Theory of Tunneling Spectroscopy of d-Wave Superconductors

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A tunneling theory for a normal metal–insulator–d-wave superconductor junction is presented. In contrast to the s-wave superconductor, the tunneling conductance spectra strongly depend on the tunneling direction relative to the crystalline axes, and do not always represent the bulk density of states. Zero-bias conductance peaks are expected in ab-plane tunneling. The present theory systematically explains various experimental results in the tunneling spectroscopy of high-T_c superconductors.

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Tunneling spectroscopy is one of the best high-resolution probes for analyzing the electronic states of superconductors [1]. Many experiments using tunneling junctions have been performed to clarify the energy gap profile of superconductors. Simultaneously, theoretical studies have continued to reveal the physics of tunneling effects. However, except for a few cases of heavy fermion superconductors [2,3], most theories have dealt with isotropic s-wave superconductors. Today, the symmetry of the pair potential of high-T_c superconductors has attracted attention [4,5], and several groups have proposed d-wave symmetry for this [6–9]. Therefore it is important to construct a tunneling theory of anisotropic superconductors, especially of d-wave systems.

Experimentally, zero-bias conductance peaks (ZBCP's) have been observed as well as gaplike spectra by using scanning tunneling spectroscopy (STS) and thin-film tunnel junctions [10–13]. The ZBCP's are frequently observed in ab-plane tunneling junctions, and are rarely observed in c-axis-oriented junctions. Although the ZBCP's vanish above the critical temperature of the superconductor, it has not yet been clarified whether the ZBCP's originate in the symmetry of the pair potential or not. We consider that the existence of ZBCP's gives an important clue to identify the symmetry of the pair potential. In this Letter, the tunneling theory of the normal metal–insulator–anisotropic even-parity superconductor ($N/I/S$) junction is presented. In particular, the normal metal–insulator–d-wave superconductor ($N/I/d$) junction is investigated as a prototype of anisotropic even-parity superconductors. The tunneling conductance is calculated by extending the previous theory of Blonder *et al.* [14] to consider the anisotropy of the pair potentials [2,3]. It is found that the tunneling conductance strongly depends on the angle between the normal to the interface and the crystalline axes of the anisotropic superconductor. Specifically, the existence of the ZBCP's as well as the gaplike conductance spectra [15–17] are naturally and systematically explained by assuming d-wave symmetry in the framework of the present theory.

For the simplest model calculation, we consider a two-dimensional $N/I/S$ junction with perfectly flat interfaces in the clean limit. In this model, the interface is perpendicular to the x axis and is located at $x = 0$. The barrier potential at the interface has a delta-function form $H\delta(x)$. 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. Quasiparticle states in inhomogeneous anisotropic even-parity superconductors can be described by the Bogoliubov–de Gennes equations [3,18],

$$\begin{aligned} Eu(\boldsymbol{x}_1) &= h_0 u(\boldsymbol{x}_1) + \int d\boldsymbol{x}_2 \Delta(\boldsymbol{s},\boldsymbol{r}) v(\boldsymbol{x}_2)\,, \\ Ev(\boldsymbol{x}_1) &= -h_0 v(\boldsymbol{x}_1) + \int d\boldsymbol{x}_2 \Delta^*(\boldsymbol{s},\boldsymbol{r}) u(\boldsymbol{x}_2)\,, \end{aligned} \tag{1}$$

where $\boldsymbol{s} = (\boldsymbol{x}_1 - \boldsymbol{x}_2)$, $\boldsymbol{r} = (\boldsymbol{x}_1 + \boldsymbol{x}_2)/2$, and $h_0 = -\hbar^2\nabla^2_{x_1}/2m - \mu$, with μ the chemical potential. The energy of the quasiparticle E is measured from the Fermi energy E_F.

