Impurity resonance states in noncentrosymmetric superconductor CePt₃Si: A probe for Cooper-pairing symmetry

Bin Liu[1] and Ilya Eremin[1,2]

[1]*Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany*
[2]*Institute für Mathematische und Theoretische Physik, TU-Braunschweig, D-38106 Braunschweig, Germany*

Motivated by the recent discovery of noncentrosymmetric superconductors, such as CePt₃Si, CeRhSi₃, and CeIrSi₃, we investigate theoretically the impurity resonance states with coexisting s-wave and p-wave pairing symmetries. Due to the nodal structure of the gap function, we find single nonmagnetic impurity-induced resonances appearing in the local density of state. In particular, 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. Our results show that the scanning tunneling microscopy can shed light on the particular structure of the superconducting gap in noncentrosymmetric superconductors.

I. INTRODUCTION

Recent discoveries of superconductivity (SC) in the systems that possess a lack of inversion symmetry such as CePt₃Si (Ref. 1) with $T_c \simeq 0.75$ K, and more recently CeRhSi₃,[2] CeIrSi₃,[3] Li(Pd$_{1-x}$,Pt$_x$)₃B,[4] UIr,[5] and Y₂C₃ (Ref. 6), have raised an interest in the theoretical investigation of superconductivity in these systems. Among interesting questions, the most important one is concerned with the underlying symmetry of the superconducting order parameter. In particular, in all these materials, there is a nonzero potential gradient ∇V averaged in the unit cell due to lack of inversion symmetry, which results in the anisotropic spin-orbit interaction. Its general form can be determined by a group theoretical argument,[7] which, as it has been found, leads to many interesting properties.[8–14] For example, on general grounds, there is a mixing of the spin-singlet and spin-triplet superconducting states due to the lack of inversion. In CePt₃Si the pairing symmetry has been studied theoretically[9–13] and it is believed that the $s+p$-wave superconducting state is realized. Frigeri *et al.*[11] pointed out that the spin-orbit interaction could determine the direction of the **d** vector as $\mathbf{d} \| \vec{l}$ ($\vec{l}$ is the vector of the Rashba spin-orbit coupling), for which the highest transition temperature was obtained. A microscopic calculation with the detailed structure of the Fermi surface[13] seems to confirm that the $s+p$-wave state is the most probable one. The experimental studies of the temperature dependencies of the spin-lattice relaxation,[15] the magnetic penetration depth,[16] and the thermal-conductivity measurements[17] are also consistent with this conjecture.

It is known that the nonmagnetic as well as the magnetic impurities in the conventional and unconventional superconductors already have been proven to be a useful tool in distinguishing between various symmetries of the superconducting state.[18] For example, in the conventional isotropic s-wave superconductor, the single magnetic impurity-induced resonance state is located at the gap edge, which is known as Yu-Shiba-Rusinov state.[19] In the case of unconventional superconductor with $d_{x^2-y^2}$-wave symmetry of the superconducting state, the nonmagnetic impurity-induced

bound state appears near the Fermi energy as a hallmark of $d_{x^2-y^2}$-wave pairing symmetry.[20] The origin of this difference is understood as being due to the nodal structure of two kinds of SC order: in the $d_{x^2-y^2}$-wave case, the phase of Cooper-pairing wave function changes sign across the nodal line, which yields finite density of states (DOSs) below the superconducting gap, while in the isotropic s-wave case, the density of states is gapped up to energies of about Δ_0 and thus the bound state can appear only at the gap edge. In principle the formation of the impurity resonance states can also occur in unconventional superconductors if the nodal line or point does not exist at the Fermi surface of a superconductor, as it occurs for isotropic nodeless p-wave and/or d_x+id_y-wave superconductors for the large value of the potential strength.[21] Therefore, scanning tunneling microscopy (STM) measurements of the impurity states can provide important messages about the pairing symmetry in the relevant systems. In the noncentrosymmetric superconductor with the possible coexistence of s-wave and p-wave pairing symmetries, it is very interesting to see what the nature of the impurity state is 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. Previously, the effect of nonmagnetic impurity scattering has been studied in the noncentrosymmetric superconductors with respect to the suppression of T_c (Ref. 22) and the behavior of the upper critical field.[23]

