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Influence of the Impurity-scattering on Zero-bias Conductance Peak in Ferromagnet/Insulator/*d*-wave Superconductor Junctions

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Effects of impurity-scattering on a zero-bias conductance peak in ferromagnet/insulator/*d*-wave superconductor junctions are theoretically studied. The impurities are introduced through the random potential in ferromagnets near the junction interface. As in the case of normal-metal/insulator/*d*-wave superconductor junctions, the magnitude of zero-bias conductance peak decreases with increasing the degree of disorder. However, when the magnitude of the exchange potential in ferromagnet is sufficiently large, the random potential can enhance the zero-bias conductance peak in ferromagnetic junctions.

KEYWORDS: Andreev reflection, *d*-wave superconductor, zero-energy states, zero-bias conductance peak, disorder, ferromagnet, spin-polarized tunneling
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1. Introduction

In recent years, spin-dependent transport properties in hybrid structures consisting of the colossal magneto resistance (CMR) materials and high-T_C superconductors have received considerable theoretical and experimental attention because the latest progress of nano-technologies enables such structures. In hybrid structures involving high-T_C superconductors, it is well known that the zero-energy states (ZES) formed at a surface of superconductors affect transport properties. For instance, a large peak can be seen in the conductance at the zero-bias voltage in normal-metal/insulator/high-T_C superconductor junctions.[1–9] The ZES are also responsible for the low-temperature anomaly of the Josephson current in unconventional superconductor junctions.[10–12] In unconventional superconductors, the pair potential changes its sign depending on a direction of a quasiparticle's motion.[13–15] The origin of the ZES is an interference effect of a quasiparticle in the presence of the sign-change in the pair potential. The retro-reflectivity of Andreev reflection[16] (AR) supports the interference effect.[17]

When we compare the theoretical results with experiments, we should know effects of random potentials on the conductance because a quasiparticle suffers the random impurity-scattering near interfaces in real junctions. Very recently, we study effects of impurity-scattering on the conductance in diffusive normal-metal/insulator/*d*-wave superconductor (DN/I/*d*-SC) junctions in numerical simulations.[18,19] At the same time, the full resistance of the disordered junctions is derived from a microscopic theory.[20] The existence of the ZES induces the quite novel interference feature peculiar to the unconventional superconductors where the pair potential changes its sign on the Fermi surface. In the presence of the ZES, with the increase of the resistance in the normal diffusive region, R_D, the full resistance R does not show the reentrant behavior, i.e. $(\mathrm{d}R/\mathrm{d}R_D) > 0$ at $R_D = 0$ which is completely different from that in the diffusive normal metal/insulator/*s*-wave superconductor (DN/I/*s*-SC) junctions where reentrant behavior $(\mathrm{d}R/\mathrm{d}R_D) < 0$ at $R_D = 0$ is expected.[21] In the extreme case, with (110) oriented junction of *d*-wave superconductor, where quasiparticles always feel ZES at the interface, R can be expressed as $R_D + R_{R_D=0}$,[20] which indicates the absence of the proximity effect.[22]

In clean ferromagnet/insulator/ *d*-wave superconductor (FM/I/*d*-SC) junctions, it is pointed out that the retro-reflectivity of AR is suppressed by the exchange potential in FM.[23–27] Since the momentum of quasiparticle parallel to the interface is conserved in clean junctions, an Andreev reflected hole with down-spin cannot trace the original path of an incident electron with up-spin. As a consequence, the zero-bias conductance peak (ZBCP) in FM/I/*d*-SC junctions decreases with increasing the exchange potential. In addition to the basic physical point of view, FM/I/*d*-SC junctions have a possibility to be used as a measuring tool of the spin-polarization in FM. In FM/I/conventional superconductor junctions, generally speaking, the conductance mainly depends on both the potential barrier at the interface and the spin-polarization in FM. Thus a relation between the conductance and the spin-polarization is unclear when we lack definite information on the potential barrier. When a superconductor is a *d*-wave superconductor, however, it may be possible to say that there is a one-to-one correspondence between a height of ZBCP and a degree of spin-polarization in FM.[28] This is because the ZBCP in *d*-wave junctions is a result of the resonant tunneling of a quasiparticle through the junction, therefore, it does not depend on the potential barrier. Thus the ZBCP depends only on the spin-polarization. The above argument, however, was valid only when the junctions are in the clean limit. In real junctions, impurity-scattering inevitably exists in the FM and may affect the zero-bias conductance. Therefore, we need to study effects of the impurity-scattering in FM on a relation between the ZBCP and the exchange potential.

