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Tunneling Density of States in Superconductor/d-wave Superconductor Proximity Junction

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초전도체와 d-wave 초전도체 근접효과 접합에서의 터널링 상태밀도함수

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Abstract

We have calculated the tunneling density of states (TDOS) of a metal/d-wave superconductor proximity junction, where the metal stands for the normal metal, s-wave superconductor, and d-wave superconductor. The tunneling direction is through the *ab*-plane of the d-wave superconductor. Because of the sign change in the order parameter experienced in the multiple Andreev reflection, there appears a finite TDOS at zero bias for d_{xy} geometry, which results in the anomalous zero bias conductance peak(ZBCP). For d_{x2-y2} geometry, however, no TDOS peak appears at zero bias. We have calculated TDOS for various crystal orientation of HTSC and compared with the experimental conductance.

Keywords : Superconductor, Proximity junction, Tunneling, Density of State, d-wave superconductor

I. Introduction

In the case of conventional low-temperature superconductors, electron tunneling experiments have provided key proofs of the validity of the BCS theory and Eliashberg equation. From the tunneling experiment, one can obtain the density of states (DOS) at the tunneling interface with very high resolution (in the sub-meV range). Temperature or magnetic field dependence of the energy gap can also be obtained from tunneling measurements. When the elastic tunneling is the only conducting channel through an insulating barrier in metal-insulator -superconductor, tunneling data display specific features related to the interaction responsible for the pairing of electrons in the superconductor such as the phonon spectra in low-T_c superconductors. Thus

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the tunnel junction acts as a spectrometer and quantitative comparisons can be made between theories and experiments with a high degree of accuracy.

Tunneling measurements also played a key role in understanding the quasiparticle interference effect in a proximity junction composed of a normal metal /superconductor or superconductor/superconductor in an intimate contact with each other. Bound states or periodic oscillations appear in the tunneling density of states (TDOS) as a result of the Andreev reflection at the normal/superconductor interface. Numerous tunneling experiments have been carried out to probe the DOS of the high-T_c superconductors (HTSC) [1],[2] on energy scales relevant to the superconductive energy gap (from a few meV to a few tens of meV), to look for specific pairing excitations, and more recently, to test the symmetry of the order parameter through Josephson experiments.

Unfortunately, early tunneling measurements on cuprates, including vacuum tunneling measurements, showed puzzling and conflicting results among various research groups. The conductance data revealed departures from simple BCS predictions; i) zero bias conductance is rather high and often shows even a peak structure, ii) sub-gap conductance is not flat at low temperature, often linear, and sometimes displayed anomalous structure, iii) conductance at high bias is quite asymmetric and frequently showing a linear bias dependence. As to the high bias conductance, recent data on Bi2212 samples displayed flat or slightly decreasing curve. Often, BTK model calculation is employed to explain these anomalous conductance behaviors in HTSC. In BTK model calculation, tunnel junction is assumed to have a NID structure in the limit of the vanishing tunneling barrier. Thus BTK model calculation deals with primarily the reflection and transmission of the quasiparticle at the intimate contact between N and S layer rather than the tunneling of the quasiparticle. Therefore, BTK model calculation cannot be applied to the case of a strong tunneling barrier such as in the vacuum tunneling case.

To elucidate the puzzling conductance behavior in the proximity junction, we calculated the tunneling density of states of N/S bilayer when S is a d-wave superconductor and the tunneling direction is along ab-plane. Zero-bias conductance peaks and characteristic DOS peaks are obtained only in specific junction geometries where a phase change of π occurs by the Andreev reflection at the interface. We compare our results with available experimental data.

II. Tunneling Density of States

The smeared tunneling density of states (TDOS) for a bulk s-wave superconductor in BCS theory is given by [3]

$$N_s(E) = N(0)\,\mathrm{Re}\left[\frac{E}{\sqrt{(E - i\Gamma)^2 - \Delta^2(E)}}\right] \quad (1)$$

where Γ represents the quasiparticle's lifetime effect. Almost all conventional superconductors show TDOS given by Eq. (1). For strong coupling superconductors, one can extract the energy dependence of gap function $\Delta(E)$ and the energy dependence of the Eliashberg function $\alpha^2(E)F(E)$ from the tunneling measurement, thereby one can look for the interaction mechanism in the superconducting medium.

