Correlation between specular Andreev reflection and zero-energy states in normal-metal/*d*-wave-superconductor junctions

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We report the effects of interfacial roughness on a zero-bias conductance peak (ZBCP) in normal-metal/*d*-wave-superconductor junctions. The roughness spoils to specularity of the junction interface, and causes a diffuse Andreev reflection of a quasiparticle. The ZBCP decreases linearly with a decreasing rate of the specular Andreev reflection at the interface. A sensitivity of the ZBCP to the roughness strongly depends on a transparency of the junctions. In low transparent junctions, the ZBCP disappears even in the regime of weak roughness. We also find a splitting of the ZBCP owing to the interfacial roughness in low transparent junctions.

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I. INTRODUCTION

In recent years, transport properties in junctions of anisotropic superconductors[1–3] have attracted much attention because high-T_c superconductors may have $d_{x^2-y^2}$-wave pairing symmetries.[4,5] One of the most important features in anisotropic superconductor junctions is the formation of zero-energy states (ZES's) at the normal-metal/superconductor (NS) interface.[6] ZES's are the origin of the zero-bias conductance peak (ZBCP) in NS junctions,[7,8] and the low-temperature anomaly in the Josephson current in SIS junctions.[9,10] So far, the effects of roughness at the junction interface on transport properties were discussed in a number of papers[11–18] by using the quasi-classical Green-function method.[19–23] In these theories, the specularity of the NS interface is characterized by a parameter which is independent of the transparency of the junctions. The ZBCP can be seen in a regime of weak interfacial roughness. However, in the regime of strong roughness, the ZBCP disappears.[13] Different theoretical studies yielded the same conclusion.[16,18]

In this paper, we study the relationship between an amplitude of the ZBCP and a specularity of the NS interface, by using a recursive Green-function method in which effects of the randomness on the conductance can be considered with no approximation. This is one of the advantages of our method. A reason to revisit the same issue is that our conclusions are different from those in previous works. Our results show that the ZBCP decreases linearly with the decreasing rate of the specular Andreev reflection; this conclusion agrees with that in previous studies.[13,16,18] The sensitivity of the ZBCP to the interfacial roughness depends strongly on a transparency of junctions. The amplitude of the ZBCP is insensitive to the roughness when the transparency of ideal junctions is rather high. However, the ZBCP is drastically suppressed by the roughness in low transparent junctions; this implies a difficulty in observing the ZBCP in scanning tunnel microscopy (STM). Moreover we find a splitting of the ZBCP owing to the roughness in low transparent junctions.

This paper is organized as follows. In Sec. II, we describe the NS junctions on two-dimensional square lattice. Numerical results of the conductance and the specular reflection rate of the Andreev reflection are shown in Sec. III. In Sec. IV, the discussion is given. In Sec. V, we summarize the paper.

II. CONDUCTANCE OF NS JUNCTIONS

Let us consider a normal-metal/d-wave superconductor junction on the two-dimensional square lattice, as shown in Fig. 1(a). The width of the junction is $W_J a_0$, where a_0 is the lattice constant. Open and gray circles denote lattice sites in the normal metal and those in the superconductor, respectively. The pair potential in the momentum space is sche-

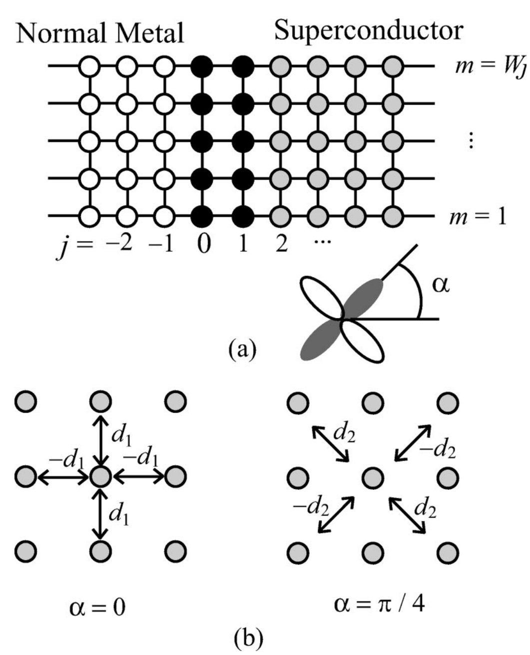

FIG. 1. The normal-metal/d-wave superconductor junction is shown in (a), where α is the orientation angle. The pair potential in Eq. (1) is schematically illustrated on the tight-binding lattice for $\alpha=0$ and $\pi/4$ in (b).

