Local electronic structure of the superconducting interface $LaAlO_3/SrTiO_3$

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Motivated by the recent discovery of superconductivity on the heterointerface $LaAlO_3/SrTiO_3$, we theoretically investigate its local electronic structures near an impurity considering the influence of Rashba-type spin-orbit interaction (RSOI) originated in the lack of inversion symmetry. We find that local density of states near an impurity exhibits the in-gap resonance peaks due to the quasiparticle scattering on the Fermi surface with the reversal sign of the pairing gap caused by the mixed singlet and RSOI-induced triplet superconducting state. We also analyze the evolutions of density of states and local density of states with the weight of triplet pairing component determined by the strength of RSOI, which will be widely observed in thin films of superconductors with surface or interface-induced RSOI, or various noncentrosymmetric superconductors in terms of point contact tunneling and scanning tunneling microscopy, and thus reveal an admixture of the spin singlet and RSOI-induced triplet superconducting states.

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Since the discovery of a high-mobility electron gas caused by electronic reconstruction at the interface $LaAlO_3/SrTiO_3$,[1] much attention has been paid to its ground state. Theoretical studies suggest the charge carrier density plays the essential role in determining the ground state.[2] The recent field-effect measurement on the $LaAlO_3/SrTiO_3$ interface[3] indicates that electrostatic tuning of the carrier density allows an on/off switching of superconductivity, and drives a quantum phase transition between a two-dimensional (2D) superconducting (SC) state[4] and an insulating state. This is analogous to the case of the cuprates superconductors, where superconductivity occurs when doping hole or electron into a Mott insulator. However, in contrast to chemical doping, the field-effect experiment only modifies the charge, revealing directly the relationship between carrier density and transition temperature T_c.[5] Therefore, the discovery of superconductivity controlled by electric field is helpful for understanding the pendent mechanism of the superconductivity, and opens the way to developing the new mesoscopic SC circuits.

Among many interesting questions the most important one concerns the underlying symmetry of the SC order parameter (OP). Compared with the conventional bulk $SrTiO_3$ superconductor with $T_c \simeq 0.4$ K,[6] the SC condensation temperature at the interface $LaAlO_3/SrTiO_3$ is only 0.2 K,[4] suggesting the different types of superconductivity in bulk and interface. In particular, due to the lack of inversion symmetry along the direction perpendicular to the interface,[1] there is a nonzero potential gradient ∇V averaged in the unit cell, which leads to the so-called Rashba-type spin-orbit interaction (RSOI).[7] The resulting RSOI changes the nature of single-electron states, namely, it leads to the lifting of spin degeneracy and the splitting of the energy bands. In this case, superconductivity is weakened or even suppressed according to Anderson's theorem,[8] which may explain the lower T_c in the interface compared to the bulk. Another key point is that the RSOI induced by broken inversion symmetry breaks the parity, the mixed singlet and triplet SC states may be possible. This characteristic feature is the same as the noncentrosymmetric superconductors, such as $CePt_3Si$,[9] $CeRhSi_3$,[10] and $Li(Pd_{1-x},Pt_x)_3B$,[11,12] where a mixing of the spin-singlet and triplet states has been discussed due to the absence of inversion symmetry.[13–16] Therefore, we expect a singlet-triplet mixing of pairing states can be realized in the SC interface $LaAlO_3/SrTiO_3$.

In this paper, we investigate the local electronic structures near an impurity considering the influence of RSOI in the SC interface, which is expected to be especially important for distinguishing the conventional superconductors from unconventional ones with the variation in the sign of OP on the Fermi surface (FS).[17]