When a normal metal (N) and a superconductor (S) are in an intimate electrical contact as in an experimental geometry of the N/S proximity junction, an energy gap is induced in the N side and slightly reduced in S side as a result of Cooper pair diffusion across the N/S boundary. This phenomenon was verified by many transport and thermodynamic measurements including tunneling conductance measurement, which showed rich variety of structures. In addition to the Cooper pair diffusion, periodic conductance peaks commonly known as Tomasch oscillation and/or McMillan-Rowell oscillation appear in the experimental geometry of proximity electron tunneling spectroscopy (PETS), as in CE-I-N/S or CE-I-S/N. Here CE stands for the counter-electrode which could be either a normal or superconducting material. Furthermore, there appears phonon structures of N and S material reflected in the variation of the energy gap.

In order to explain the PETS data quantitatively, one should compute the tunneling density of states of N/S or S/N bilayer at the tunneling side in contact

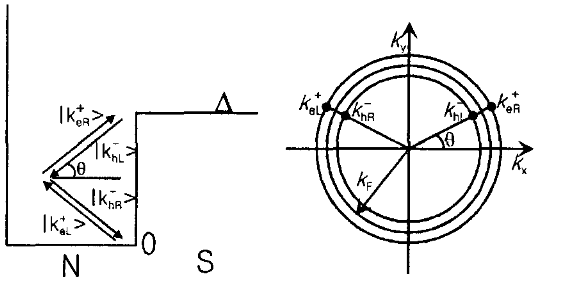

Fig. 1. Schematic representation (a) of the quasiparticle reflection process involved in N/S proximity junction. An injected electron-like quasiparticle $|k^+_R\rangle$ is Andreev -reflected to $|k^-_R\rangle$ at the N/S interface which is subsequently reflected to $|k^-_L\rangle$ at the tunneling barrier. θ is the injection angle. Four quasiparticle states involved in the interference in N side (b).

with the insulating barrier. For the conventional SC, TDOS can be obtained by Green's function method [4]-[6] which includes the Andreev reflection at the interface.

But for non s-wave superconductors, the energy gap experienced by quasiparticles with different momenta on the Fermi surface can be different in the magnitude and even the sign depending on the incident tunneling angle, making it difficult to apply Green's function approach. Therefore, recent theoretical approaches are concentrated on methods which can follow quasiparticle trajectories, such as Bogoliubov de Gennes equation[7] and quasiclassical Green's function method[8]-[10] which eliminated irrelevant details varying on the Fermi length scale.

Due to its chemically active surface and short coherence length, HTSC junctions are not easy to make and thus it is hard to find a relevant model system to simulate the experimental data. For this reason, different geometries such as DID, DND, NID junctions and N/D contacts are employed as model systems following BTK model calculation, where D represents a superconductor with a d-wave symmetry.

In this paper we will consider CE-I-N/D structure with a clean N/D interface. This model simulates the situation where superconductivity of the d-wave superconductor is suppressed on the surface due to the oxygen deficiency, for example, and counter -electrode is evaporated onto the surface with an artificial or natural oxide barrier inbetween.

Our calculation of TDOS is based on the Bogoliubov de Gennes equation. Here the quasiparticle wavefunction for electron-like or hole-like states is given as

$$\left|k^{\pm}_{R,L}\right\rangle = \begin{pmatrix} u \\ v \end{pmatrix} \exp\left[ik^{\pm}_{R,L}x\right] \qquad (2)$$

in the spinor space. Here u and v represent electron and hole component of the quasiparticle state,

$$u = \frac{1}{\sqrt{2}}\sqrt{1 \pm \frac{\Omega}{E}}, \quad v = \frac{1}{\sqrt{2}}\sqrt{1 \mp \frac{\Omega}{E}}. \qquad (3)$$

The quasiparticle momentum $k^{\pm} = k_F \pm \Omega/hv_F + i/l_N$ is the momentum corresponding to the electron-like (+) and hole-like (-) quasiparticle state, $\Omega = \sqrt{E^2 - \Delta^2}$, and l_N the mean free path of the quasiparticle. Here the subscripts R, L represents the position of quasiparticle momentum as shown in Fig. 1.