In this paper we investigate theoretically the impurity resonance states where both s-wave and p-wave Cooper pairings coexist. Due to the nodal structure of gap function as a result of the interference between the spin-triplet and the spin-singlet components of the superconducting order parameters, we find that a single nonmagnetic impurity-induced resonance state appears in the local density of state (LDOS). In particular, 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. Our results show that the scanning tunneling microscopy can shed light on the particular structure of the superconducting gap in noncentrosymmetric superconductors.

II. MODEL AND *T*-MATRIX FORMULATION

Theoretical models of the superconducting state in CePt$_3$Si are based upon the existence of a Rashba-type spin-orbit coupling (RSOC).[9] Therefore, following previous consideration,[11] we start from a single orbital model with RSOC,

$$H = \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}} c_{\mathbf{k}s}^{\dagger} c_{\mathbf{k}s} + \alpha \sum_{\mathbf{k}ss'} \mathbf{g}_k \cdot \sigma_{\mathbf{ss'}} c_{\mathbf{k}s}^{\dagger} c_{\mathbf{k}s'}, \qquad (1)$$

where $c_{\mathbf{k}s}^{\dagger}$ ($c_{\mathbf{k}s}$) is the fermion creation (annihilation) operator with spin s and momentum $\mathbf{k}$. Here, $\varepsilon_{\mathbf{k}}$ is the tight-binding-energy dispersion,

$$\begin{aligned} \varepsilon_{\mathbf{k}} = {} & 2t[\cos(k_x) + \cos(k_y)] + 4t_1 \cos(k_x)\cos(k_y) \\ & + 2t_2[\cos(2k_x) + \cos(2k_y)] \\ & + \{2t_3 + 4t_4[\cos(k_x) + \cos(k_y)] \\ & + 4t_5[\cos(2k_x) + \cos(2k_y)]\}\cos(k_z) + 2t_6 \cos(2k_z) - \mu, \end{aligned}$$
$$(2)$$

which reproduces the so-called β band of CePt$_3$Si, as obtained from the band-structure calculations.[7,13] The electron hopping parameters are $(t, t_1, t_2, t_3, t_4, t_5, t_6, n) = (1, -0.15, -0.5, -0.3, -0.1, -0.09, -0.2, 1.75)$ and the electron density per site n is used to determine the chemical potential.[13]

The second term of Eq. (1) is the RSOC interaction where α denotes the coupling constant and the vector function $\mathbf{g}_{\mathbf{k}}$ is assumed in the following form $\mathbf{g}_{\mathbf{k}} = (-\sin k_y, \sin k_x, 0)$. This term removes the usual Kramers degeneracy between the two
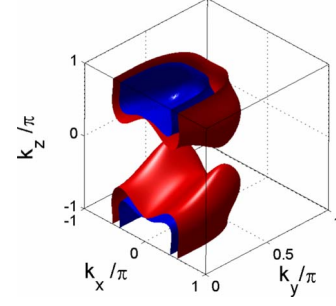

FIG. 1. (Color online) The calculated Fermi surface using Eq. (1) and the spin-orbit coupling constant $\alpha = 0.3t$.

spin states at a given $\mathbf{k}$ and leads to a quasiparticle dispersion $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} \pm \alpha |\mathbf{g}_{\mathbf{k}}|$ with $|\mathbf{g}_{\mathbf{k}}| = \sqrt{\mathbf{g}_{\mathbf{k}x}^2 + \mathbf{g}_{\mathbf{k}y}^2 + \mathbf{g}_{\mathbf{k}z}^2}$, splitting the Fermi surface (FS) into two sheets. Based on the above hopping parameters and RSOC constant $\alpha = 0.3t$, the resulting FS is shown in Fig. 1, where the main characteristic features of the FS has been successfully reproduced.[7]