We assume that the pair potential is

$$\Delta(\boldsymbol{k},\boldsymbol{r}) = \Delta(\gamma)\Theta(x)\,, \quad \exp(i\gamma) \equiv \boldsymbol{k}/|\boldsymbol{k}| \tag{2}$$

using a wave vector $\boldsymbol{k}$, which is Fourier transform of $\boldsymbol{s}$, and $\Theta(x)$ is the Heaviside step function. In the weak coupling limit, $\boldsymbol{k}$ is fixed on the Fermi surface ($|\boldsymbol{k}| = k_F$). Two component wave functions $u(\boldsymbol{r})$ and $v(\boldsymbol{r})$ can be written as

$$\begin{aligned} \Psi(\boldsymbol{r}) &= \begin{pmatrix} u(\boldsymbol{r}) \\ v(\boldsymbol{r}) \end{pmatrix} \\ &= \exp(ik_F y \sin\gamma) \left[\begin{pmatrix} u_1(\gamma,x) \\ v_1(\gamma,x) \end{pmatrix} \exp(ik_F x \cos\gamma) \right. \\ &\qquad \left. + \begin{pmatrix} u_2(\gamma,x) \\ v_2(\gamma,x) \end{pmatrix} \exp(-ik_F x \cos\gamma) \right]. \end{aligned} \tag{3}$$

The envelope functions $u_j(\gamma,x)$ and $v_j(\gamma,x)$ ($j = 1,2$)

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obey

$$Eu_j(\gamma,x) = -\left[\frac{i\hbar^2\sigma k_F\cos\gamma}{m}\frac{d}{dx} - H\delta(x)\right]u_j(\gamma,x) + \Delta(\gamma_j)\Theta(x)v_j(\gamma,x),$$
$$Ev_j(\gamma,x) = \left[\frac{i\hbar^2\sigma k_F\cos\gamma}{m}\frac{d}{dx} - H\delta(x)\right]v_j(\gamma,x) + \Delta^*(\gamma_j)\Theta(x)u_j(\gamma,x), \quad (4)$$

with $\sigma = 1$, $\gamma_j = \gamma$ for $j = 1$, and $\sigma = -1$, $\gamma_j = \pi - \gamma$ for $j = 2$.

Suppose an electron is injected from the normal metal with angle θ. The reflection and transmission processes at the interface of the $N/I/S$ junction are schematically illustrated in Fig. 1. We have taken care of the fact that the momentum parallel to the interface and the group velocity are both conserved at the interface. The electron injected from the normal metal is reflected as an electron (normal reflection) and a hole (Andreev reflection) [19]. The transmitted holelike quasiparticle and electronlike quasiparticle experience different effective pair potentials $\Delta(\theta_+)$ and $\Delta(\theta_-)$, respectively, with $\theta_+ = \theta$ and $\theta_- = \pi - \theta$. This is a feature peculiar to anisotropic superconductors and gives rise to an anomalous interference effect in the tunneling conductance, as shown below.

The reflection coefficients of the Andreev reflection $a(E,\theta)$ and normal reflection $b(E,\theta)$ are determined by

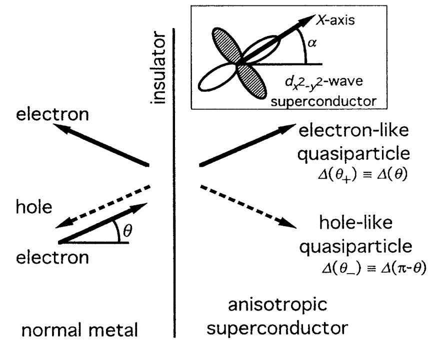

FIG. 1. Schematic illustration of the reflection and transmission processes at the interface. In this figure the quantities θ and α express the injection angle of the electron and the angle between the normal vector of the interface and the x axis of the $d_{x^2-y^2}$-wave superconductor, respectively.

the boundary conditions

$$\Psi(\boldsymbol{r})|_{x=0_-} = \Psi(\boldsymbol{r})|_{x=0_+},$$
$$\left.\frac{d\Psi(\boldsymbol{r})}{dx}\right|_{x=0_-} = \left.\frac{d\Psi(\boldsymbol{r})}{dx}\right|_{x=0_+} - \frac{2mH}{\hbar^2}\Psi(\boldsymbol{r})\Big|_{x=0_+}. \quad (5)$$