Starting with a quasiparticle moving from left (I-N interface) to the right (N/D interface) inside N ($|k^+_R\rangle$ in Fig. 1), we trace the trajectory of the quasiparticle as it is reflected (Andreev or specular) from each interface ($|k^+_R\rangle \to |k^-_R\rangle \to |k^-_L\rangle \to |k^+_L\rangle \to |k^+_R\rangle$). Note here that the group velocity of quasiparticle states $|k^-_R\rangle$ and $|k^+_L\rangle$ is negative (moving toward tunneling barrier). We can sum each quasiparticle wavefunction as a geometric series. By calculating interference between the incoming quasiparticle wavefunction and the quasiparticle wavefunction moving left at the I-N interface, we can obtain TDOS at the tunneling barrier.

III. N/S bilayer

For the isotropic conventional superconductor, the s-wave energy gap Δ_S has no angle dependence. Let us define the normal direction of the interface as x-axis and let I-N interface be at $x = -d$ and N/S interface at $x = 0$. Incident angle θ is the angle between the quasiparticle trajectory and the interface normal. Incident angle θ should have no effect on the qualitative feature of TDOS, but affect the amplitude and period of the oscillation in TDOS, for the effective length of the N layer is different depending on the incident angle.

For an incoming (moving right) electron-like quasiparticle state $|k^+_R\rangle$, the Andreev-reflected quasiparticle state at the N/S interface can be represented as $r|k_R^->$. The Andreev reflection coefficient r obtained from the continuity condition of the wave function at N/S interface, $|k^+_R> + r|k^-_R> = t|k'^+_R>$, is

$$r(E)=\frac{R_N\Delta_S-R_S\Delta_N}{R_NR_S-\Delta_N\Delta_S} \quad (4)$$

where $R_{N,S}$ and $\Omega_{N,S}$ are defined as

$$R_{N,S}=E+\Omega_{N,S},\ \ \Omega_{N,S}=\sqrt{E^2-\Delta_{N,S}^2} \quad (5)$$

and t and k' is the transmission coefficient and the quasiparticle's momentum in S side.

Successive specular reflection at the I-N interface inverts the quasiparticle momentum from k^-_R to k^-_L with an additional phase change thus making the quasiparticle wave function as

$$re^{i\theta_1}|k_L^-> \quad (6)$$

where $k^-_L = -k_F - \Omega/\hbar v_F + i/l_N$ as shown in Fig. 1 and θ_l is the phase change of the quasiparticle necessary for the continuity condition at the tunneling barrier (x=-d). Note that the group velocity of the hole-like state k^-_L is positive.

Quasiparticle wave function counting each successive reflection at $x=0$ (Andreev reflection) and at $x=-d$ (specular reflection) can be represented as an infinite series

$$|k\rangle=|k_R^+\rangle+r\,|k_R^->+re^{i\theta_1}|k_L^-\rangle+ r^2e^{i\theta_1}|k_L^+\rangle+r^2e^{i(\theta_1+\theta_2)}|k_R^+\rangle+\cdots\cdots \quad (7)$$

where θ_l and θ_2 are again the additional phase changes necessary for the continuity of the wavefunction at I-N interface for hole-like and electron-like quasiparticles, respectively. One can easily obtain phase changes

$$\theta_1+\theta_2=\frac{4\Omega_N d}{\hbar v_{FN}\cos\theta}, \quad (8)$$

from the continuity condition of electron-like (θ_2) and hole-like (θ_l) quasiparticles at x=-d. As we can see, each of the first four terms in Eq. (7) is repeated with the factor $r^2e^{i(\theta_1+\theta_2)}$ multiplied at each succession. These terms are summed up to give

$$|k_{total}> \;=\; \frac{1}{1-\psi^2}[(|k_R^+>+re^{i\theta_1}|k_L^->) + (r|k_R^->+r^2e^{i\theta_1}|k_L^+>)] \quad (9)$$