In this paper, effects of the randomness on the ZBCP in FM/I/d-SC junctions are studied numerically by using the recursive Green function method. It is naively expected that the height of the ZBCP in disordered FM/I/d-SC junctions might be smaller than that in clean junctions. Contrary to expectations, we found that the random potential enhances the height of ZBCP when the polarization of ferromagnets is sufficiently large. We also study a full resistance R of the junction as a function of the length of disordered region in the FM. In contrast to the case of DN/I/s-SC junction, reentrant behavior is hard to be expected in the case of DN/I/d-SC junction with ZES. When the magnitude of the polarization in FM is not large, full resistance R can be expressed as $R_{\rm D} + R_{R_{\rm D}=0}$ as well as that in DN/I/d-SC junction. We also study the relation between the tunneling conductance and the polarization in FM. The calculated results show that a relation between the height of the ZBCP and the magnitude of the exchange potential is insensitive to the random potential when ferromagnets are near half-metallic, and the length of the disordered region is sufficiently short.

This paper is organized as follows. In §2, the model and formulations are presented. The numerical results are shown in §3. In §4, we summarize this paper.

2. Formulation

We consider a FM/I/d-SC junction on the two-dimensional square lattice as shown in Fig. 1(a). Periodic boundary conditions are assumed in the direction parallel to the interface and the width of the junction is Ma, where a is the lattice constant. We describe the FM/I/d-SC junction by the mean-field (BCS) Hamiltonian $\mathcal{H}$ on the single-orbital tight-binding model,

$$\begin{aligned}\mathcal{H} = &-t \sum_{l,m,l',m',\sigma} \left(c^{\dagger}_{l',m',\sigma} c_{l,m,\sigma} + \text{H.c.} \right) \\ &+ \sum_{l,m,\sigma} \left(v_{l,m} - v_{\sigma} \right) c^{\dagger}_{l,m,\sigma} c_{l,m,\sigma} - \mu \hat{n} \\ &- \sum_{l,m,l',m'} \left(\Delta^{m,m'}_{l,l'} c^{\dagger}_{l,m,\downarrow} c^{\dagger}_{l',m',\uparrow} + \text{H.c.} \right) \end{aligned} \quad (1)$$

where (l, m) are lattice indices, $c_{l,m,\sigma}(c^{\dagger}_{l,m,\sigma})$ is the annihilation (creation) operator of an electron at (l, m) with spin σ $(= \uparrow$ or $\downarrow)$, $\hat{n}$ is the number operator and μ is the chemical potential of a junction. In the first term, the summation $\sum_{l,m,l',m'}$ runs over nearest-neighbor sites, and t is the nearest-neighbor hopping integral. In this paper, the length is measured in units of the lattice constant a and the energy is measured in units of t. We introduce the pair potential between the next nearest neighbor sites to describe the junction with $\alpha = \pi/4$ where the α is the angle between the (100) direction of high-$T_{\rm c}$ superconductors and the junction interface normal. As shown in Fig. 1(b), the pair potential $\Delta^{m,m'}_{l,l'}$ is given by

$$\Delta^{m,m'}_{l,l'} = \begin{cases} \Delta_0 & : \ l = l' \pm 1, m = m' \pm 1 \\ -\Delta_0 & : \ l = l' \pm 1, m = m' \mp 1 \\ 0 & : \ \text{otherwise} \end{cases} \quad (2)$$