We start from a two-dimensional minimal tight-binding model with the RSOI to describe the 2D electronic gas generated at the interface $LaAlO_3/SrTiO_3$,[1,15,18] due to the interface which is composed by Ti $3d_{xy}$ electrons.[19] It is given by

$$H = \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s} + \lambda \sum_{\mathbf{k}ss'} \mathbf{g}_{\mathbf{k}} \cdot \sigma_{ss'} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s'}, \quad (1)$$

where $c^{\dagger}_{\mathbf{k}s}$ ($c_{\mathbf{k}s}$) is the fermion creation (annihilation) operator with spin s and momentum $\mathbf{k}$. Here,

$$\varepsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] - \mu \quad (2)$$

is the tight-binding energy dispersion. The second term is the RSOI interaction where λ denotes the coupling constant and the spin-orbital vector function $\mathbf{g}_{\mathbf{k}}$ has the form of $\mathbf{g}_{\mathbf{k}} = (-\sin k_y, \sin k_x, 0)$.[7] Then applying the unitary 2×2 matrix

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ \frac{\mathbf{g_{k1}} + \mathbf{i g_{k2}}}{|\mathbf{g_k}|} & -\frac{\mathbf{g_{k1}} + \mathbf{i g_{k2}}}{|\mathbf{g_k}|} \end{pmatrix}, \quad (3)$$

we can diagonalize Eq. (1) into the band representation

$$H = \sum_{\mathbf{k}\nu} \xi_{\mathbf{k}\nu} a^{\dagger}_{\mathbf{k}\nu} a_{\mathbf{k}\nu} \quad (4)$$

with the band dispersion

$$\xi_{\mathbf{k}\pm} = \varepsilon_{\mathbf{k}} \pm \lambda |\mathbf{g}_{\mathbf{k}}|. \quad (5)$$

As shown in Fig. 1, the RSOI term lifts the spin degeneracy by generating two bands with reversal spin orientation.

In the superconducting state, the presence of RSOI breaks

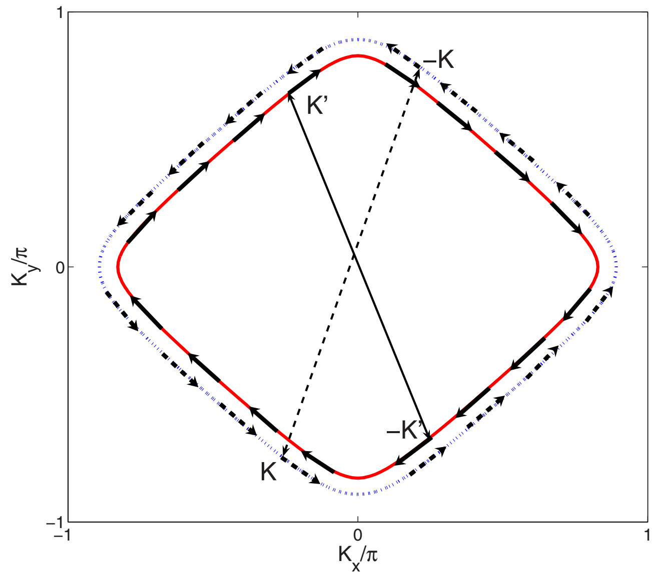

FIG. 1. (Color online) Fermi surfaces for $\mathbf{g_k} = (-\sin k_y, \sin k_x, 0)$ with reversal spin orientation at $\lambda/t = 0.1$. The solid and dotted double arrows denote the Cooper pairing within each Fermi surface.

the parity and, therefore, mixes the singlet (even parity) and triplet (odd parity) Cooper-pairing states. We parametrize the 2×2 pairing-potential matrix by

$$\Delta_{\mathbf{k}} = (\Delta_s \sigma_0 + \mathbf{d_k} \cdot \sigma)(i\sigma_2), \tag{6}$$

where spin-singlet Δ_s (s wave) is assumed reasonably up to the interface because of the conventional BCS bulk $SrTiO_3$ superconductor.[6] According to weak coupling calculations in the noncentrosymmetric superconductors,[15] the RSOI-induced triplet $\mathbf{d_k}$ vector parallel to $\mathbf{g_k}$ gives the highest T_c as long as the pairing interaction stabilizes the gap function with the same momentum dependence as that of $\mathbf{g_k}$. Thus, we define $\mathbf{d_k} = d_0 \mathbf{g_k}/|\mathbf{g_k}|$ in the following calculations. Then the mean field BCS Hamiltonian has the matrix form