By solving the Bogoliubov–de Gennes equations, these coefficients are found to be

$$a(E,\theta) = \frac{4\cos^2\theta\sqrt{E+\Omega_-}\sqrt{E-\Omega_+}\exp(-i\phi_+)}{(4\cos^2\theta + Z^2)\sqrt{E+\Omega_+}\sqrt{E+\Omega_-} - Z^2\sqrt{E-\Omega_+}\sqrt{E-\Omega_-}\exp[i(\phi_- - \phi_+)]},$$
$$b(E,\theta) = \frac{-Z(Z+2i\cos\theta)\{\sqrt{E+\Omega_+}\sqrt{E+\Omega_-} - \sqrt{E-\Omega_+}\sqrt{E-\Omega_-}\exp[i(\phi_- - \phi_+)]\}}{(4\cos^2\theta + Z^2)\sqrt{E+\Omega_+}\sqrt{E+\Omega_-} - Z^2\sqrt{E-\Omega_+}\sqrt{E-\Omega_-}\exp[i(\phi_- - \phi_+)]}, \quad (6)$$

with

$$\exp(i\phi_\pm) = \Delta(\theta_\pm)/|\Delta(\theta_\pm)|, \quad \Omega_\pm = \sqrt{E^2 - |\Delta(\theta_\pm)|^2}, \quad (7)$$

where $Z = 2mH/\hbar^2 k_F$.

Using these coefficients, the normalized tunneling conductance is calculated according to the formula given by Blonder, Tinkham, and Klapwidjk [14]

$$\sigma(E) = \frac{\bar\sigma_S(E)}{\bar\sigma_N(E)}, \qquad \bar\sigma_i(E) = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} d\theta\,\tilde\sigma_i(E,\theta) \quad (i = S,N),$$
$$\tilde\sigma_S(E,\theta) \equiv 1 + |a(E,\theta)|^2 - |b(E,\theta)|^2, \qquad \tilde\sigma_N(E,\theta) \equiv \frac{4\cos^2\theta}{4\cos^2\theta + Z^2}, \quad (8)$$

where $\bar\sigma_N(E)$ is the tunneling conductance in the normal state. The quantity $\tilde\sigma_S(E,\theta)$ is given as

$$\tilde\sigma_S(E,\theta) = \frac{16(1+|\Gamma_+|^2)\cos^4\theta + 4Z^2(1-|\Gamma_+\Gamma_-|^2)\cos^2\theta}{|4\cos^2\theta + Z^2\{1 - \Gamma_+\Gamma_-\exp[i(\phi_- - \phi_+)]\}|^2}, \quad (9)$$

where

$$\Gamma_\pm = \frac{E}{|\Delta(\theta_\pm)|} - \sqrt{\left(\frac{E}{|\Delta(\theta_\pm)|}\right)^2 - 1}.$$

For large Z, the denominator vanishes when $1 = \Gamma_+\Gamma_-\exp[i(\phi_- - \phi_+)]$. This condition coincides with the equation giving the energy of bound states of a quasiparticle formed at the surface of a semi-infinite superconductor [20,21]. If this is satisfied, the $\tilde{\sigma}_S(E,\theta)$ becomes 2 and is independent of Z. For comparison with the above conductance results, we have also calculated the bulk density of states of anisotropic superconductors (NDOS) normalized by those in the normal state

$$\sigma_0(E) = \frac{1}{2\pi}\int_{-\pi/2}^{\pi/2} d\theta \left(\frac{E}{\sqrt{E^2 - |\Delta(\theta_+)|^2}} + \frac{E}{\sqrt{E^2 - |\Delta(\theta_-)|^2}}\right). \quad (10)$$

To this point the calculations have been for general anisotropic superconductors. In the following, $\sigma(E)$ is calculated for various specific types of pair potential symmetries.