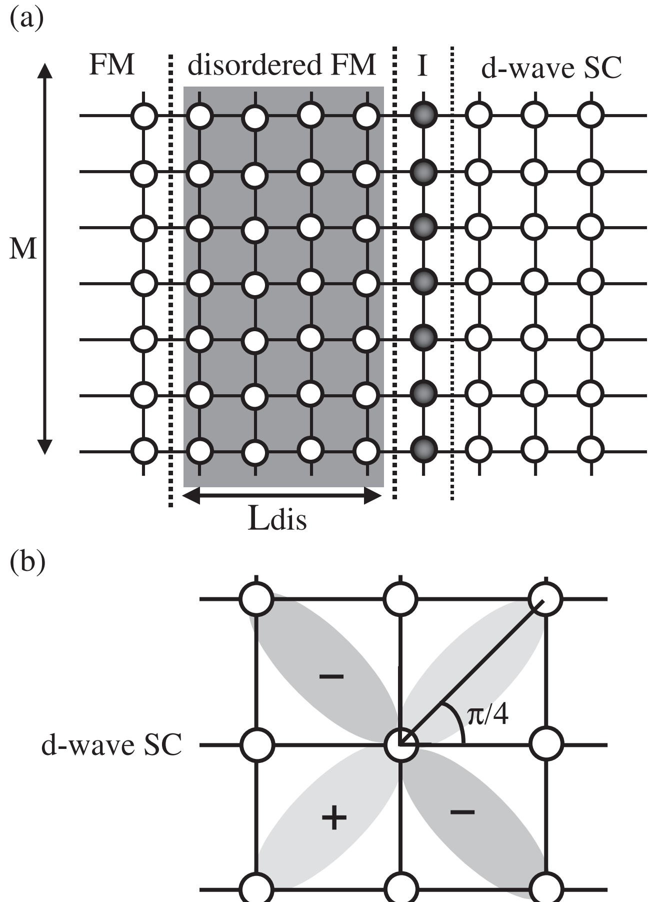

Fig. 1. Schematic figure of (a) disordered ferromagnetic metal/insulator/d-wave superconductor junction and (b) pair potential of d-wave superconductor.

where Δ_0 is the amplitude of the pair potential at the zero temperature. We note that the tight-binding model does not correspond to the two-dimensional CuO_2 plane in high-$T_{\rm C}$ 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 keeping the pair potential between the nearest neighbor sites and rotating the square lattice by 45°. 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. The exchange potential in FM is defind by $V_{\rm ex} = (v_{\uparrow} - v_{\downarrow})/2$, where $v_{\uparrow(\downarrow)}$ is the spin-dependent potential of an electron with $\sigma = \uparrow(\downarrow)$. The impurity potntial in FM is considered through on-site potential $v_{l,m}$ which takes random values uniformly distributed within a range of $-V_{\rm dis}/2 \le v_{l,m} \le V_{\rm dis}/2$ in a disordered region as shown in Fig. 1(a). In an insulator, $v_{l,m}$ is set to be $V_{\rm ins}$ independent of (l, m). Far from the interface, $v_{l,m}$ is taken to be zero.

By applying the Bogoliubov transformation, $\mathcal{H}$ in eq. (1) is diagonalized and we obtain the Bogoliubov–de Gennes equation which is numerically solved by using the recursive Green function technique.[17–19,29,30] In this method, the real-space Green function $\mathcal{G}^{m,m'}_{l,l'}$ is calculated without any approximation for the random potential: this is an advantage of the recursive Green function method. Using the Kubo formula,[31,32] the conductance is expressed in terms of the Green's functions

$$G = \frac{e^2}{h}\frac{t^2}{2}\sum_{\sigma}\sum_{m=1}^{M}\sum_{n=1}^{2M}\Big(\bar{\mathcal{G}}^{m,n}_{l,l+1}\bar{\mathcal{G}}^{n,m}_{l,l+1} + \bar{\mathcal{G}}^{m,n}_{l+1,l}\bar{\mathcal{G}}^{n,m}_{l+1,l} - \bar{\mathcal{G}}^{m,n}_{l,l}\bar{\mathcal{G}}^{n,m}_{l+1,l+1} - \bar{\mathcal{G}}^{m,n}_{l+1,l+1}\bar{\mathcal{G}}^{n,m}_{l,l}\Big), \quad (3)$$

