Theory of tunneling spectroscopy in superconducting Sr_2RuO_4

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A theory for tunneling spectroscopy in a normal-metal–insulator–triplet-superconductor junction is presented. We assume two kinds of nonunitary triplet-superconducting states which are the most promising states for Sr_2RuO_4. The calculated conductance spectra show zero-bias peaks as well as gap structures. The existence of residual components in the spectra reflect the nonunitary properties of superconducting states. [S0163-1829(97)01437-9]

Recent discovery of superconducting in Sr_2RuO_4 (Ref. 1) provides us with an example of a noncuprate layered perovskite material that exhibits superconductivity. Since this compound is isostructural to the cuprate superconductors, the electronic properties in the normal state[2] and superconducting state[3] are highly anisotropic. The rather large residual density of states of quasiparticles at low temperatures is indicated by several experiments.[4,5] Furthermore, there are several evidences which support the indications of ferromagnetic spin fluctuations.[6] Based on these facts, some theories[7,8] proposed that the nonunitary triplet pairing superconducting states are realized in Sr_2RuO_4. Since the triplet pairing states have strong anisotropy in k space, novel interference effects of the quasiparticles are expected to occur at boundaries and surfaces. To determine the symmetry of the pair potential definitively, it is important to predict the spectra of tunneling experiments which play a significant role to identify the d-wave symmetry in the high-T_C superconductors.[9–11]

Recently a tunneling conductance formula for normal-metal–insulator–anisotropic singlet superconductor junctions was presented.[9,11] Even in the case of a spin-singlet superconductor, when the pair potential becomes anisotropic[12] and changes its sign on the Fermi surface, zero-energy states[14] appear at the surface depending on the orientation of the surface. The formation of the zero-energy states[14] induces zero-bias conductance peaks in tunneling spectroscopy, which were actually observed in the experiments of high-T_C superconductors.[10,13] By assuming $d_{x^2-y^2}$-wave symmetry of the pair potentials, not only the zero-bias conductance peaks but also gaplike spectra were systematically explained.[9–11] However, the tunneling conductance for normal-metal–insulator–triplet superconductor ($N/I/TS$) junction is not well-clarified yet.

In the present paper, we present a formulation of the tunneling conductance spectra of $N/I/TS$ junction by extending the previous one for anisotropic singlet superconductors.[9–11] Although the superconducting states of Sr_2RuO_4 are not clarified yet, we will choose two kinds of triplet p-wave pair potentials (E_u states) which are proposed by Machida *et al.*[8] and Sigrist and Zhitomirsky.[7] A large variety of conductance spectra including zero-bias conductance peaks is obtained depending on the tunneling directions. Thus, the tunneling spectroscopy measurements are one of the useful methods to identify the pairing symmetry of Sr_2RuO_4.

For the calculation, we assume an $N/I/TS$ junction model in the clean limit with a semi-infinite double-layer structure. We also assume a nearly two-dimensional Fermi momentum by restricting the z component of the Fermi surface to the region given by $-\bar{\delta}<\sin^{-1}(k_{Fz}/k_F)<\bar{\delta}$. The flat interface is