In the case of s-wave superconductors, when $\Delta(\theta_+)$ and $\Delta(\theta_-)$ are substituted by Δ_S in Eqs. (6)–(9), the previous results [14] of a normal metal–insulator–s-wave superconductor junction are completely reproduced. By choosing infinite Z, we can show analytically that $\sigma(E)$ becomes $\sigma_0(E)$. However, this does not always hold true in anisotropic superconductors.

In the case of d-wave superconductors, we calculate $\sigma(E)$ for various values of Z. As shown in the inset of Fig. 1, α is the angle between the normal to the interface and the X axis of the d-wave superconductor. Here, the X axis is defined to be the direction along which the magnitude of the pair potential becomes maximum, and the crystal a axis is taken along the X axis when the symmetry is $d_{x^2-y^2}$ wave. When the transmitted quasiparticle is in the crystal ab plane, the effective pair potentials $\Delta(\theta_+)$ and $\Delta(\theta_-)$, for the $d_{x^2-y^2}$-wave case, can be expressed as [22]

$$\Delta(\theta_+) = \Delta_0\cos(2\theta - 2\alpha), \quad \Delta(\theta_-) = \Delta_0\cos(2\theta + 2\alpha). \quad (11)$$

As seen in Fig. 2, $\sigma(E)$ of the normal metal–insulator–$d_{x^2-y^2}$-wave superconductor junction shows various energy dependences. For $Z = 0$, $\sigma(E)$ does not depend on α at all, and decreases from 2 with increasing E [23]. For nonzero α and Z, $\sigma(E)$ at $E = 0$ is enhanced compared with the case of $Z = 0$. Comparing curves C and D in Figs. 2(b) and 2(c), it should be remarked that, for large Z, $\sigma(E)$ does not approach the NDOS $\sigma_0(E)$, contrary to the conventional tunneling spectra of s-wave superconductors [14].

The Z and α dependence of $\sigma(E)$ at $E = 0$ can be understood from

$$\tilde{\sigma}_S(0,\theta) = \frac{32\cos^4\theta}{|4\cos^2\theta + Z^2\{1 + \exp[i(\phi_- - \phi_+)]\}|^2}. \quad (12)$$

For a $d_{x^2-y^2}$-wave superconductor with $\alpha = 0$, $\Delta(\theta_+)$ and $\Delta(\theta_-)$ have the same sign independent of θ, and $\exp[i(\phi_- - \phi_+)] \to 1$ for any θ. In such a case, $\tilde{\sigma}_S(0,\theta)$ and $\tilde{\sigma}_S(0)$ are inversely proportional to Z^4 for large Z. In general, $\tilde{\sigma}_N(E)$ in Eq. (8) is inversely proportional to Z^2 for large Z. For these reasons, for both the s-wave case and the $d_{x^2-y^2}$-wave case with $\alpha = 0$, σ_0 vanishes for large Z, and we cannot expect zero-bias enhancement. However, for nonzero α, if $\pm\pi/4 + \alpha > \theta > \pm\pi/4 - \alpha$ with $\pi/2 > \theta > -\pi/2$, $\pi/4 > \alpha > 0$, $\Delta(\theta_+)$ and $\Delta(\theta_-)$ have different signs from each other. In such a case, $\exp[i(\phi_- - \phi_+)] \to -1$ and $\tilde{\sigma}_S(0,\theta) \to 2$ regardless of Z. It can be shown exactly from Eqs. (8) and (12) that $\tilde{\sigma}_S(0) \to 8\alpha/\pi$ with $\pi/4 > \alpha > 0$ and $\tilde{\sigma}_S(0) \to 4 - 8\alpha/\pi$ with $\pi/2 > \alpha > \pi/4$ and also $\sigma(0)$ is proportional to Z^2 for larger Z. This is an explicit explanation of the enhancement of ZBCP's with increasing barrier height (or Z). However, this enhancement is limited for $E = 0$, and if E deviates from zero for large Z, $\tilde{\sigma}_S(E,\theta)$ and $\tilde{\sigma}_S(E)$ are proportional to the inverse of Z^2.