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. A full symmetry analysis[7,13] shows that s-wave pairing $\Delta_s = \Delta_0[\cos(k_x) + \cos(k_y)]$ and p-wave triplet pairing states with order parameter $\mathbf{d}_{\mathbf{k}}$ parallel to the $\mathbf{g}_{\mathbf{k}}$ vector ($\mathbf{d}_{\mathbf{k}} = d_0\mathbf{g}_{\mathbf{k}}$) are able to coexist. Following previous estimations,[13] we have taken the odd-parity component $\mathbf{d}_{\mathbf{k}} = d_0(-\sin k_y, \sin k_x, 0)$. Then the mean-field BCS Hamiltonian for this system has the matrix form

$$H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \alpha(\mathbf{g}_{k_x} - i\mathbf{g}_{k_y}) & -\mathbf{d}_{k_x} + i\mathbf{d}_{k_y} & \Delta_s \\ \alpha(\mathbf{g}_{k_x} + i\mathbf{g}_{k_y}) & \varepsilon_{\mathbf{k}} & -\Delta_s & \mathbf{d}_{k_x} + i\mathbf{d}_{k_y} \\ -\mathbf{d}_{k_x} - i\mathbf{d}_{k_y} & -\Delta_s^* & -\varepsilon_{\mathbf{k}} & \alpha(\mathbf{g}_{k_x} + i\mathbf{g}_{k_y}) \\ \Delta_s^* & \mathbf{d}_{k_x} - i\mathbf{d}_{k_y} & \alpha(\mathbf{g}_{k_x} - i\mathbf{g}_{k_y}) & -\varepsilon_{\mathbf{k}} \end{pmatrix}. \qquad (3)$$

The inverse of the single-particle Green's function is defined as

$$g^{-1}(\mathbf{k}, i\omega_n) = i\omega_n I - H_{\mathbf{k}}, \qquad (4)$$

where I is the 4×4 identity matrix. Taking the inverse of Eq. (3), we find

$$g(\mathbf{k}, i\omega_n) = \begin{pmatrix} G(\mathbf{k}, i\omega_n) & F(\mathbf{k}, i\omega_n) \\ F^{\dagger}(\mathbf{k}, i\omega_n) & -G^t(-\mathbf{K}, -i\omega_n) \end{pmatrix}, \qquad (5)$$

where

$$G(\mathbf{k}, i\omega_n) = \sum_{\tau = \pm 1} \frac{1 + \tau(\vec{\mathbf{g}}_{\mathbf{k}} \cdot \sigma)}{2} G_{\tau}(\mathbf{k}, i\omega_n), \qquad (6)$$

$$F(\mathbf{k}, i\omega_n) = \sum_{\tau = \pm 1} \frac{1 + \tau(\vec{\mathbf{g}}_{\mathbf{k}} \cdot \sigma)}{2} i\sigma_y F_{\tau}(\mathbf{k}, i\omega_n), \qquad (7)$$

and

$$G_{\tau}(\mathbf{k}, i\omega_n) = \frac{i\omega_n + \epsilon_{\tau}}{(i\omega_n)^2 - E_{\mathbf{k}\tau}^2}, \qquad (8)$$

$$F_{\tau}(\mathbf{k}, i\omega_n) = \frac{\Delta_{\tau}}{(i\omega_n)^2 - E_{\mathbf{k}\tau}^2}. \qquad (9)$$