matically depicted in the lower figure, where α denotes the orientation angle between the a axis of high-T_c superconductors and the normal of the junction interface. We describe the NS junction by the mean-field (BCS) Hamiltonian,

$$H = -t \sum_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle,\sigma} c^{\dagger}_{\boldsymbol{r},\sigma} c_{\boldsymbol{r}',\sigma} + \sum_{\boldsymbol{r},\sigma} (\epsilon_{\boldsymbol{r}} + 4t - \mu_F) c^{\dagger}_{\boldsymbol{r},\sigma} c_{\boldsymbol{r},\sigma} - \sum_{\{\boldsymbol{r},\boldsymbol{r}'\}} [\Delta_0(\boldsymbol{r}',\boldsymbol{r}) c_{\boldsymbol{r},\downarrow} c_{\boldsymbol{r}',\uparrow} + \text{H.c.}], \quad (1)$$

where $\boldsymbol{r} = (j,m)$ is the lattice index and $c^{\dagger}_{\boldsymbol{r},\sigma}$ $(c_{\boldsymbol{r},\sigma})$ is the creation (annihilation) operator of an electron at $\boldsymbol{r}$ with spin $\sigma(=\uparrow$ or $\downarrow)$. The summation $\Sigma_{\langle \boldsymbol{r},\boldsymbol{r}'\rangle}$ runs over nearest-neighbor sites, and t is the nearest-neighbor hopping integral. In a direction parallel to the NS interface, the periodic boundary condition is applied. The energy is measured in units of t from the chemical potential of the junction. The difference in energy between the band edge and the chemical potential corresponds to the Fermi energy μ_F. The length is measured in units of a_0. We assume that the on-site potential $\epsilon_{\boldsymbol{r}}$ is zero far from the interface, (i.e., $j \leqslant -2$ and $3 \geqslant j$). At the interface, an uniform potential barrier is introduced as $\epsilon_{\boldsymbol{r}} = V_b$ for $j=0$ and 1, as shown by solid circles in Fig. 1(a). The roughness near the interface is described by the on-site potential, given randomly in ranges of

$$-V_N/2 < \epsilon_{\boldsymbol{r}} < V_N/2 \quad \text{for} \quad j=-1, \quad (2)$$

$$-V_S/2 < \epsilon_{\boldsymbol{r}} < V_S/2 \quad \text{for} \quad j=2, \quad (3)$$

where V_N and V_S represent a degree of roughness in the normal metal and that in the superconductor, respectively. In d-wave superconductors, the pair potential has site-off-diagonal elements depending on the orientation angle α. When $\alpha=0$, the pair potential has finite values among the nearest-neighbor sites, as shown in Fig. 1(b), where $d_1 = f_1\Delta_0$ with $f_1 = t/\mu_F$, and Δ_0 is the amplitude of the pair potential at zero temperature. The pair potential remains finite among the next-nearest-neighbor sites for $\alpha=\pi/4$, where $d_2 = f_2\Delta_0$ with $f_2 = (t/\mu_F)/\sqrt{8t/\mu_F - 1}$. Thus $\{\boldsymbol{r},\boldsymbol{r}'\}$, in the last term of Eq. (1), represents the nearest- or next-nearest-neighbor sites depending on α. We introduce the factors f_1 and f_2 for the maximum value of the gap being Δ_0 independent of μ_F. We note that the tight-binding model does not correspond to the two-dimensional CuO_2 plane in high-T_C superconductors. The tight-binding lattices represent the two-dimensional space. In our model, we introduce the pair potential between the next-nearest-neighbor sites to describe junctions with $\alpha=\pi/4$. An alternative way to describe the $\pi/4$ junction is to keep the pair potential between the nearest-neighbor sites and to rotate the square lattice by 45°.[24] There are no essential differences between results in the two models when we focus on the formation of the ZES. This is because the ZES is a consequence of the d-wave symmetry of the pair potential. When we discuss effects of a shape of the Fermi surface, however, the model employed in Ref. 24 is more suitable than ours to describe the CuO_2 plane.