where $\bar{\mathcal{G}} = \mathcal{G}(E - i0) - \mathcal{G}(E + i0)$ and $\bar{\mathcal{G}}_{l,l'}$ is a $2M \times 2M$ matrix. Since the DC conductance does not depend l, l is taken to be far away from the disordered region in numerical simulations. In what follows, we calculate the ensemble average of the conductance $\langle G \rangle$ over a number of samples which have different random impurity-configurations.

3. Results

Throughout this paper, we fix $M = 32$, $\Delta_0 = 0.001t$, $\mu = -2.5t$ and use 1000 samples to carry out the ensemble average.

In Figs. 2A, 2B, and 2C, the ensemble average of the conductance $\langle G \rangle$ at the zero-bias voltage (ZBCP) is plotted as a function of $V_{\rm dis}$ for several choices of $V_{\rm ex}$, where $V_{\rm ins}$ is fixed at 5.0. The length of the disordered region is $L_{\rm dis} = 2.0$, 5.0, and 10.0 in Figs. 2A, 2B, and 2C, respectively. The curve (a) are results of N/I/*d*-SC junctions (i.e., $V_{\rm ex} = 0.0$). We consider the exchange potential in ferromagnet as $V_{\rm ex} = 0.25$, 0.5, 0.75, 1.0 and 1.4 in curves (b), (c), (d), (e), and (f), respectively. In clean FM/I/*d*-SC, (i.e., $V_{\rm dis} = 0$), the results show that the height of the ZBCP decreases with increasing the exchange potential. In a previous paper, we showed that the specular Andreev reflection is a source of the ZES at the junction interface.[17] It is known that the presence of the time-reversal symmetry in systems leads to the specular Andreev reflection or the retro reflectivity of a holelike quasiparticle.[21] In FM/I/*d*-SC, however, the specular Andreev reflection is suppressed even in the limit of the zero-bias voltage because the exchange potential in ferromagnet breaks the time-reversal symmetry. In N/I/*d*-SC junctions, the height of the ZBCP monotonically decreases with increasing $V_{\rm dis}$ as shown in curves (a). This is because the tunneling conductance is suppressed by the existence of diffusive metal since $\langle G(eV = 0)\rangle$ is given by

$$\langle G(eV = 0)\rangle = \frac{1}{R_{\rm D} + R_{\rm B}}$$

with $R_{\rm B} = R_{R_{\rm D}=0}$, where R, $R_{\rm D}$ and $R_{\rm B}$ denotes the full resistance, resistance in the diffusive metal, and resistance from the insulating barrier, respectively.[20] However, in the presence of $V_{\rm ex}$, the results show that the height of the ZBCP first increases with increasing $V_{\rm dis}$ then decreases as shown in Fig. 2A(c)–2A(f). The same tendency can be also found in Figs. 2B and 2C for large $V_{\rm ex}$ such as curve (f). This novel feature can not be understood by the simple summation of resistance $R_{\rm D}$ and $R_{\rm B}$ and is considered to be an interference effect of a quasiparticle. When $V_{\rm ex}$ is sufficiently large, the retro-reflection is strongly suppressed by the exchange potential in clean junctions. In the presence of disorder, however, the propagation path of an incident spin-up electron and that of reflected spin-down hole is determined rather by the random potential than by the exchange potential when $V_{\rm ex} \sim V_{\rm dis}$. Thus the retro-reflectivity seems to be recovered when $L_{\rm dis}$ is sufficiently small.