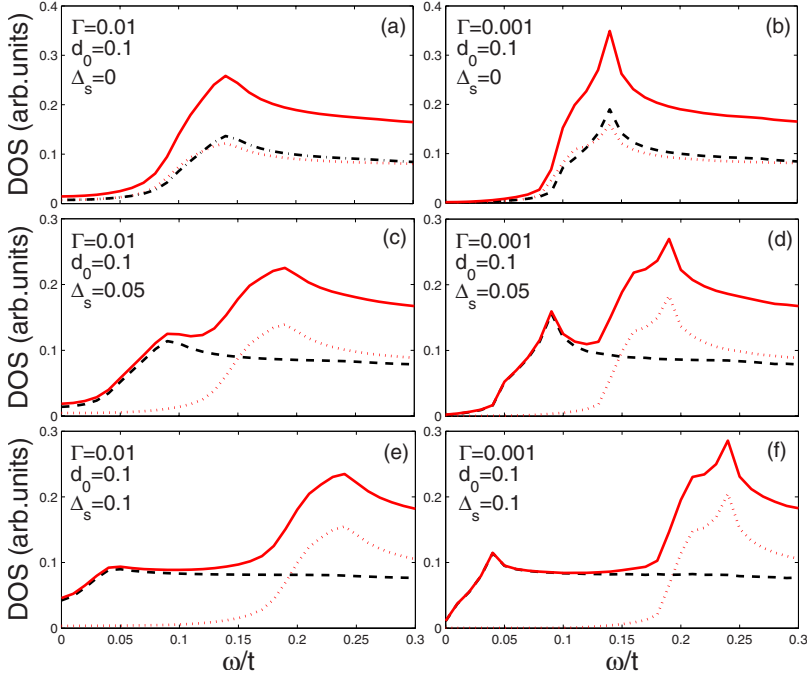Here, the single-particle excitation energy is

FIG. 2. (Color online) The evolution of the local density of states for various ratios between coexisting isotropic s-wave and p-wave Cooper-pairing states. The left and right panels refer to the different values of the damping constant Γ. The dashed and the dotted curves denote the contribution of the different bands, and the straight curve refers to the total density of states. The parameters of the gaps and the damping Γ are given in terms of hopping integral t.

$$E_{\mathbf{k}\tau} = \sqrt{\epsilon_\tau^2 + |\Delta_\tau|^2}, \tag{10}$$

with

$$\epsilon_\tau = \epsilon_{\mathbf{k}} + \tau\alpha|\mathbf{g_k}|; \Delta_\tau = \Delta_{\mathbf{k}} + \tau|\mathbf{d_k}|, \tag{11}$$

and the unit vector is $\vec{\mathbf{g}}_{\mathbf{k}} = \mathbf{g_k}/|\mathbf{g_k}|$.

For completion the equations above have to be supplemented by the self-consistency equation that determines the symmetry of the superconducting gap and the superconducting transition temperature. For the sake of simplicity and also because this is not critical for our further analysis, we consider the superconducting order parameter as a given parameter. At the same time, recent studies based on the helical spin fluctuation mediated Cooper-pairing find two stable superconducting phases with either dominantly $s+p$-wave or $p+d+f$-wave symmetry of superconducting order parameter.[13,24,25] In the following we adopt the former one for our calculation.

The next step is to obtain Green's function in the presence of a single impurity site. The impurity scattering is given by

$$H_{imp} = U_0 \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma}, \tag{12}$$

Where, without loss of generality, we have taken a single-site nonmagnetic impurity of strength U_0 located at the origin, $r_i = 0$. Then the site dependent Green's function can be written in terms of the T-matrix formulation[21,26,27] as

$$\zeta(i,j;i\omega_n) = \zeta_0(i-j;i\omega_n) + \zeta_0(i,i\omega_n)T(i\omega_n)\zeta_0(j,i\omega_n), \tag{13}$$

where

$$T(i\omega_n) = \frac{U_0\rho_3}{1 - U_0\rho_3\zeta_0(0,0;i\omega_n)}, \tag{14}$$

and

$$\zeta_0(i,j;i\omega_n) = \frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_{ij}}g(k,i\omega_n), \tag{15}$$

with ρ_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 local density of state, which can be measured in the STM experiment, has been obtained as

$$N(r,\omega) = -\frac{1}{\pi}\sum_i \text{Im } \zeta_{ii}(r,r;\omega + i\eta), \tag{16}$$

where η denotes an infinitely small positive number.