$$H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} & \lambda g_k^* & -d_k^* & \Delta_s \\ \lambda g_k & \varepsilon_{\mathbf{k}} & -\Delta_s & d_k \\ -d_k & -\Delta_s^* & -\varepsilon_{\mathbf{k}} & \lambda g_k \\ \Delta_s^* & d_k^* & \lambda g_k^* & -\varepsilon_{\mathbf{k}} \end{pmatrix} \tag{7}$$

with complex notations $g_k = \mathbf{g_{k1}} + \mathbf{i}\mathbf{g_{k2}}$, $d_k = \mathbf{d_{k1}} + \mathbf{i}\mathbf{d_{k2}}$, and corresponding complex conjugates g_k^*, d_k^*. Finally the single-particle Green's function is obtained as

$$g(\mathbf{k}, i\omega_n) = \begin{pmatrix} G(\mathbf{k}, i\omega_n) & F(\mathbf{k}, i\omega_n) \\ F^\dagger(\mathbf{k}, i\omega_n) & -G^t(-\mathbf{k}, -i\omega_n) \end{pmatrix}, \tag{8}$$

where

$$G(\mathbf{k}, i\omega_n) = \sum_{\tau=\pm 1} \frac{1 + \tau(\vec{\mathbf{g}}_{\mathbf{k}} \cdot \sigma)}{2} G_\tau(\mathbf{k}, i\omega_n), \tag{9}$$

$$F(\mathbf{k}, i\omega_n) = \sum_{\tau=\pm 1} \frac{1 + \tau(\vec{\mathbf{g}}_{\mathbf{k}} \cdot \sigma)}{2} i\sigma_2 F_\tau(\mathbf{k}, i\omega_n), \tag{10}$$

and

$$G_\tau(\mathbf{k}, i\omega_n) = \frac{i\omega_n + \xi_{\mathbf{k}\tau}}{(i\omega_n)^2 - E_{\mathbf{k}\tau}^2}, \tag{11}$$

$$F_\tau(\mathbf{k}, i\omega_n) = \frac{\Delta_\tau}{(i\omega_n)^2 - E_{\mathbf{k}\tau}^2}. \tag{12}$$

Here, the SC quasiparticle excitation energy is

$$E_{\mathbf{k}\tau} = \sqrt{\xi_{\mathbf{k}\tau}^2 + |\Delta_\tau|^2}, \tag{13}$$

where $\Delta_\tau = \Delta_s + \tau|\mathbf{d_k}|$ are the SC gaps on the energy bands and thus automatically include both inter- and intra-band pairings in the original electron operator $c_{\mathbf{k}s}$, and $\vec{\mathbf{g}}_{\mathbf{k}} = \mathbf{g_k}/|\mathbf{g_k}|$ is the unit vector. Then we get the density of states (DOS)

$$\rho(\omega) = -\frac{1}{\pi} \mathrm{Im} \sum_{\tau,\mathbf{k}} G_\tau(\mathbf{k}, i\omega_n)|_{i\omega_n \to \omega + i0^+}. \tag{14}$$