The Hamiltonian in Eq. (1) is diagonalized by the Bogoliubov transformation

$$\begin{bmatrix} c_{\boldsymbol{r},\uparrow} \\ c^{\dagger}_{\boldsymbol{r},\downarrow} \end{bmatrix} = \sum_{\lambda} \begin{bmatrix} u_{\lambda}(\boldsymbol{r}) & -v^{*}_{\lambda}(\boldsymbol{r}) \\ v_{\lambda}(\boldsymbol{r}) & u^{*}_{\lambda}(\boldsymbol{r}) \end{bmatrix} \begin{bmatrix} \gamma_{\lambda,\uparrow} \\ \gamma^{\dagger}_{\lambda,\downarrow} \end{bmatrix}, \quad (4)$$

where $\gamma^{\dagger}_{\lambda,\sigma}$ $(\gamma_{\lambda,\sigma})$ is the creation (annihilation) operator of a Bogoliubov quasiparticle. On the two-dimensional lattice, the wave function $(u_{\lambda}, v_{\lambda})$ obeys the Bogoliubov–de Gennes equation,[25] which we solve by using the recursive Green-function method.[26] The details of the simulation were given in Refs. 27 and 28. In the recursive Green-function method, we can numerically calculate the transmission and reflection coefficients of the NS junction. The differential conductance is given by[30,29]

$$G(eV) = \frac{dI}{dV} = \frac{2e^2}{h} \sum_{l,l'} [\delta_{l,l'} - |r^{ee}_{l,l'}|^2 + |r^{he}_{l,l'}|^2], \quad (5)$$

where l and l' indicate propagating channels, and $r^{ee}_{l,l'}$ and $r^{he}_{l,l'}$ are the normal and the Andreev reflection coefficients of a quasiparticle, respectively. These reflection coefficients depend on the energy of an incident quasiparticle eV, where V is the bias voltage applied to the NS junction. The specularity of the NS interface is estimated from a specular reflection rate of the Andreev reflection:[31]

$$S_A \equiv \sum_{l} |r^{he}_{l,l}|^2 / \sum_{l,l'} |r^{he}_{l,l'}|^2. \quad (6)$$

In the absence of roughness at the interface, (i.e., $V_N = V_S = 0$), S_A becomes unity; this corresponds to the perfect specular NS interface. In quasiclassical Green-function approaches,[13,16,18] the specularity of the interface is characterized by a parameter or a function. In our method, however, the specular reflection rate is not a parameter but one of the obtained results in the simulation as well as the conductance.

III. RESULTS

In Fig. 2, we calculate $\langle S_A\rangle$ as a function of the V_N and V_S for $\alpha=0$ in (a) and for $\alpha=\pi/4$ in (b), where $W_J=50$, $\mu_F=2.0t$, $\Delta_0=0.01t$, and $\langle\cdots\rangle$ denotes the ensemble average of the random configuration. The bias voltage is fixed at $eV=0$ and the barrier potential is $V_b=2.0t$. Here we consider two types of junctions:

$$V_N = 0 \quad \text{and} \quad V_S \neq 0 \quad (7)$$

and

$$V_N \neq 0 \quad \text{and} \quad V_S = 0. \quad (8)$$

In Eq. (7), the interfacial roughness is introduced only in the superconductor. The calculated results in these junctions are shown by solid circles in Figs. 2(a) and 2(b). We consider the roughness only in the normal metal in Eq. (8). The results in these junctions are shown with open circles. For $\alpha=0$ in Fig. 2(a), $\langle S_A\rangle$ of junctions with the roughness in the superconductor is slightly larger than that with the roughness in the normal metal. We have confirmed that the same tendency can