III. NUMERICAL RESULTS AND DISCUSSIONS

A. Density of state

Before considering the effect of the impurity, it is useful to analyze first the DOS in the superconducting state, which is expressed as

$$\rho(\omega) = -\frac{1}{\pi}\text{Im}\sum_{i,\mathbf{k}} g_{ii}(\mathbf{k},\omega). \tag{17}$$

As we already have mentioned above, it is not necessary to calculate the magnitude of the gap functions self-consistently since we are mainly interested in the qualitative properties arising from the gap structure. We first consider the situation when the s-wave part of the total superconducting gap is momentum independent, $\Delta_s = \Delta_0$. In Fig. 2 we show the evolution of the density of state in positive frequencies for various values of the s-wave component of the superconducting
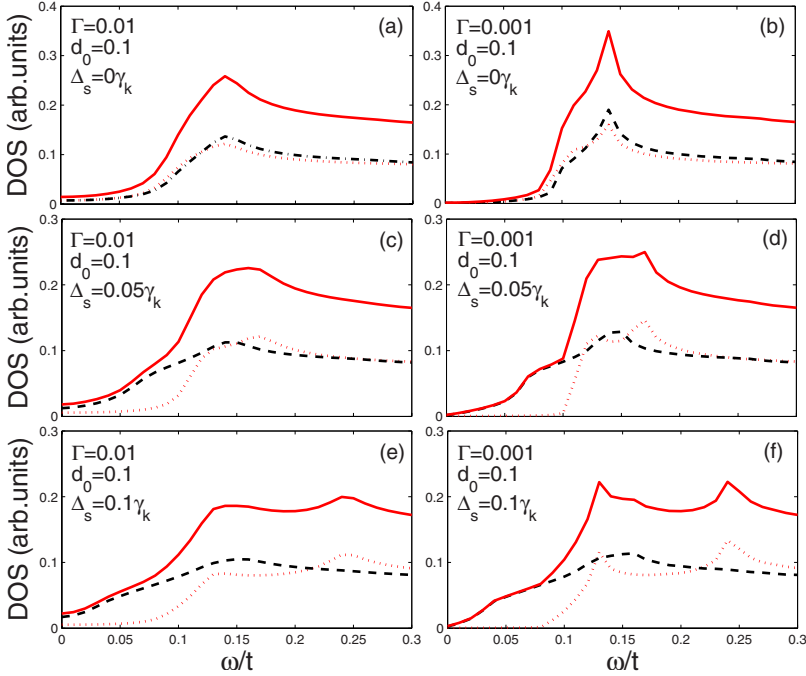
FIG. 3. (Color online) The evolution of the local density of states for various ratios between coexisting anisotropic s-wave and p-wave Cooper-pairing states. The left and right panels refer to the different values of the damping constant Γ. The dashed and the dotted curves denote the contribution of the different bands, and the straight curve refers to the total density of states. The parameters of the gaps and the damping Γ are given in terms of hopping integral t.

gap. In particular, for zero value of the s-wave component, the superconducting gap is purely determined by the p-wave superconducting gap with the point node at the Fermi surfaces of the corresponding bands at $(k_x=0, k_y=0)$. This gap structure is the same for both bands splitted by the spin-orbit coupling. With increasing value of the isotropic s-wave gap, one finds that the total superconducting gap in one of the bands increases with the total superconducting gap $\Delta_s + |\mathbf{d_k}|$ while it decreases effectively for the other band for which the total gap is $\Delta_s - |\mathbf{d_k}|$. Once both s-wave and p-wave superconducting gaps are the same, the accidental node forms at one of the band and the behavior of the density of states changes to a linear at low energy reflecting the formation of the line of node. We further note that density of states shows only slight electron-hole asymmetry.

In Fig. 3 we show, however, a similar evolution of the density of states now that the s-wave component of the superconducting gap is momentum dependent, $\Delta_s = \Delta_0 (\cos k_x + \cos k_y) = \Delta_0 \gamma_{\mathbf{k}}$.[28] Interestingly enough, here the node in the density of states forms already when the p-wave superconducting gap component is zero (see also Fig. 5) and is the result of the initial momentum structure of the s-wave superconducting gap that yields point 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 gaps, 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 is shifted by introducing the moderate component of the p-wave gap.