where ψ^2 is defined as $\psi^2\equiv r^2(E)e^{-2\gamma}e^{2i\phi_N}$ and $\phi_N=\frac{2\Omega_N d}{\hbar v_{FN}\cos\theta}\equiv\frac{R\Omega_N}{\cos\theta}$. Here $\gamma=\frac{2d}{l_N\cos\theta}$ was inserted to include the effect of a finite mean free path of the quasiparticle in the normal layer. Terms in the first parenthesis represent quasiparticles moving to the right, and the second, to the left. Calculating the interference of the latter with the injected quasiparticle wave function $|k^+_R>$ at $x = -d$ and multiplying that with the *unperturbed* background DOS of N, we get TDOS at the I-N interface

$$N_N(E)=\mathrm{Re}\left\{\left(\frac{E}{\Omega_N}\right)\left[1+2\frac{(\Delta_N/E)\psi+\psi^2}{1-\psi^2}\right]\right\}. \quad (10)$$

This TDOS obtained from the multiply reflected quasiparticle wavefunction shows strong and weak oscillations corresponding to ψ and ψ^2 terms in the modification of TDOS as shown in Fig. 2, where d is the N-layer thickness, l is the mean free path, and R is the relative thickness of the N-layer defined as $R(meV^{-1})=3.04\cdot10^{-3}\times d(nm)/v_F(10^8cm/\mathrm{sec})$. The TDOS obtained in this work is exactly the same as that obtained by a Green's function method of

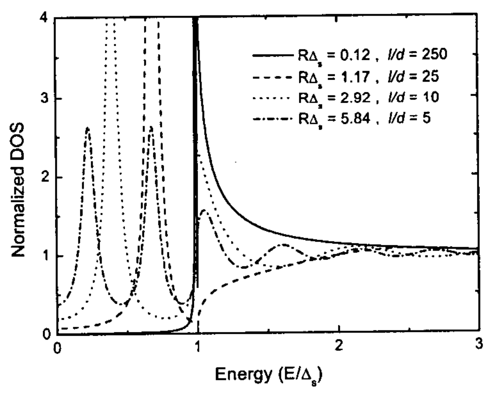

Fig. 2. TDOS of an N/S bilayer for several N layer thickness and mean free path. There appear bound states inside of the gap energy Δ_s due to Andreev reflection at the N/S interface.

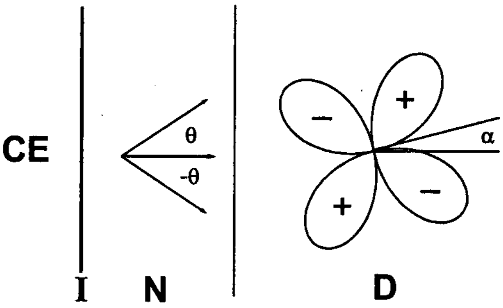

Fig. 3. Configuration of our model system. θ is the incident angle of the quasiparticle and α is the angle between d_{xy} order parameter and the interface normal.

Wolfram[4]-[6], thus assuring the validity of this approach.

IV. N/D bilayer

Now let us consider the case of N side being a superconductor having s-wave symmetry while the S overlayer having d-wave symmetry. We assume, for simplicity, that the magnitude of the N-layer energy gap is 20 % compared to that of the overlayer superconductor ($\Delta_D = 5\Delta_N$). Unlike N/S proximity junction, the apparent energy gap perceived by the Andreev reflected quasiparticle is different from that perceived by the incoming quasiparticle due to the anisotropy of the energy gap in d-wave superconductor.

Let α be the angle between d_{xy} order parameter and the interface normal as shown in Fig. 3. Thus $\alpha=0$ and $\alpha=\pi/4$ correspond to d_{xy} and d_{x2-y2} symmetries, respectively, of the order parameter in S layer. Then the gap perceived by $|k^+_R\rangle$ at the N/D interface is $\Delta_D(\theta)=\Delta_o \sin 2(\theta-\alpha)$, while the gap perceived by $|k^-_L\rangle$ is $\Delta_D(-\theta)=-\Delta_o \sin 2(\theta+\alpha)$. This results in different reflection coefficients,

$$r^+(E,\theta)=\frac{R_N\Delta_D(\theta)-R_S\Delta_N}{R_NR_S-\Delta_N\Delta_D(\theta)},$$

$$r^-(E,-\theta)=\frac{R_N\Delta_D(-\theta)-R_S\Delta_N}{R_NR_S-\Delta_N\Delta_D(-\theta)}\exp\left(\frac{i4d\Omega_N \sin^2\theta}{\eta v_F\cos\theta}\right) \tag{11}$$

at the N/D interface for incoming waves $|k^+_R\rangle$ and $|k^-_L\rangle$, respectively.