In Fig. 2, we show the calculated DOS for the ratio α

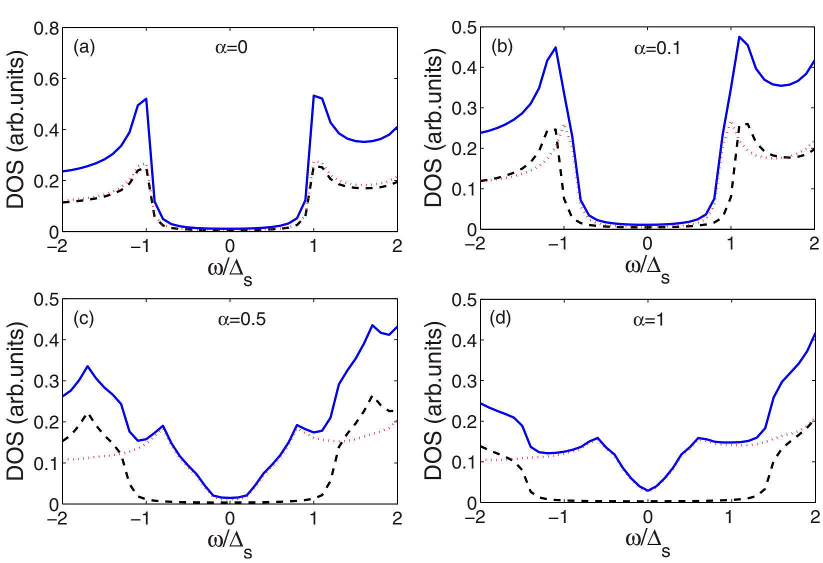

FIG. 2. (Color online) Evolution of DOS with the ratio $\alpha = d_0/\Delta_s$ between singlet s-wave and triplet pairing gaps. The dashed and dotted curve denotes the contribution of the different bands and the solid curve refers to the total DOS.

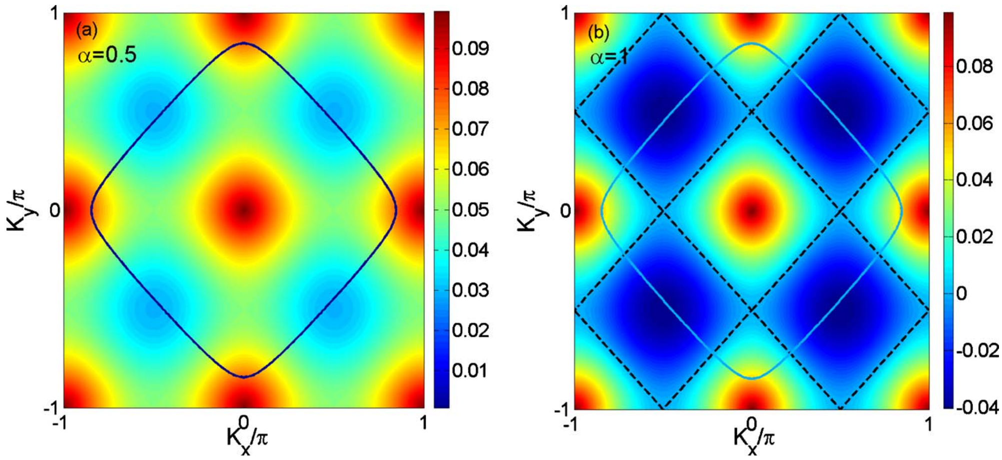

FIG. 3. (Color online) Mixed singlet and triplet pairing gap functions for $\Delta_s - |\mathbf{d}_\mathbf{k}|$ in the first Brillouin zone at (a) $\alpha=0.5$ and (b) $\alpha=1$. The solid line denotes Fermi surface of band $\xi_{\mathbf{k}-}$, and the dashed line in (b) indicates the formation of the line of node.

$=d_0/\Delta_s$ between the magnitudes of triplet and singlet OP ranging from 0 to 1, since the singlet pairing component is expected to be dominant near half-filling compared to the RSOI-induced triplet pairing in the interface $LaAlO_3/SrTiO_3$.[20] In the absence of RSOI [Fig. 2(a)], namely, for zero value of the triplet pairing component, the total SC gap is purely determined by the singlet *s*-wave gap without node on the FS. The "U"-shaped DOS structure is the same for both bands, and is a typical feature of the conventional Bardeen-Cooper-Schrieffer superconductors. Upon introducing and increasing the weight of the anisotropic triplet pairing component, one finds that the total SC gap in one of the bands increases with the value $\Delta_s + |\mathbf{d}_\mathbf{k}|$ while it decreases effectively for the other band for which the total gap is $\Delta_s - |\mathbf{d}_\mathbf{k}|$. Therefore, the DOS in both bands are still gapped near the Fermi energy [Figs. 2(b) and 2(c)]. When the singlet *s*-wave and triplet pairing SC gaps are the same, the accidental node forms at one of the bands and the DOS changes to a linear behavior at low energy reflecting the formation of the line of node [Fig. 2(d)]. We propose that point contact tunneling can probe the DOS so that reveal the mixed singlet and triplet pairing states. The corresponding momentum dependence of the mixed singlet and triplet pairing gap functions for Δ_- has been plotted in Fig. 3 for $\alpha=0.5$ and $\alpha=1$ (Δ_+ is always positive without node on the FS and thus not plotted here). It is clearly shown that the line node has occurred at sufficient large $\alpha=1$ [dashed line in Fig. 3(b)].