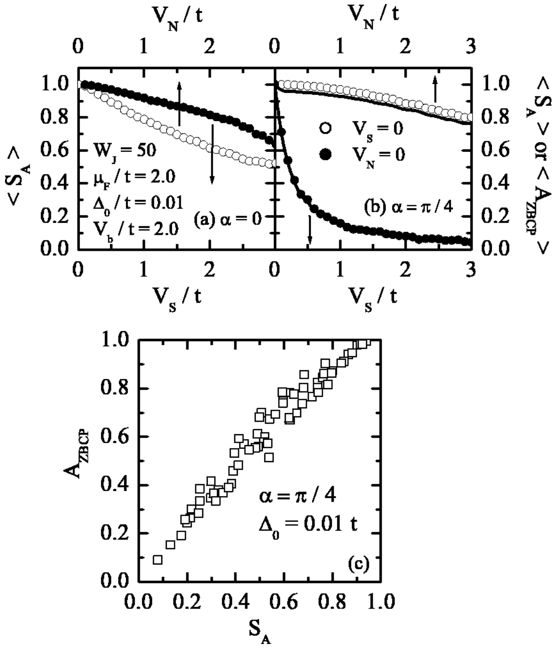

FIG. 2. The specular reflection rate is shown as a function of the roughness at the NS interface for $\alpha=0$ and $\pi/4$ in (a) and (b), respectively. Here the bias-voltage is fixed at zero. We introduce the roughness only on the superconductor side (●). The roughness is considered only on the normal metal side (○). In (b), the normalized amplitude of the ZBCP is shown by solid lines.

be seen in the s-wave NS junctions. On the other hand, for $\alpha=\pi/4$ in Fig. 2(b), $\langle S_A \rangle$ with the roughness in the superconductor is much smaller than that with the roughness in the normal metal. Thus the roughness at a surface of the superconductor drastically suppresses the specular Andreev reflection for $\alpha=\pi/4$. The most important difference between Figs. 2(a) and 2(b) is the formation of the ZES at the NS interface. In addition to the specular reflection rate, we also calculate the amplitude of the ZBCP defined by

$$A_{\rm ZBCP}=\frac{G(eV=0,V_N,V_S)}{G(eV=0,V_N=0,V_S=0)}, \tag{9}$$

which becomes unity in the absence of the interfacial roughness. In Fig. 2(b), we plot $\langle A_{\rm ZBCP} \rangle$ for the two types of junctions with solid lines. The results show that $\langle S_A \rangle$ and $\langle A_{\rm ZBCP} \rangle$ are closely related to each other. When we compare Figs. 2(a) and 2(b), it is also found that $\langle S_A \rangle$ depends on the orientation angle even if the degree of roughness is equal.

In Fig. 3, we show $A_{\rm ZBCP}$ for $\alpha=\pi/4$ as a function of S_A for several choices of W_J, μ_F, V_N, V_S, and V_b, where eV/t and Δ_0/t are fixed at 0.0 and 0.01, respectively. In this figure, $A_{\rm ZBCP}$ and S_A are calculated results before the ensemble average. The figure shows that $A_{\rm ZBCP}$ increases almost linearly with increasing S_A, irrespective of the parameters such as the degree of disorder and the Fermi energy. The results again indicate the strong correlation between the specular Andreev reflection of a quasiparticle and the formation of the ZES. Thus we conclude that the specular Andreev reflection plays an essential role in the formation of the ZES. The anisotropy (sign change) in the pair potential is the origin of the ZES. A quasiparticle can detect the anisotropy only when an incident angle of an incoming wave is memorized in an outgoing wave.

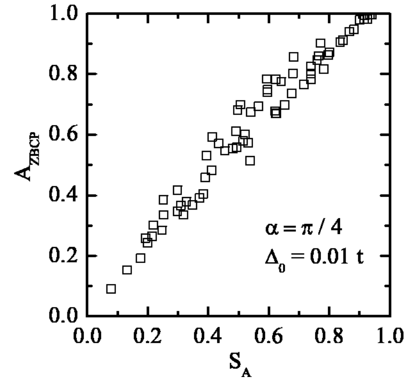

FIG. 3. A relation between the amplitude of the ZBCP and the specular reflection rate is shown for $\alpha=\pi/4$, where the bias voltage is fixed at zero. These are results before the ensemble average.