The resulting TDOS in this case can be expressed in a way similar to Eq. (10) but with a minor modification of r^2 being replaced by r^+r^-,

$$N_N(E,\theta)=\mathrm{Re}\left\{\left(\frac{E}{\Omega_N}\right)\left[1+\frac{2}{1-\psi^2}\left(\frac{\Delta_N}{E}r^+e^{i\phi_N-\gamma}+\psi^2\right)\right]\right\} \tag{12}$$

Here ψ^2 is defined as

$$\psi^2\equiv\frac{R_N\Delta_D(\theta)-R_S\Delta_N}{R_NR_S-\Delta_N\Delta_D(\theta)}\frac{R_N\Delta_D(-\theta)-R_S\Delta_N}{R_NR_S-\Delta_N\Delta_D(-\theta)}e^{-2\gamma}e^{2i\phi_n}.$$

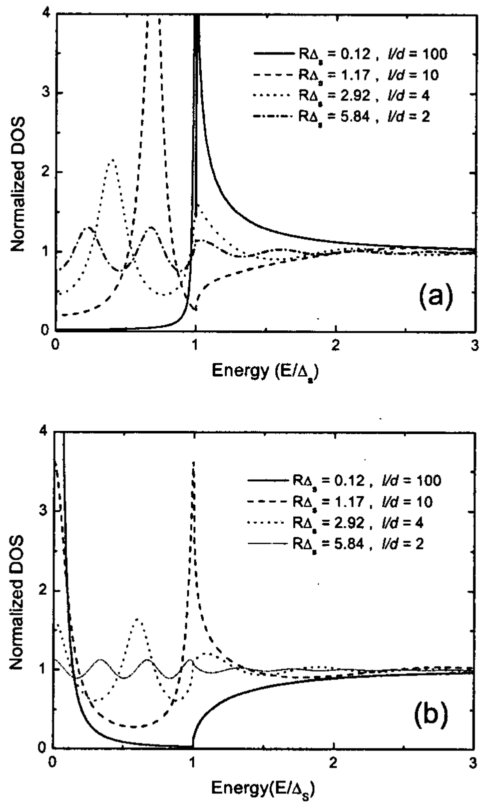

Fig. 4. (a) TDOS of N/d_{x2-y2} bilayer and (b) TDOS of N/d_{xy} bilayer. TDOS of N/d_{xy} shows a bound state at zero bias whereas TDOS of N/d_{x2-y2} does not show a bound state at zero bias.

This minor modification in the reflection coefficients r^+ and r^- can produce a significant change in the TDOS because of the sign change in the reflection coefficient depending on the incident angle. For example, in the case of N-layer being normal ($\Delta_N=0$), Andreev reflection coefficients reduce to

$$r^+(E,\theta) = \mathrm{sgn}(\Delta_D(\theta))\left[\frac{E-\Omega_D(\theta)}{E+\Omega_D(\theta)}\right]^{1/2},$$

$$r^-(E,-\theta) = \mathrm{sgn}(\Delta_D(-\theta))\left[\frac{E-\Omega_D(-\theta)}{E+\Omega_D(-\theta)}\right]^{1/2} \exp\left(\frac{i4dE\sin^2\theta}{\hbar v_F\cos\theta}\right) \quad (13)$$

with the resulting TDOS

$$N_N(E,\theta) = \mathrm{Re}\left\{\left[1+2\frac{\psi^2}{1-\psi^2}\right]\right\} \quad (14)$$

The position of bound states that can be obtained from the zero of the denominator $1-\psi^2$ in Eq. (14) can be different from N/S case due to the sign change of the reflection coefficient in N/D junction. Figure 4(a) shows TDOS when D is a d_{x2-y2} superconductor ($\alpha=\pi/4$) and Figure 4(b) when D is a d_{xy} superconductor ($\alpha=0$). As can be seen in Figure 4(a) for d_{x2-y2} symmetry, the TDOS has the same structure of N/S case[4], because in this case Andreev reflected quasiparticles with incident angle θ and $-\theta$ feel the same energy gap at N/d_{x2-y2}. When the incident angle θ is $\pi/4$, the quasiparticle *feels* no gap (gap node) and TDOS becomes flat.