In order to detect the sign reversal pairing in the mixed singlet and triplet pairing SC interface $LaAlO_3/SrTiO_3$, we calculate the local density of states (LDOS) in the presence of a single impurity site. The impurity scattering is given by

$$H_{\text{imp}} = V_0 \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma}, \tag{15}$$

where without loss of generality we have taken a single-site nonmagnetic impurity of strength V_0 located at the origin. Then the site dependent Green's function can be written in terms of the *T*-matrix formulation[17] as

$$\zeta(i,j;i\omega_n) = \zeta_0(i-j;i\omega_n) + \zeta_0(i,i\omega_n)T(i\omega_n)\zeta_0(j,i\omega_n), \tag{16}$$

where

$$T(i\omega_n) = \frac{V_0\rho_3}{1 - V_0\rho_3\zeta_0(0,0;i\omega_n)} \tag{17}$$

$$\zeta_0(i,j;i\omega_n) = \frac{1}{N}\sum_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{R}_{\mathbf{ij}}} g(k,i\omega_n), \tag{18}$$

with ρ_i being the Pauli spin operator, and $\mathbf{R}_\mathbf{i}$ the lattice vector, $\mathbf{R}_{\mathbf{ij}}=\mathbf{R}_\mathbf{i}-\mathbf{R}_\mathbf{j}$. Finally, the LDOS, which can be measured in the scanning tunneling microscopy experiment, has been obtained as

$$\rho(r,\omega) = -\frac{1}{\pi}\sum_i \text{Im}\,\zeta_{ii}(r,r;\omega+i\eta), \tag{19}$$

where η denotes an infinitely small positive number.

In Figs. 4(a)–4(d) we display the LDOS near a nonmagnetic impurity for various weight ratios α and scattering strengths V_0. Obviously, in the case of pure singlet *s*-wave pairing, the LDOS only has two impurity resonance peaks at gap edges $\pm\Delta_s$ for any scattering strength, which is known as Yu-Shiba-Rusinov states.[21] Upon increasing the weight of triplet pairing, the impurity resonance peaks at $\pm\Delta_-$ shift to low energies when the $|\Delta_-|$ decreases to 0 [Fig. 4(b)]. In Fig. 4(c), although the line node has formed on the FS, the rather small gap value $|\Delta_-|=0.04\Delta_s$ makes the impurity-induced resonance peaks visible only for very large scattering strength V_0. When the triplet pairing component is dominant [$\alpha=2$ in Fig. 4(d)], the in-gap impurity resonance states are clearly shown. These impurity resonance states are originated in the Andreev's bound states[17] due to the quasiparticle scattering on the FS with the reversal sign of the pairing gap. Since the triplet paring is induced by RSOI and the magnitude is determined by the strength of RSOI dependent of materials,[20,22] the above evolution of LDOS with the weight of triplet pairing component is expected to widely take place in thin films of superconductors with interface or surface-