Within the same formalism, we can also obtain $\sigma(E)$ for $(s + d_{x^2-y^2})$-wave and extended s-wave superconductors where the pair potentials are expressed as $\Delta_S + \Delta_0\cos(2\theta)$ and $\Delta_S + \Delta_0\cos(4\theta)$, respectively. In the case of a $(s + d_{x^2-y^2})$-wave superconductor, when $\Delta_0 > \Delta_S$ is satisfied, since $\Delta(\theta_+)$ and $\Delta(\theta_-)$ change sign on the Fermi surface

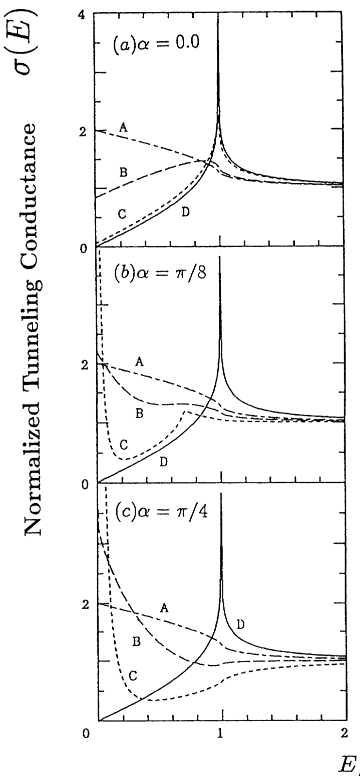

FIG. 2. Normalized tunneling conductance $\sigma(E)$ plotted as a function of E/Δ_0 for a normal metal–insulator–$d_{x^2-y^2}$-wave superconductor junction with the transmitted quasiparticles in the crystal ab plane: (a) $\alpha = 0$, (b) $\alpha = \pi/8$, and (c) $\alpha = \pi/4$. $A: Z = 0$, $B: Z = 1$, $C: Z = 5$, and $D: \sigma_0(E)$.

and $\exp[i(\phi_- - \phi_+)] \rightarrow -1$ for some θ, we can also expect a ZBCP to occur. The ZBCP's are also expected for extended s-wave superconductors under the same conditions. However, in such a case, the α dependence of $\sigma(E)$ is qualitatively different, since there are eight nodes on the Fermi surface. It should be noted that the existence of a ZBCP does not always imply that the symmetry of the pair potential is $d_{x^2-y^2}$ wave [21]. In the case of a $(s + id_{x^2-y^2})$-wave superconductor, since $\exp[i(\phi_- - \sigma_+)] \neq -1$ is satisfied for all θ, ZBCP's do not occur.

In the case of c-axis tunneling, $\sigma(E)$ can be obtained within the same scheme by extending our theory to a three-dimensional system. In this model, the interface is perpendicular to the z axis and is located at $z = 0$. Taking account of the electronic structure of high-T_c superconductors, we assume that the pair potential depends on the azimuthal angle φ in the xy plane as $\Delta_0 \cos(2\varphi)$. In this case, the holelike quasiparticle and the electronlike quasiparticle transmitted into the superconductor experience the same effective pair potentials for all directions and consequently ZBCP's are not expected. The qualitative features of the Z dependence of $\sigma(E)$ are almost the same as those in Fig. 2(a).