In the TDOS of N/D junction with d_{xy} symmetry as in Figure 4(b), however, there appears a *zero bias conductance peak* (ZBCP) whenever the incident angle θ is not equal to 0. This is because the energy gap experienced by quasiparticles $|k^+_R\rangle$ and $|k^-_L\rangle$ at the N/D interface is different, i.e., $\Delta_D(\theta) \propto \sin 2\theta$ and $\Delta_D(-\theta) \propto -\sin 2\theta$ for electron-like state $|k^+_R\rangle$ and hole-like state $|k^-_L\rangle$, respectively.

One can understand the origin of ZBCP by regarding the N/S bilayer as a potential well problem. Since the tunneling barrier acts as a mirror for the quasiparticle, the potential well width will be twice of the N layer thickness. For N/d_{x2-y2}, the potential well depth is simply the energy gap Δ_{dx2-y2} and hence even the lowest bound state energy is greater than zero. But for N/d_{xy}, the potential drop (energy gap difference) at $x = 0$ and $-2d$ has a different sign which allows a bound state with $E=0$, that effectively produces a ZBCP. The appearance of ZBCP in the high T_c superconductor proximity junction was reported in many literatures[7]-[10].

In the case of N side being a s-wave superconductor (S/D proximity junction), TDOS is given by Eq. (4) and (5) with modifications such as replacing r^2 by r^+r^- and $2\Omega_N$ by $\Omega_N(\theta) + \Omega_N(-\theta)$. TDOS is similar to that of N/D bilayer, but shows some differences. Density of states is shifted by Δ_s as one can expect. Resonance peak heights are increased for every other peak. This is because *2d* oscillation (Tomasch oscillation) is present in this case in addition to the *4d* oscillation (McMillan -Rowell oscillation). When D is d_{xy} superconductor, the density of states shows a peak just at the energy gap of N layer. This can be understood in the same footing with ZBC observed in the N/d_{xy} bilayer.

V. D′/D bilayer

An interesting phenomenon can arise if N-layer has d-wave superconductivity (D′/D junction). That is, an additional complexity occurs because quasiparticles impinging on the tunneling barrier (I-D′) after being reflected from D′/D interface can now acquire a finite probability for the Andreev reflection in addition to the usual specular reflection. This unusual Andreev reflection at the tunneling barrier can happen because the quasiparticle that is reflected specularly at the tunneling barrier perceives different pair potentials before and after the reflection at I-D′ due to the anisotropic energy gap in D′.

Thus the hole-like quasiparticle $|k_R^-\rangle$ which is moving toward tunneling barrier splits into two quasiparticle states $|k_R^+\rangle$ (Andreev reflected) and $|k_L^-\rangle$ (specularly reflected) upon reaching I-D′ interface. And these quasiparticles experience Andreev reflection at D′/D interface and bounce back as $|k_R^-\rangle$ and $|k_L^+\rangle$, respectively. Both $|k_R^-\rangle$ and $|k_L^+\rangle$ can generate $|k_R^+\rangle$ and $|k_L^-\rangle$ with different amplitudes at the I-D′ interface, and they will bounce back as $|k_R^-\rangle$ and $|k_L^+\rangle$ again at D′/D interface. This process will go on indefinitely. To trace and sum all the terms in a closed form is rather difficult in this case since the number of the reflected terms at the tunneling barrier is doubled every time a quasiparticle hits the I-D′ interface. One can overcome this difficulty by introducing a matrix representation. If we define a_n and b_n as the amplitude of n-th reflected quasiparticle states $|k_R^- >$ and $|k_L^+ >$, respectively at each succession, they are related by the relation

$$\begin{pmatrix} a_{n+1} \\ b_{n+1} \end{pmatrix} = e^{-2d/l} \begin{pmatrix} r_{NS}^+ r_{IN}^+ e^{i\theta_3} & r_{NS}^+ t_{IN}^- e^{i\theta_5} \\ r_{NS}^- t_{IN}^+ e^{i\theta_4} & r_{NS}^- r_{IN}^- e^{i\theta_6} \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix} \qquad (15)$$

Here reflection coefficients (*r's*) and phase factors (*θ's*) are similarly defined as for the N/S case, and transmission coefficients (*t's*) are newly introduced. Note that *t's* appear only in the off-diagonal sites.