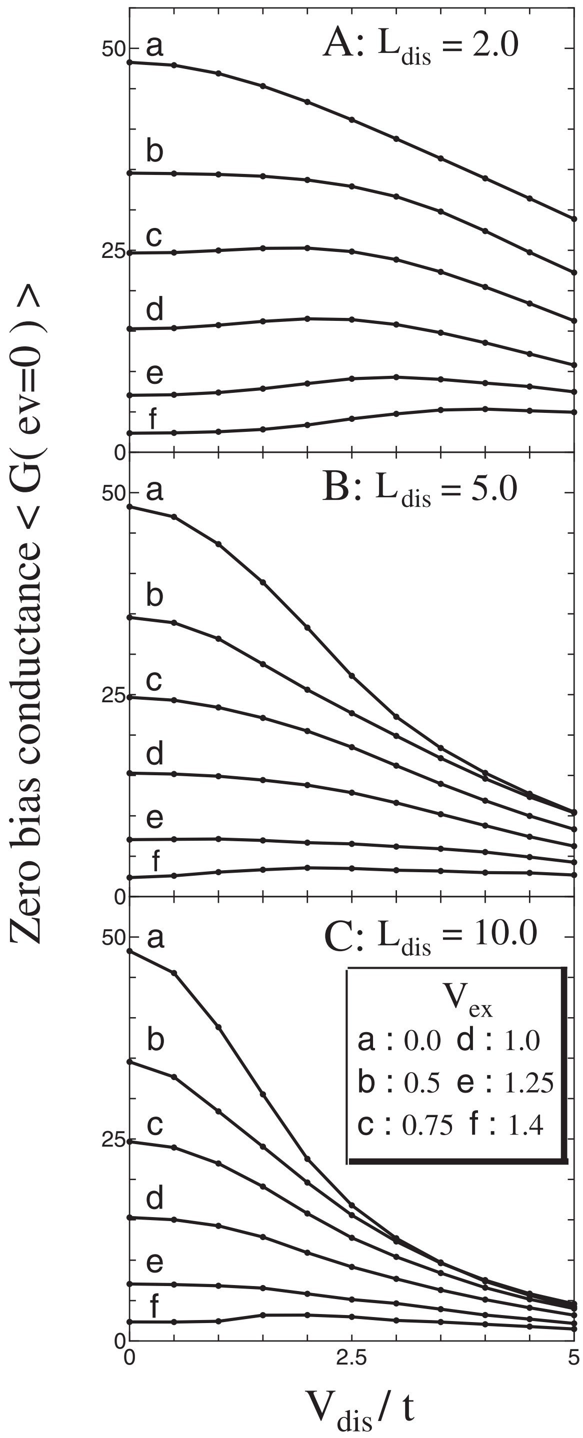

Fig. 2. The zero-bias conductance peak is plotted as a function of $V_{\rm dis}$. The length of random region $L_{\rm dis}$ are 2.0, 5.0, and 10.0 in A, B, C, respectively. The magnitude of the exchange potential $V_{\rm ex}$ are 0, 0.25, 0.5, 0.75, 1.0 and 1.40, in *a*, *b*, *c*, *d*, *e* and *f*, respectively.

In order to clarify this feature, we concentrate on the $L_{\rm dis}$ dependence of the full resistance R. When the magnitude of $V_{\rm ex}$ is not so large, resistance increases linearly with the increase of $L_{\rm dis}$ as shown in Fig. 3. The results qualitatively agree with those in N/I/*d*-SC junctions. Since the resistance from the disordered region $R_{\rm D}$ is proportional to $L_{\rm dis}$, the full resistance of the junction R is given by $R_{\rm D} + R_{R_{\rm D}=0}$.[20] However, with the further increase of $V_{\rm ex}$, the resistance

