnetic impurities in the conventional and unconventional superconductors already have been proven to be a useful tool to distinguish between various symmetries of the superconducting state[12, 16, 17, 18]. Therefore, STM measurements of the impurity states can provide important messages about the pairing symmetry in the revelent systems. In the noncentrosymmetric superconductor with possible
coexistence of s-wave and p-wave pairing symmetry, it is very interesting to see what is the nature of the impurity state, and whether a low energy resonance state can still occur around the impurity through changing the dominant role played by each of the pairing components.

2. Model and T-matrix formulation
Following previous consideration[8, 12] we start from a single orbital model with Rashba spin-orbit coupling (RSOC), $H = \sum_{k} \varepsilon_{k} c_{k}^{\dagger} c_{k} + \alpha \sum_{k \sigma, k' \sigma'} g_{k} \cdot \sigma \sigma' c_{k}^{\dagger} c_{k' \sigma'}$. In the superconducting state, the presence of RSOC breaks the parity and, therefore, mixes the singlet (even parity) and triplet (odd parity) Cooper-pairing states, $\Delta = (\Delta_{s} \sigma_{0} + d_{k} \cdot \sigma) (i \sigma_{2})$. Then the mean field BCS Hamiltonian for this system has the matrix form

$$
H_{k} = \begin{pmatrix}
\varepsilon_{k} & \Delta_{k} \\
\alpha(g_{k} \cdot \mathbf{d}_{k} - i \mathbf{d}_{k} \cdot \mathbf{g}_{k}) & (\Delta_{k} - \varepsilon_{k})
\end{pmatrix},
$$

where the tight-binding energy dispersion $\varepsilon_{k} = 2t(\cos(k_{x}) + \cos(k_{y})) + 4t_{1} \cos(k_{x}) \cos(k_{y}) + 2t_{2}(\cos(2k_{x}) + \cos(2k_{y})) + [2t_{3} + 4t_{4}(\cos(k_{x}) + \cos(k_{y})) + 4t_{5}(\cos(2k_{x}) + \cos(2k_{y}))] \cos(k_{z}) + 2t_{6} \cos(2k_{z}) - \mu$ with $(t, t_{1}, t_{2}, t_{3}, t_{4}, t_{5}, t_{6}, n) = (1, -0.15, -0.5, -0.3, -0.1, -0.09, -0.2, 1.75)$ reproduces the so-called $\beta$-band of CePt$_{3}$Si$_{2}$[4, 10, 12]. $\alpha$ denotes the coupling constant and the vector function $g_{k}$ is assumed in the following form $g_{k} = (-\sin k_{y}, \sin k_{x}, 0)$. A full symmetry analysis[4, 10] shows that s-wave pairing $\Delta_{s} = \Delta_{0}(\cos(k_{x}) + \cos(k_{y}))$ and p-wave triplet pairing state with order parameter $d_{k}$ parallel to the $g_{k}$ vector, $d_{k} = d_{0}g_{k}$ are able to coexist. Then we obtain the single-particle Green’s function as

$$
g(k, i\omega_{n}) = \begin{pmatrix}
G(k, i\omega_{n}) \\
F^{\dagger}(k, i\omega_{n})
\end{pmatrix},
$$

where $G(k, i\omega_{n}) = \sum_{\tau = \pm 1} \frac{1+\tau g_{k} \cdot \sigma}{2} \frac{i\omega_{n} + \epsilon_{\tau}}{\epsilon_{\tau} - E_{k\tau}}$, and $F(k, i\omega_{n}) = \sum_{\tau = \pm 1} \frac{1+\tau g_{k} \cdot \sigma}{2} i \sigma_{y} \frac{\Delta_{\tau}}{(i\omega_{n})^{2} - E_{k\tau}^{2}}$. Here, the single-particle excitation energy is $E_{k\tau} = \sqrt{\epsilon_{\tau}^{2} + |\Delta_{\tau}|^{2}}$ with $\epsilon_{\tau} = \varepsilon_{k} + \tau \alpha |g_{k}| |\Delta_{\tau}| = \Delta_{k} + \tau |d_{k}|$, and the unit vector is $\hat{g}_{k} = g_{k}/|g_{k}|$.