B. Impurity resonance states

In view of complicated band structure arising in CePt$_3$Si from the Rashba spin-orbit coupling and the corresponding

interference effect for the superconducting gap, the density of states in a clean case that can be accessed by the tunneling experiments cannot give a precise information on the exact structure of the superconducting gap in the noncentrosymmetric superconductors. At the same time, an introduction of the nonmagnetic impurity can give additional important information on the symmetry of the superconducting gap in such a material. In terms of Eq. (16), the T matrix can be written as

$$T^{-1}(i\omega_n) = U_0^{-1} - \rho_3 \zeta_0(0,0;i\omega_n), \qquad (18)$$

and the position of the impurity resonant state is given by det $T^{-1}=0$. We first study the situation of the isotropic s-wave superconducting gap coexisting with p wave. In Fig. 4 we show the calculated density of states without impurity and also the local density of states with an impurity on the nearest-neighbor site (0,1,0). Without the s-wave component, the density of states shows the formation of the impurity-induced resonant bound states that appear symmetrically in energy at the positive and negative sides of the LDOS. Clearly these resonant bound states arise due to unconventional nature of the p-wave superconducting gap and the nodal points at the Fermi surface. One clearly sees that upon increasing of the isotropic s-wave contribution, the bound state shifts toward the edge of the superconducting gap, implying the zero density of states for energies lower than Δ_0.

In Fig. 5 we show the corresponding local density of states for the coexisting anisotropic s-wave and p-wave superconducting gaps. In the present case, for any value of the s-wave and p-wave gaps, there are nodal points at the Fermi surface, resulting either from the internal structure of the anisotropic s-wave gap, the point nodes from the p-wave state, or a nodal line at one of the bands that arises due to interference of the p-wave and s-wave gaps. Therefore, the impurity-induced bound state occurs for all ratios between
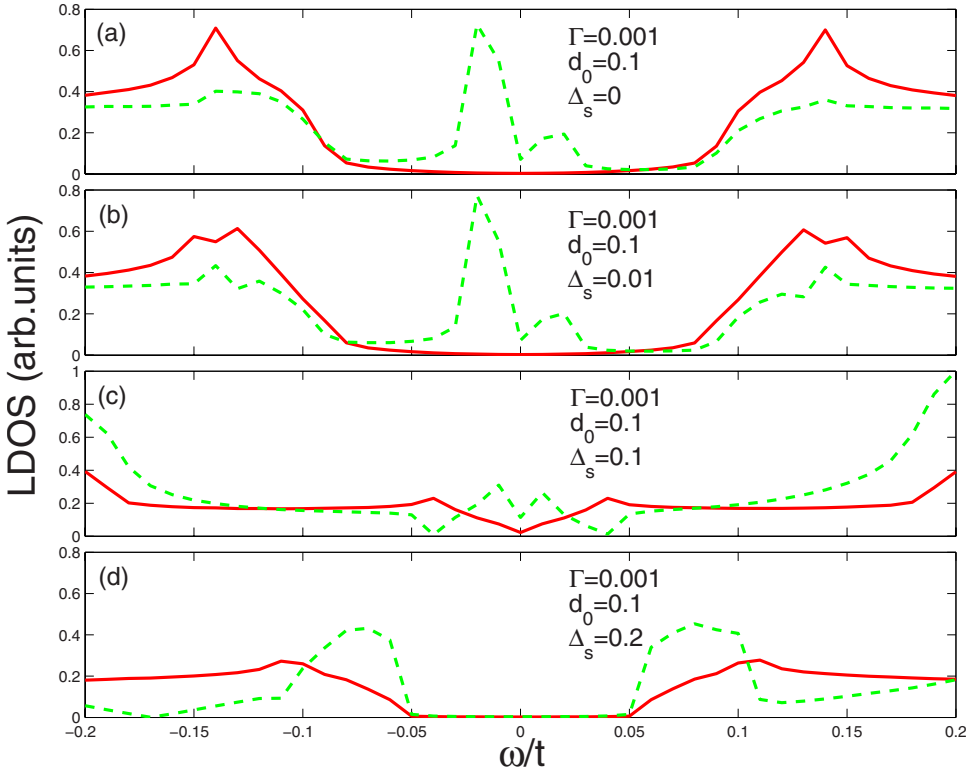
FIG. 4. (Color online) The LDOS for coexisting isotropic s-wave and p-wave Cooper-pairing states for various ratios of the parameters. The straight (red) curves refer to the calculated density of states without impurity and the dashed (green) curves refer to the LDOS at the $(0,1,0)$ position. Here, we use $U_0 = 5t$.

the p-wave and s-wave gaps. Note, that in case of pure anisotropic s-wave gap due to the nodal structure on both of the bands, the impurity-induced bound state becomes visible only for very large values of the potential scattering strength U_0.