Since the ZES are insensitive to the roughness in the normal metal, we consider the interfacial roughness only on the superconductor side in the following (i.e., $V_N=0$). In Figs. 4(a), 4(b), and 4(c), we show the conductance for $\alpha=\pi/4$ as a function of the bias voltage for several choices of V_S, where $W_J=50$, $\mu_F=2.0t$, and $\Delta_0=0.01t$. The results are normalized by the normal conductance of the perfect junc-

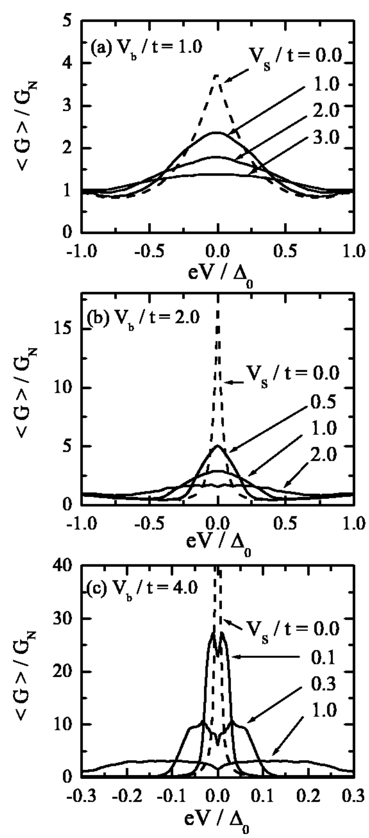

FIG. 4. The differential conductances are shown as functions of the bias voltages, where $\alpha=\pi/4$ and V_N is fixed at 0. The barrier potential is $V_b/t=1.0$, 2.0, and 4.0 in (a), (b), and (c), respectively.

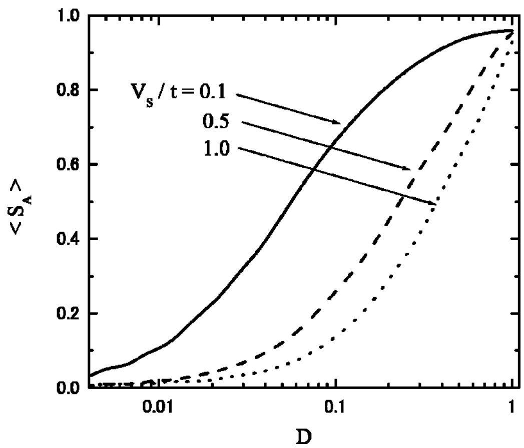

FIG. 5. The specular reflection rate is plotted as a function of the transparency of the junctions D for several V_S. Here D is calculated from the normal conductance of the ideal junctions.

tions (G_N). The barrier potential is $V_b/t=1.0$, 2.0 and 4.0 in Figs. 4(a), 4(b), and 4(c), respectively. In low barrier junctions in Fig. 4(a), the broad ZBCP can be seen even in the presence of the roughness. When the barrier potential is increased, the ZBCP rapidly decreases with increasing the interfacial roughness as shown in Fig. 4(b). In the presence of strong roughness, the peak structure disappears and the conductance becomes almost independent of eV as shown in the curve for $V_S/t=2.0$. In Fig. 4(c), the barrier potential is increased more, where a scale of the horizontal axis is changed for clarity and the normalized ZBCP for $V_S=0$ is about 198. The ZES becomes more sensitive to the roughness. As a result, the zero-bias conductance decreases to 10% even in the regime of weak roughness such as $V_S/t=0.1$. A sensitivity of the ZES to the interfacial roughness depends strongly on the transparency of the ideal insulating layer, which is given by

$$D=G_N/G_0, \tag{10}$$

where G_0 is the Sharvin conductance of the wire in the absence of the potential barrier and the roughness. We note that D is also one of the calculated results in the simulation. In the present calculation, the values of D are about 0.5 for $V_b/t=1.0, 0.1$ for $V_b/t=2.0$ and 0.01 for $V_b/t=4.0$ in Figs. 4(a), 4(b), and 4(c), respectively.