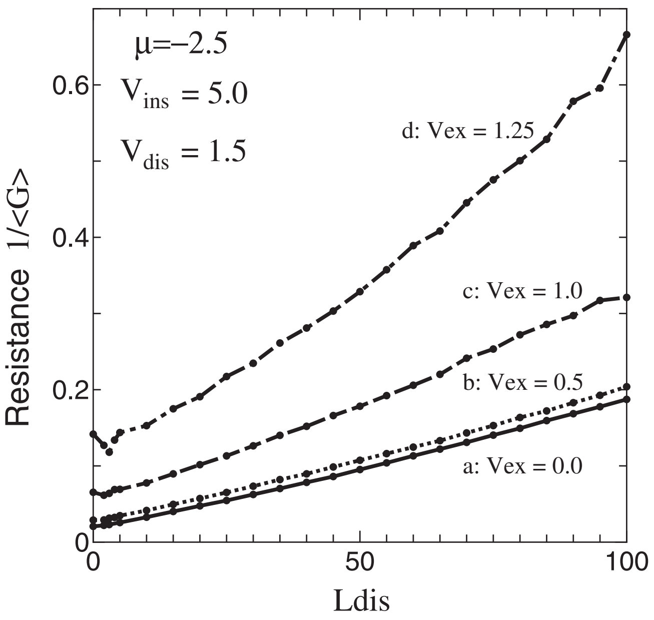

Fig. 3. Resistance at zero-bias voltage as a function of $L_{\rm dis}$ for $V_{\rm ins} = 5$ and $E_{\rm F} = 1.5$. The magnitude of the disorder potentials is $V_{\rm dis} = 1.5$. The length of the disorder region $L_{\rm dis}$ is *a*: $V_{\rm ex} = 0.0$, *b*: $V_{\rm ex} = 0.5$, *c*: $V_{\rm ex} = 1.0$ and *d*: $V_{\rm ex} = 1.25$.

deviates from the linear relation. For sufficiently large $V_{\rm ex}$ such as 1.25 in Fig. 3, R first decreases for $L_{\rm dis} < 5$ then increases. In this case, the randomness in FM opens available channels of the resonant tunneling and reduces the full resistance.

The ZBCP in *d*-wave junctions is a result of the resonant tunneling of a quasiparticle through the junction. Therefore, the height of the ZBCP does not depend on the potential barrier in the absence of the exchange potential. The resonant tunneling, however, is suppressed by the exchange potential, which leads to the fact that the height of the ZBCP depends on the potential barrier. From this fact, we discussed a relation between a height of ZBCP and a degree of spin-polarization in a previous paper.[28] However the argument above is valid for clean junctions because the random potentials were not taken into account. In this paper, we address this issue. Figure 4 shows a relation between the normalized ZBCP $\langle G(eV = 0)\rangle$ and $V_{\rm ex}$ for $V_{\rm dis} = 1$ in (a) and 0.5 in (b), where $V_{\rm ins}$ is fixed at 5 because of the height of ZBCP $\langle G(eV = 0)\rangle$ does not depend on the barrier potential. In this figure, $L_{\rm dis}$ is chosen to be smaller than the mean free path of diffusive region which is estimated to be about 80 for (a) $V_{\rm dis} = 0.5$ and 20 for (b) $V_{\rm dis} = 1.0$. The solid line is the result of a clean junction ($V_{\rm dis} = 0$). The dotted ($L_{\rm dis} = 2$), dot-dashed ($L_{\rm dis} = 5$) and dashed ($L_{\rm dis} = 10$) lines denote the results of disordered junctions. The magnitude of $L_{\rm dis}$ is sufficiently smaller than that of the mean free path. The height of the ZBCP decreases monotonically with increasing $V_{\rm ex}$ irrespective of the degree of disorder. When the exchange potential is small, the height of the ZBCP depends on the random potential as well as on the potential barrier. This feature can be understood from an equation $\langle G(eV = 0)\rangle^{-1} = R_{\rm B} + R_{\rm D}$. Since the resonant tunneling can still occur for small $V_{\rm ex}$, $R_{\rm B}$ is not much larger than $R_{\rm D}$. Thus we can not find a clear relation between the exchange potential and the height of the ZBCP for small