To obtain TDOS we need to sum up terms like $\sum_{n=1}^{\infty} a_n$ and $\sum_{n=1}^{\infty} b_n$, and this can be accomplished easily through a unitary transformation of the matrix.

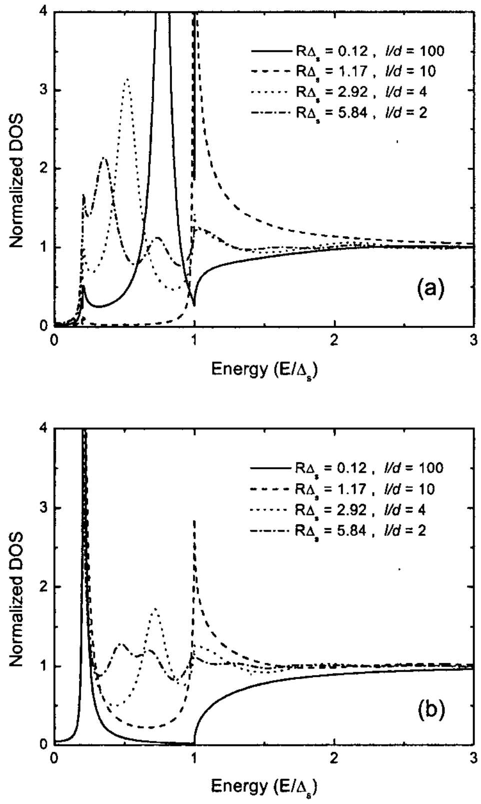

Fig. 5. (a) TDOS of d_{x2-y2} /d_{x2-y2} bilayer and (b) TDOS of d_{xy} /d_{xy} bilayer. Similar to S/d junction, there appear DOS peak just above the induced gap for d_{xy} symmetry.

Practically it will be very difficult to realize D′/D proximity junction except for the case of intermediate state (vortex) of HTSC and the case of a HTSC with a degraded surface layer where the surface superconductivity is reduced by, for example, the oxygen deficiency. In this case, the orientation of the energy gap in D′/D will be the same although the magnitude could be different. For this reason, we have calculated TDOS in D′/D with the same orientation of the energy gap.

Figure 5(a) is the case when d_{x2-y2} superconductivity is induced in the metal in contact with d_{x2-y2} superconductor, and Figure 5(b) shows TDOS when d_{xy} superconductivity is induced in the metal in contact with d_{xy} superconductor. Characteristic features are similar to those when s-wave in induced in the N side, such as suppressed DOS below induced gap in d_{x2-y2} superconductor and DOS peak just above the induced gap for d_{xy} superconductor.

VI. Summary

From the quasiparticle wavefunction based on the Bogoliubov de Gennes equation, we obtained TDOS for various N/S bilayer proximity junctions such as N/d_{x2-y2}, N/d_{xy}, S/d_{x2-y2}, S/d_{xy}, d_{x2-y2}/d_{x2-y2}, and d_{xy}/d_{xy} by counting all the successive Andreev reflections at N/S interface and specular reflection at the tunneling barrier side. Subsequent interference between incoming and reflected quasiparticle wave generates a geometric resonance effect. In the simplest case of N/S and S/S, TDOS obtained in this work reproduces exactly the same result obtained by the Green's function method. In addition, this method can be applied easily to the proximity junction composed of anisotropic superconductors. We found ZBCP in the N/d_{xy} bilayer and DOS peak just above the energy gap in the S/d_{xy} and d_{xy}/d_{xy} bilayers as a result of phase change of π in the order parameter perceived by Andreev reflected quasiparticles at the interface of the bilayer. However, there appears no ZBC peak in the case of

N/d_{x2-y2} or S/d_{x2-y2} bilayer junction, which we can understand quite naturally. This result can be applied to the analysis of anisotropic flux flow resistance in HTSC.

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