In this Letter, the tunneling conductance of quasiparticles injected from a normal metal into an anisotropic superconductor is investigated. The well known previous result that the tunneling spectra of an s-wave superconductor approaches the NDOS for large barrier height parameter Z does not hold any more in the tunneling spectroscopy of an anisotropic superconductor, especially of a d-wave superconductor. In ab-plane tunneling, when the orientational angle α between the x axis of the $d_{x^2-y^2}$-wave superconductor and the interface normal is nonzero, ZBCP's occur. These peaks cannot be explained from the NDOS of the bulk $d_{x^2-y^2}$-wave superconductor. Instead, they occur when the effective pair potentials felt by the electronlike quasiparticle and the holelike quasiparticle have different signs. ZBCP's can also be expected for superconductors in which the pair potential changes its sign on the Fermi surface, e.g., certain kinds of s-wave or $s + d_{x^2-y^2}$-wave superconductors. The peak becomes higher as Z increases, and larger than 2 for sufficiently large Z. It vanishes above T_c, since it originates from the symmetry of the pair potential. These features of the ZBCP's are consistent with the experimental results for $YBa_2Cu_3O_{7-\delta}$ observed by STS at low temperature [21]. Furthermore, the gaplike spectra, which have been observed experimentally [15–17], are naturally derived within our formalism.

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[1] E.L. Wolf, *Principles of Electron Tunneling Spectroscopy* (Oxford University Press, New York, 1985).
[2] A. Millis, D. Rainer, and J. Sauls, Phys. Rev. B **38**, 4504 (1998).
[3] Chr. Bruder, Phys. Rev. B **41**, 4017 (1990).
[4] P. Chaudhari and Shawn-Yu Lin, Phys. Rev. Lett. **72**, 1084 (1994).
[5] A.G. Sun, D.A. Gajewski, M.B. Maple, and R.C. Dynes, Phys. Rev. Lett. **72**, 2267 (1994).
[6] P. Monthoux, A.V. Balatsky, and D. Pines, Phys. Rev. B **47**, 6069 (1993).
[7] D.A. Wollman, D.J. van Harlingen, W.C. Lee, D.M. Ginsberg, and A.J. Leggett, Phys. Rev. Lett. **71**, 2134 (1993).
[8] C.C. Tsuei, J.R. Kirtley, C.C. Chi, L.S. Yu-Jahnes, A. Gupta, T. Shaw, J.Z. Sun, and M.B. Ketchen, Phys. Rev. Lett. **73**, 593 (1994).
[9] M. Sigrist and T.M. Rice, J. Phys. Soc. Jpn. **61**, 4283 (1992).
[10] J. Geerk, X.X. Xi, and G. Linker, Z. Phys. B **73**, 329 (1988).
[11] T. Walsh, Int. J. Mod. Phys. **6**, 125 (1992).
[12] I. Iguchi, Physica (Amsterdam) **185–189C**, 241 (1991).
[13] S. Kashiwaya, M. Koyanagi, M. Matuda, and K. Kajimura, Physica (Amsterdam) **194–196B**, 2119 (1994).
[14] G.E. Blonder, M. Tinkham, and T.M. Klapwidjk, Phys. Rev. B **25**, 4515 (1982).
[15] T. Hasegawa and K. Kitazawa, J. Phys. Chem. Solids **54**, 1351 (1993).
[16] J. Lesueur, L.H. Greene, W.L. Feldmann, and A. Inam, Physica (Amsterdam) **191C**, 325 (1992).
[17] C. Manabe, M. Oda, and M. Ido (to be published).
[18] C.R. Hu, Phys. Rev. Lett. **72**, 1526 (1994).
[19] A.F. Andreev, Zh. Eksp. Teor. Fiz. **46**, 1823 (1964) [Sov. Phys. JETP **19**, 1228 (1964)].
[20] M. Matusmoto and H. Shiba, J. Phys. Soc. Jpn. (to be published).
[21] S. Kashiwaya, Y. Tanaka, M. Koyanagi, and K. Kajimura, Phys. Rev. B **51**, 1350 (1995).
[22] In the case of a d_{xy}-wave superconductor, the angle between the x axis and the a axis is $\pi/4$. The effective pair potentials $\Delta(\theta_+)$ and $\Delta(\theta_-)$ can be expressed by substituting α in Eq. (11) for $\alpha + \pi/4$. Determination of the value of α is beyond the scope of this paper.
[23] Y. Koyama and H. Ebisawa, J. Phys. Soc. Jpn. (to be published).