To obtain the local density of states (LDOS) around a single impurity site, we apply T-matrix formulation[19, 20, 21] to get the site dependent Green’s function as

$$
\zeta(i, j; i\omega_{n}) = \zeta_{0}(i - j; i\omega_{n}) + \zeta_{0}(i, i\omega_{n}) T(i\omega_{n}) \zeta_{0}(j, i\omega_{n}),
$$

where $T(i\omega_{n}) = \frac{U_{i\omega_{n}}}{1 - U_{i\omega_{n}} \zeta_{0}(0, i\omega_{n})}$, and $\zeta_{0}(i, j; i\omega_{n}) = \frac{1}{N} \sum k e^{i \mathbf{k} \cdot \mathbf{R} \mathbf{i}} g(k, i\omega_{n})$ with $\rho_{i}$ being the Pauli spin operator, and $\mathbf{R}_{i}$ is the lattice vector, $\mathbf{R}_{ij} = \mathbf{R}_{i} - \mathbf{R}_{j}$. Finally, the LDOS which can be measured in the STM experiment is written as

$$
N(r, \omega) = \frac{1}{\pi} \sum_{i} \text{Im} \zeta_{i\omega}(r; \omega + i\eta),
$$

where $\eta$ denotes an infinitely small positive number.

3. Results
In the left column of Fig. 1, considering first the situation when the s-wave part of the total superconducting gap is momentum independent, $\Delta_{s} = \Delta_{0}$, we plot the density of states (DOS) without impurity and also the LDOS with an impurity on the nearest neighbor site $(0, 1, 0)$. The evolution of the DOS for various values of the s-wave component indicates that for $\Delta_{s} = 0$ the superconducting gap is purely determined by the p-wave superconducting gap with point node,
the DOS behaves to be "U" shape (Fig. 1a and 1b). With increasing value of the isotropic $s$-wave gap, once both $s$-wave and $p$-wave superconducting gaps are the same, the accidental node forms and the behavior of the DOS changes to a linear at low energy reflecting the formation of the line of node (Fig. 1c). Finally when $s$-wave gap is larger than $p$-wave one, the U-shaped DOS behavior suggests zero density of states for energies lower than $\Delta_0$ (Fig. 1d). While for LDOS around an impurity, the LDOS shows the formation of the impurity induced resonant states that appear at the positive and negative energy. Clearly these resonant states arise due to unconventional nature of the $p$-wave superconducting gap and the nodal points at the Fermi surfaces. One clearly sees that upon increasing of the isotopic $s$-wave contribution the resonant states shift towards the edge of the superconducting gap (Fig. 1d).

In the right column of Fig. 1 we show a similar evolution of the DOS without impurity and the LDOS with an impurity on the nearest neighbor site $(0, 1, 0)$, however, now the $s$-wave component of the superconducting gap is momentum dependent, $\Delta_s = \Delta_0 (\cos k_x + \cos k_y) = \Delta_0 \gamma_k$. Interestingly enough, here the node in the DOS forms already when the $p$-wave superconducting gap component is zero and is the result of the initial momentum structure of the $s$-wave superconducting gap that yields nodes on the Fermi surface. This is unique to the anisotropic $s$-wave superconducting gap. By introducing the interference between $s$-wave and $p$-wave gap the position of the node is shifted to the different points of the Brillouin Zone, however, here the nodal structure of the superconducting gap is not a result of the interference effect between $p$-wave and $s$-wave of the superconducting gap but arises already in the pure anisotropic $s$-wave symmetry and shifted by introducing the moderate component of the $p$-wave gap. The
corresponding LDOS shows that for any value of the $s$-wave and $p$-wave gap, because there are nodal points at the Fermi surface resulting either from the internal structure of the anisotropic $s$-wave gap, point nodes from the $p$-wave state, or a nodal line that arises due to interference of the $p$-wave and $s$-wave gap, the impurity induced state always occurs near the Fermi energy (Fig. 1e-h). Note, that in case of pure anisotropic $s$-wave gap due to the nodal structure the impurity induced state becomes visible only for a very large values of the potential scattering strength $U_0$.

4. Summary

In summary, we have investigated theoretically the non-magnetic impurity induced resonance states in the superconductors without inversion symmetry using as an example CePt$_3$Si, which is believed to have a line node in the energy gap arising from the coexistence of $s$-wave and $p$-wave pairing symmetry. Analyzing the local density of states, we find that a single nonmagnetic impurity-induced resonance states is highly probable in non-centrosymmetric superconductors. We show that further STM experiments may reveal the exact symmetry of the superconducting gap in these systems.

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