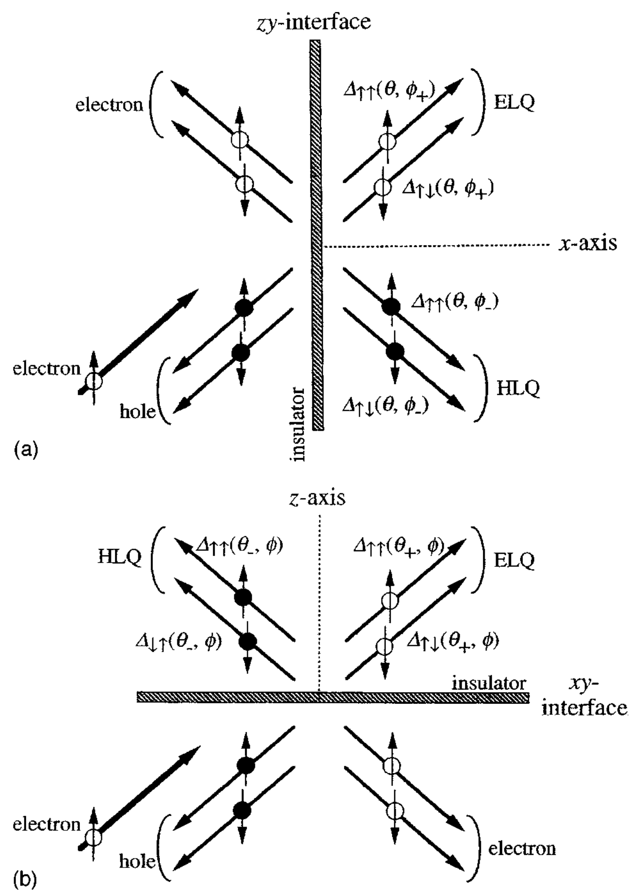

FIG. 1. Schematic illustration of the reflection and the transmission process of the quasi-particle at the interface of the junction with z-y plane interface (a) and x-y plane interface (b). The θ and ϕ are the polar angle and azimuthal angle, respectively.

perpendicular to the x axis, and is located at $x=0$ [Fig. 1(a)]. The barrier potential at the interface has a δ-functional form $H\delta(x)$, where $\delta(x)$ and H are the δ function and its amplitude, respectively. Similarly, we consider an alternative situation that the flat interface is perpendicular to the z axis and is located at $z=0$ [Fig. 1(b)]. The Fermi wave number k_F and the effective mass m are assumed to be equal both in the normal metal and in the superconductor. The wave function of the quasiparticles in inhomogeneous anisotropic superconductors is given by the solution of the Bogoliubov–de Gennes (BdG) equation.[12,14] Although this equation includes a nonlocal pair potential with two position coordinates for the Cooper pairs, we assume that the effective pair potential is given by

$$\Delta_{\rho\rho'}(\mathbf{k},\mathbf{r})=\begin{cases}\Delta_{\rho\rho'}(\theta,\phi)\Theta(x), & z\text{-}y \text{ plane interface,}\\ \Delta_{\rho\rho'}(\theta,\phi)\Theta(z), & x\text{-}y \text{ plane interface,}\end{cases}\quad \frac{k_x+ik_y}{|\mathbf{k}|}=\sin\theta e^{i\phi},\quad \frac{k_z}{|\mathbf{k}|}=\cos\theta, \tag{1}$$

where θ is the polar angle and ϕ is the azimuthal angle in the x-y plane. The quantities ρ and ρ' denote spin indices. This pair potential is rather simplified by applying the quasiclassical approximation and by ignoring the pair-breaking effect at the interface.[12] In Eq. (1), $\mathbf{k}$ is a wave vector of the relative motion of the Cooper pairs and is fixed on the Fermi surface ($|\mathbf{k}|=k_F$). The quantities $\Theta(x)$, $\Theta(z)$, and $\mathbf{r}$ are the Heaviside step functions and the center-of-mass coordinate of the pair potentials, respectively.

Suppose an electron is injected from the normal metal with angles θ and ϕ. We have taken care of the fact that the momentum parallel to the interface is conserved at the interface. The electron injected from the normal metal is reflected as an electron (normal reflection) and a hole (Andreev reflection). When the interface is perpendicular to the x axis (z-y plane interface) [Fig. 1(a)], the transmitted holelike quasiparticle (HLQ) and electronlike quasiparticle (ELQ) feel different effective pair potentials $\Delta_{\rho\rho'}(\theta,\phi_+)$ and $\Delta_{\rho\rho'}(\theta,\phi_-)$, with $\phi_+=\phi$ and $\phi_-=\pi-\phi$. On the other hand, in the case when the interface is perpendicular to the z axis (x-y plane interface), two kinds of quasiparticles feel $\Delta_{\rho\rho'}(\theta_+,\phi)$ and $\Delta_{\rho\rho'}(\theta_-,\phi)$, with $\theta_+=\theta$ and $\theta_-=\pi-\theta$ [Fig. 1(b)], respectively. The coefficients of the Andreev reflection $a_{\rho\rho'}(E,\theta,\phi)$ and normal reflection $b_{\rho\rho'}(E,\theta,\phi)$ are determined by solving the BdG equations under the following boundary conditions:

$$\Psi(\mathbf{r})|_{x=0_-}=\Psi(\mathbf{r})|_{x=0_+},$$

$$\left.\frac{d\Psi(\mathbf{r})}{dx}\right|_{x=0_-}=\left.\frac{d\Psi(\mathbf{r})}{dx}\right|_{x=0_+}-\frac{2mH}{\hbar^2}\Psi(\mathbf{r})|_{x=0_-} \tag{2}$$

for the z-y plane interface and

$$\Psi(\mathbf{r})|_{z=0_-}=\Psi(\mathbf{r})|_{z=0_+},$$

$$\left.\frac{d\Psi(\mathbf{r})}{dz}\right|_{z=0_-}=\left.\frac{d\Psi(\mathbf{r})}{dz}\right|_{z=0_+}-\frac{2mH}{\hbar^2}\Psi(\mathbf{r})|_{z=0_-} \tag{3}$$

for the x-y plane interface. Using the obtained coefficients, the normalized tunneling conductance is calculated according to the formula given by our previous works:[9,11]

$$\sigma(E)=\begin{cases}\dfrac{\int_{\pi/2-\delta}^{\pi/2}\int_{-\pi/2}^{\pi/2}(\sigma_{S,\uparrow}+\sigma_{S,\downarrow})\sigma_N \sin^2\theta\cos\phi\, d\theta\, d\phi}{\int_{\pi/2-\delta}^{\pi/2}\int_{-\pi/2}^{\pi/2}2\sigma_N\sin^2\theta\cos\phi\, d\theta\, d\phi}, & z\text{-}y \text{ plane interface,}\\[2ex] \dfrac{\int_{\pi/2-\delta}^{\pi/2}\int_0^{2\pi}(\sigma_{S,\uparrow}+\sigma_{S,\downarrow})\sigma_N\sin\theta\cos\theta\, d\theta\, d\theta}{\int_{\pi/2-\delta}^{\pi/2}\int_0^{2\pi}2\sigma_N\sin\theta\cos\theta d\theta d\phi}, & x\text{-}y \text{ plane interface,}\end{cases} \tag{4}$$

where σ_N denotes the normal-state tunneling conductance given by

$$\sigma_N=\begin{cases}\dfrac{\sin^2\theta\cos^2\phi}{\sin^2\theta\cos^2\phi+Z^2}, & z\text{-}y \text{ plane interface,}\\[2ex] \dfrac{\cos^2\theta}{\cos^2\theta+Z^2}, & x\text{-}y \text{ plane interface,}\end{cases}\qquad Z=\frac{mH}{\hbar^2k_F}. \tag{5}$$

In the above, E denotes an energy of quasiparticles measured from Fermi energy. The quantity $\sigma_{S,\rho}$ is given as

$$\sigma_{S,\rho}=\frac{1+|a_{a\uparrow\rho}|^2+|a_{\downarrow\rho}|^2-|b_{\uparrow\rho}|^2-|b_{\downarrow\rho}|^2}{\sigma_N}. \tag{6}$$

Hereafter, following the discussions by Sigrist[7] and Machida,[8] we will choose two kinds of nonunitary pair potentials with tetragonal symmetry. These two types of E_u symmetry states are independent of k_z due to the two-dimensional nature of the Fermi surface. Both of these have a matrix form of the pair potential, with $\Delta_{\uparrow\uparrow}(\theta,\phi)=\Lambda_i(\theta,\phi)$, $\Delta_{\uparrow\downarrow}(\theta,\phi)=\Delta_{\downarrow\uparrow}(\theta,\phi)=\Delta_{\downarrow\downarrow}(\theta,\phi)=0$, where $\Lambda_i(\theta,\phi)$ is the orbital part which is reduced to depend on θ and ϕ. Two kinds of $\Lambda_i(\theta,\phi)$ are given by $\Lambda_1(\theta,\phi)=\Delta_0 \sin\theta(\sin\phi+\cos\phi)$ and $\Lambda_2(\theta,\phi)=\Delta_0 \sin\theta e^{i\phi}$, where Δ_0 is the absolute value of the pair potential in a bulk superconductor. For the abbreviation, we will call the superconducting state of the pair potential with $\Lambda_1(\theta,\phi)$ $[\Lambda_2(\theta,\phi)]$ as an $E_u(1)$ $[E_u(2)]$ state in the following. Normalized conductance $\sigma_{S,\uparrow}$ is described as follows.