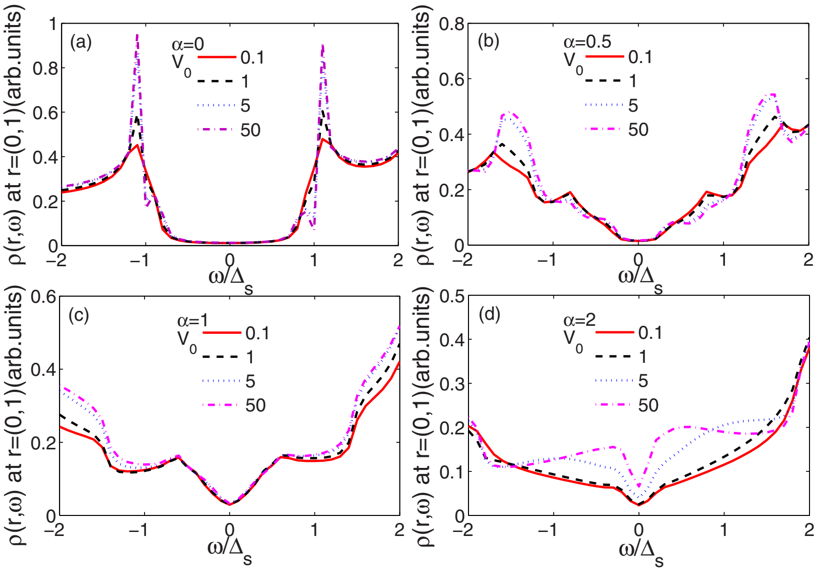

FIG. 4. (Color online) Evolution of LDOS near a nonmagnetic impurity with α for various scattering strengths V_0.

induced RSOI or various noncentrosymmetric superconductors.

We also investigate the possible mixed singlet d-wave and triplet pairing states in the superconducting interface $LaAlO_3/SrTiO_3$.[20] In Fig. 5, we plot the DOS and corresponding momentum-dependent gap functions in the mixed singlet $d_{x^2-y^2}$-wave and triplet pairing states. It is shown that upon increasing the weight of triplet pairing, the DOS always keeps a "V"-shape behavior at the low energies [Figs. 5(a)–5(c)] due to the existence of line node on the FS seen in Figs. 5(d)–5(g). Although RSOI-induced triplet pairing gap changes the shape of pure $d_{x^2-y^2}$-wave gap function, the nodal line on the FS always persists. The LDOS near an impurity in mixed singlet d-wave and triplet pairing states has been plotted in Fig. 6. We find in-gap impurity resonance states for different values of α, similar to that of the zero bias resonance peak on the Zn impurity in cuprates superconductors.[23] Compared to the case of coexisting singlet s-wave and triplet pairing states, the evolutions of DSO and LDOS in the mixed singlet d-wave and triplet pairing states with the weight of triplet pairing component exhibits different RSOI's influence on the electronic structures near an impurity, and thus can be easily differentiated by point contact tunneling or scanning tunneling microscopy.