Since A_{ZBCP} and S_A depend strongly on the barrier potential, we calculate $\langle S_A \rangle$ as a function of V_b for several choices of V_S in Fig. 5, where $\alpha=\pi/4$, $W_J=50$, and $\mu_F=2.0t$. The horizontal axis D is calculated from Eq. (10). The specular reflection rate decreases with the decreasing transparency of the ideal junctions. Since there is a linear relation between S_A and A_{ZBCP}, as shown in Fig. 3, the vertical axis in Fig. 5 corresponds to A_{ZBCP}.

IV. DISCUSSION

When we consider a relation between the specular reflection rate of the Andreev reflection and the amplitude of the ZBCP, the present results agree well with those in other theories using the quasiclassical Green-function method.[13,16,18] However, our results show that the specular reflection rate depends not only on the degree of roughness but also strongly on the transparency of junctions, as shown in Fig. 5. As a consequence, our conclusions are very different from those viewed *quantitatively* in previous studies. For instance, in a quasiclassical Green-function method,[12,13] the specularity is determined by a parameter d/l, where d is the thickness of disordered layer at a surface of superconductor and l is the mean free path in it. The ZBCP can be seen for $d/l<1.0$.[12,13] On the other hand in our results, the ZBCP disappears even in areas of weak roughness such as $d/l=0.13$ for $D=0.1$ shown in Fig. 4(b) and $d/l=0.027$ for $D=0.01$ shown in Fig. 4(c). The disagreement arises because S_A depends strongly on D, as shown in Fig. 5. The dependence of the specularity parameter on the transparency is also not taken into account in other approaches.[16,18]

It must be important to pay attention to the fact that the peak position is shifted from zero-bias in low transparent junctions as shown in Fig. 4(c). The peak can be seen around $eV/\Delta_0=0.01$ and 0.03 for $V_S/t=0.1$ and 0.3, respectively. So far a surface state which breaks time-reversal symmetry (TRS) has been considered to be a source of the peak splitting.[11,32,33] However the peak splitting in our results is purely caused by interfacial roughness in the presence of TRS.[24] We confirmed that the peak splitting tends to appear in low transparent junctions. Further investigations are needed to make clear the relation between the minimum of the conductance at the zero bias shown in Fig. 4(c) and that found in experiments.[33,34]

In general, the amplitude of the pair potential near the interface becomes smaller than its bulk value. In this study, however, we do not consider the self-consistency of the pair potential. One of us calculated the conductance of NS junctions where the pair potential is determined in a self-consistent way, and compared the results with those of a non-self-consistent pair potential.[35] The two conductances deviate from each other when the bias voltage is relatively large. However, they agree well with each other in the limit of zero bias. Thus it may be possible to infer that the characters of the ZBCP remain qualitatively unchanged even when the pair potential is determined self-consistently. However, we believe that a self-consistent study has to be made in order to make clear the relation between the suppression of the pair potential and the specular reflection rate of the Andreev reflection.

The calculated results indicate that the superconductors near the interface must be extremely clean to observe the ZBCP in STM experiments, where the barrier potential is rather high. Actually, experimental results with STM are still controversial, in particular in Nd-based high-T_c superconductors.[36,37] Although there are several experiments which reported the ZBCP, some experiments did not report it.[2] On the other hand, the ZBCP can be seen in a number of NS junctions.[2] This is probably because the potential barrier is rather low in some NS junctions. In addition to the symmetry change in the pair potential from d to $d+is$, for instance, we suggest that the effects of the interfacial roughness should be reconsidered to explain the absence of the ZBCP and the peak splitting in low transparent junctions.

V. CONCLUSION

We numerically study the effects of interfacial roughness on conductance in normal-metal/*d*-wave superconductor junctions by using the recursive Green-function method. There are two conclusions: (i) the specular Andreev reflection of a quasiparticle is indispensable to the formation of a ZES at the NS interface, and (ii) the specular Andreev reflection rate depends strongly on the transparency of the ideal junction. The first conclusion agrees with that in previous theories using a quasiclassical Green-function method. However, the second conclusion indicates that the NS junction must be clean to observe the ZBCP in low transparent junctions. We also find in low transparent junctions that the interfacial roughness causes the shift of the ZBCP.

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