$E_u(1)$:

$$\sigma_{S,\uparrow}=\begin{cases}\dfrac{1+\sigma_N|\Gamma_+|^2+(\sigma_N-1)|\Gamma_+|^2|\Gamma_-|^2}{|1+(\sigma_N-1)\Gamma_+\Gamma_-|^2}, & z\text{-}y \text{ plane interface},\\[2ex] \dfrac{1+\sigma_N|\Gamma_+|^2+(\sigma_N-1)|\Gamma_+|^4}{|1+(\sigma_N-1)\Gamma_+{}^2|^2}, & x\text{-}y \text{ plane interface},\end{cases} \tag{7}$$

$$\Gamma_\pm=\frac{\Delta_0 \sin\theta(\sin\phi\pm\cos\phi)}{E+\Omega_\pm}, \quad \Omega_\pm=\sqrt{E^2-\Delta_0^2 \sin^2\theta(\sin\phi\pm\cos\phi)^2}. \tag{8}$$

$E_u(2)$:

$$\sigma_{S,\uparrow}=\begin{cases}\dfrac{1+\sigma_N|\Gamma|^2+(\sigma_N-1)|\Gamma|^4}{|1-e^{-2i\phi}(\sigma_N-1)\Gamma^2|^2}, & z\text{-}y \text{ plane interface},\\[2ex] \dfrac{1+\sigma_N|\Gamma|^2+(\sigma_N-1)|\Gamma|^4}{|1+(\sigma_N-1)\Gamma^2|^2}, & x\text{-}y \text{ plane interface},\end{cases} \tag{9}$$

$$\Gamma=\frac{E-\Omega}{|\Delta_0 \sin\theta|}, \quad \Omega=\sqrt{E^2-\Delta_0^2 \sin^2\theta}. \tag{10}$$

While $\sigma_{S,\downarrow}$ is unity due to the absence of the effective pair potentials. This feature is peculiar to the nonunitary superconducting state. Figures 2 and 3 show the calculated conductance spectra of the two states for various barrier heights. Here, we assume that the injected electrons have equal probability weight for both up- and down-spin components, and δ is chosen as 0.05π to express the two-dimensional features of the Fermi surface. In Fig. 2(a), the magnitude of zero-bias conductance peaks increases with the increase of Z as in our previous works. The origin of the zero-bias conductance peaks is that the denominator of the conductance formula in Eq. (7) vanish in the large-Z limit for $-\pi/4<\phi<\pi/4$ (z-y plain interface). The zero-bias conductance peaks are universal properties for the junction of anisotropic superconductors independent of their parity and unitarity, where the pair potentials change sign on the Fermi surface. On the other hand, for the x-y plane interface junction, the zero-bias conductance peaks do not appear [Fig. 2(b)]. With the increase of Z, $\sigma(0)$ converges not to 0, but 0.5 due to the residual density of states on the Fermi surface of quasiparticles with down spins. In the limit of a two-dimensional Fermi surface, i.e., $\delta\to 0$,

$$\sigma_{S,\uparrow}=\mathrm{Re}\left[\frac{E}{\sqrt{E^2-\Delta_0^2[\cos\phi+\sin\phi]^2}}\right],$$

$$\sigma(E)=\frac{1}{2}\left[1+\frac{1}{2\pi}\int_0^{2\pi}\sigma_{S,\uparrow}d\phi\right] \tag{11}$$

is satisfied. The obtained $\sigma(E)$ expresses the bulk density of states of the $E_u(1)$ state superconductor. In the case of the $E_u(2)$ state with the z-y plane interface, $\sigma(E)$ becomes maximum at $E=0$. The quantity $\sigma(0)$ increases with the increase of Z. In the limit of the large magnitude of Z, $\sigma(0)$ converges to a certain value which is larger than 0.5 [Fig. 3(a)]. In this case, the denominator of $\sigma_{S,\uparrow}$ vanishes at $E=0$ only for $\phi=0$. Hence, the strong enhancement of $\sigma(0)$ with the increase Z does not occur as in Fig. 2(a). When the interface is perpendicular to the z axis, the conductance spectra have a U-shaped structure [Fig. 3(b)] for larger Z. In this case, with the decrease of δ, $\sigma(E)$ converges to the bulk DOS of the $E_u(2)$ superconductors as in Fig. 2(b).