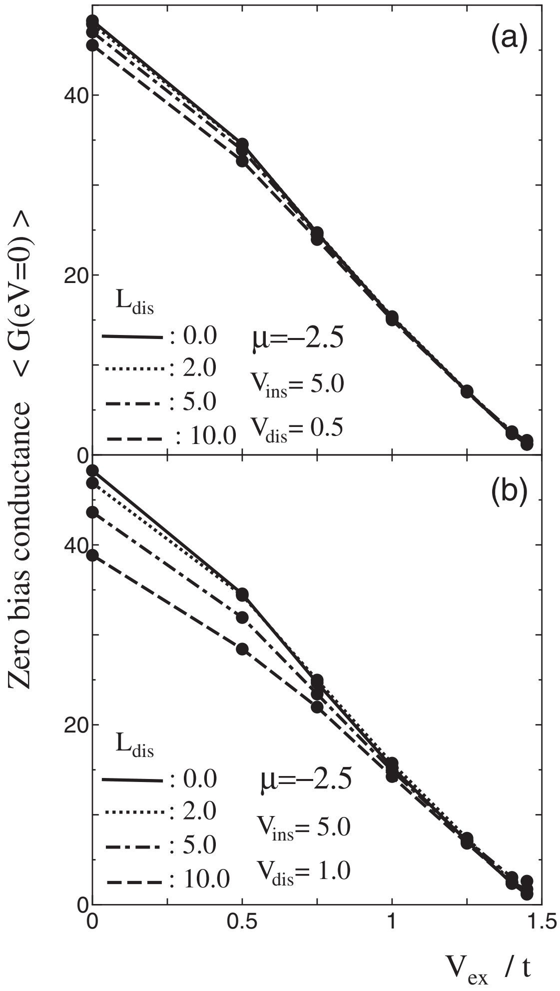

Fig. 4. The relations between the zero-bias conductance peak and the exchange potential for $V_{\rm ins} = 5$ and $E_{\rm F} = 1.5$. The magnitude of the disorder potentials is (a) $V_{\rm dis} = 0.5$ and (b) $V_{\rm dis} = 1$. The length of the disorder region $L_{\rm dis}$ is $L_{\rm dis} = 0.0$ (the solid line), $L_{\rm dis} = 2.0$ (the dotted line), $L_{\rm dis} = 5.0$ (the dot-dashed line) and $L_{\rm dis} = 10.0$ (the dashed line).

$V_{\rm ex}$. The height of the ZBCP is not so much sensitive to the disorder in the limit of large $V_{\rm ex}$, where FM are referred to as half-metals. In this case, a relation $R_{\rm B} \gg R_{\rm D}$ is satisfied because the resonant tunneling is strongly suppressed by the exchange potential. Thus the height of the ZBCP reflects $V_{\rm ex}$ and depends on the potential barrier as $\langle G(eV = 0)\rangle \sim R_{\rm B}^{-1}$.

4. Summary

In this paper, we have studied effects of disorder on the spin-polarized tunneling in ferromagnet/insulator/*d*-wave superconductor (FM/I/*d*-SC) junctions by using the recursive Green function method. Before performing a numerical simulation, we expected that the impurity-scattering decreases the zero-bias conductance peak (ZBCP) because it was reported that the exchange potential and the impurity-scattering suppress the ZBCP independently. Contrary to expectations, we found that the random impurity-scattering in FM enhances the height of ZBCP when the magnitude of the exchange potential in ferromagnet is sufficiently large. The enhancement of the ZBCP originates from the fact that the retro-reflectivity of the Andreev reflection of a quasiparticle is recovered by the impurity-scattering. We have also studied a full resistance R of the junction as a function of the length of diffusive region in the FM. When the magnitude of the polarization in FM is not strong, we find the full resistance R can be expressed as $R_D + R_{R_D=0}$ and that R has no reentrant behavior as a function of R_D. In this paper, the symmetry of the pair potential is chosen as d-wave. The possibility of the formation of $d + is$-wave state at the interface or surface of d-wave superconductor is an hottest issue.[33–36] It is actually interesting problem to study the case where $d + is$-wave state is formed at the interface of FM/I/d-SC junctions.

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