IV. SUMMARY

In summary, we have investigated theoretically the nonmagnetic impurity-induced resonance bound states in the superconductors without inversion symmetry using, as an ex-
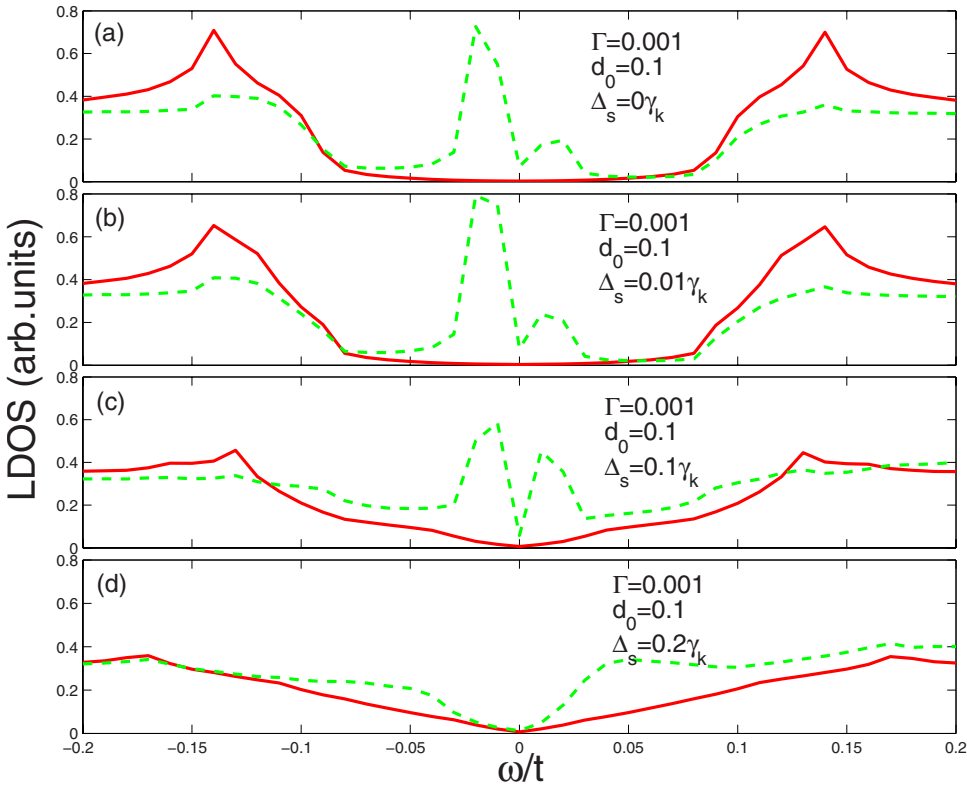

FIG. 5. (Color online) The LDOS for coexisting anisotropic s-wave (Δ) and p-wave Cooper-pairing states for various ratios of the parameters. The straight (red) curves refer to the calculated density of states without impurity and the dashed (green) curves refer to the LDOS at the $(0,1,0)$ position. Here, we use $U_0 = 5t$.

ample, 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 symmetries. Analyzing the local density of states that we found in the nodal structure of gap function, we find that a single nonmagnetic impurity-induced resonance state is highly probable in noncentrosymmetric superconductors. We show that further STM experiments may reveal the exact symmetry of the superconducting gap in these systems.

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[28] Note that both the nodal and the isotropic s-wave components of the total superconducting gap may coexist in the microscopic theory of the Cooper pairing. Moreover, the on-site Coulomb repulsion will tend to favor the nodal s-wave gap function.