In this paper, we have studied the properties of tunneling spectra in $N/I/TS$ junctions. Although our formula can be extended for any triplet superconducting states, the present paper only mentions the results for pairing states which are the most promising for Sr_2RuO_4. The existence of the large residual density of states of quasiparticles reflects the nonunitary superconducting states. The zero-bias conductance peaks and gap structures are obtained depending on the tunneling direction. By polarizing the injected electron with, for example, a ferromagnetic normal metal, we can selectively measure the conductance spectrum components for the corresponding spin directions. If the flat metallic spectra for the down-spin injection and gap structures (or zero-bias conductance peaks) for the up-spin injection are detected, they can be regarded as the most clear evidence for the realization of

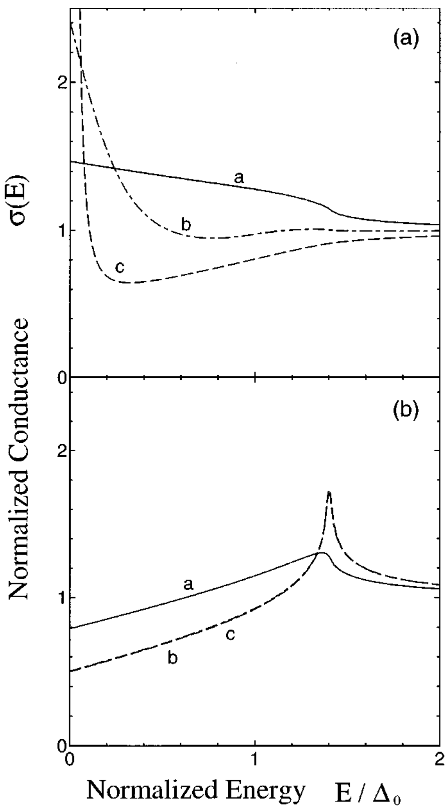

FIG. 2. Normalized tunneling conductance is plotted for the $E_u(1)$ state. (a) The x axis is perpendicular to the interface (z-y plane interface). (b) The z axis is perpendicular to the interface (x-y plane interface). a, $Z=0.1$; b, $Z=1$; c, $Z=5$.

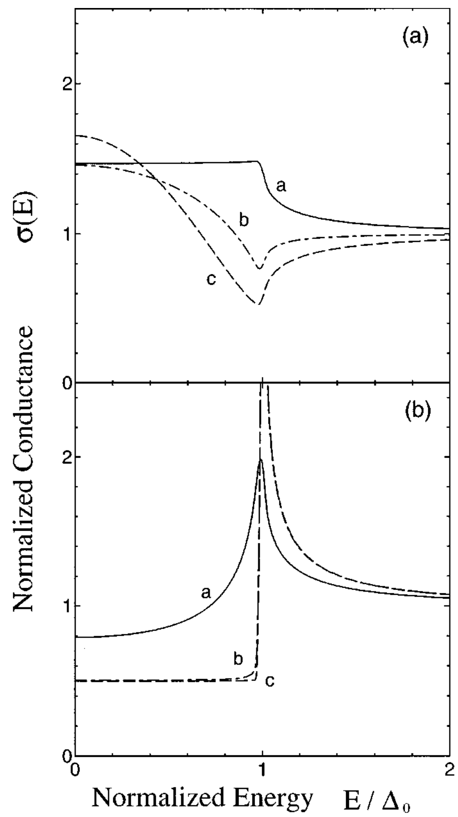

FIG. 3. Normalized tunneling conductance is plotted for the $E_u(2)$ state. (a) The x axis is perpendicular to the interface (z-y plane interface). (b) The z axis is perpendicular to the interface (x-y plane interface). a, $Z=0.1$; b, $Z=1$; and c, $Z=5$.

the nonunitary superconducting states. We hope our theory will give a guide to determine the symmetry of the pair potential in Sr_2RuO_4.

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