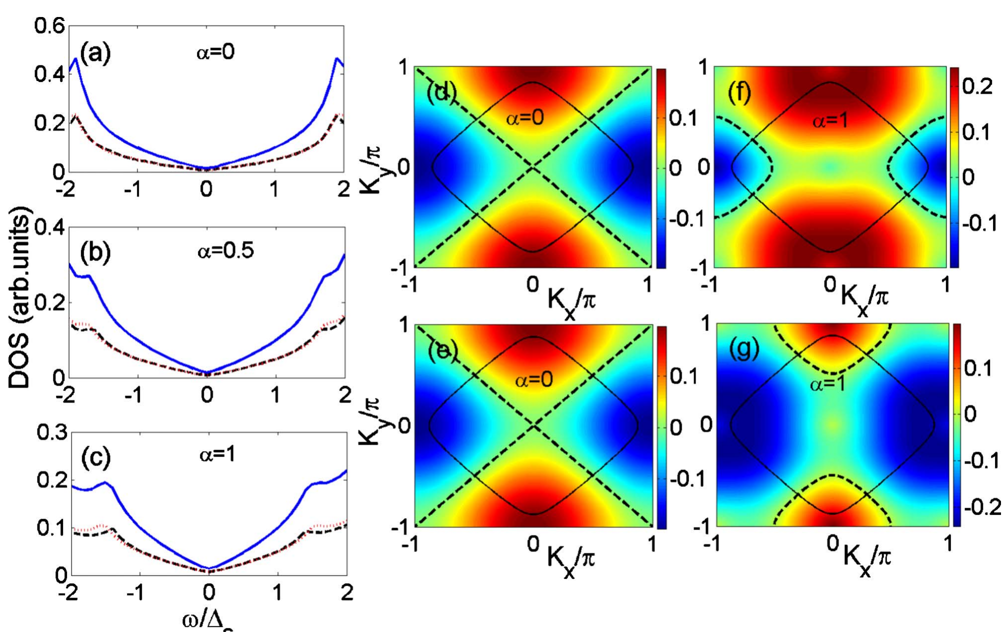

FIG. 5. (Color online) Evolution of DOS for various ratio $\alpha = d_0/\Delta_s$ between singlet $d_{x^2-y^2}$-wave and triplet Cooper-pairing states in (a), (b), and (c). The dashed and dotted curve denotes the contribution of the different bands and the solid curve refers to the total DOS. The corresponding singlet and triplet pairing gap functions in the first Brillouin zone at $\alpha=0$ for Δ_+ (d) and Δ_- (e), and $\alpha=1$ for Δ_+ (f) and Δ_- (g), where the solid line denotes corresponding Fermi surface of band $\xi_{\mathbf{k}+}$ in (d) and (f), and band $\xi_{\mathbf{k}-}$ in (e) and (g), and the dashed line indicates the node line.

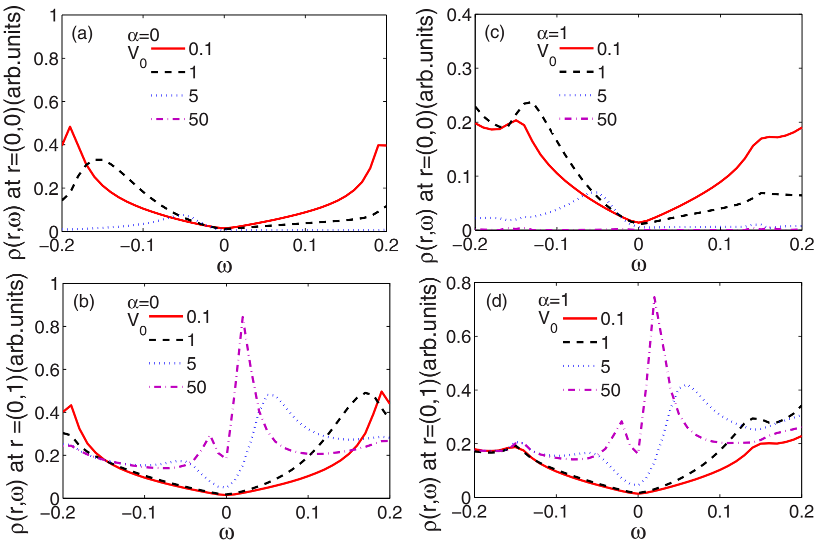

FIG. 6. (Color online) LDOS near an impurity for $\alpha=0$ and $\alpha=1$ with various scattering strengths V_0.

In summary, we study the mixed singlet and triplet cooper pairing states on the interface $LaAlO_3/SrTiO_3$ based on a minimal tight-binding model considering the influence of RSOI induced by the lack of inversion symmetry. Applying T-matrix approximation, we theoretically investigate its impurity-induced resonance states. We find that local density of states near an impurity exhibits the in-gap resonance peaks due to the quasiparticle scattering on the FS with the reversal sign of the pairing gap caused by the mixed singlet and RSOI-induced triplet cooper pairing SC state. We also reveal the evolutions of DOS and LDOS with the weight of triplet pairing component. These features will be widely observed via point contact tunneling and scanning tunneling microscopy in thin films of superconductors with interface or surface-induced RSOI or various superconductors without inversion symmetry.

Recently, the observation of superconductivity in a topological insulator Bi_2Se_3 has attracted much interest on its topological surface states due to prominent role played by spin-orbit interaction.[24] Its unconventional superconductivity has been discussed in a recent paper[25] where possible singlet or triplet pairing states was proposed. Our present approach can be directly applied to investigate its pairing symmetry and superconductivity.

Recently, we notice the magnetotransport experiment reports[26] that the RSOI is caused by the lack of inversion symmetry on the interface $LaAlO_3/SrTiO_3$ and its strength can be tuned applying an external electric field.

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