Spin-polarized quasiparticle transport in ferromagnet–d-wave-superconductor junctions with a $\{110\}$ interface

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Within a scattering framework, a theoretical study is presented for the spin-polarized quasiparticle transport in ferromagnet–d-wave-superconductor junctions with $\{110\}$ interface. We find that the subgap conductance behaviors are qualitatively different from a nonmagnetic case, due to the modification of Andreev reflection by the exchange field in the ferromagnet, and can also be significantly different from those of a ferromagnet–s-wave junction because of the sign change of the d-wave order parameter along the $\{110\}$ direction of the crystal. For a ballistic ferromagnet–d-wave-superconductor junction, a zero-bias conductance minimum is achieved. In addition, a conductance maximum at finite bias can also be evolved by interfacial scattering. For a normal-metal–ferromagnet–d-wave-superconductor junction, conductance resonances are predicted.
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Due to the past several years of experimental and theoretical efforts, it has been widely accepted that high-critical temperature (T_c) superconductors have a $d_{x_a^2-x_b^2}$-wave pairing symmetry.[1] The energy gap of such a pairing state, $\Delta_0(\hat{k}_a^2-\hat{k}_b^2)$, has a sign change at some directions of the Fermi wave vector. This feature is dramatically different from the case in a conventional s-wave superconductor. As a direct consequence of this sign change, it was predicted[2] that a sizable areal density of midgap states (i.e., states with energy arbitrarily close to the Fermi surface) exists on a $\{110\}$ surface of a $d_{x_a^2-x_b^2}$-wave superconductor. These midgap states have been used to explain[3,4] the zero-bias conductance peak observed in most high-T_c superconductor junctions. The fundamental process central to this explanation is Andreev reflection (AR),[5] that is, an electron incident with an energy below the superconducting energy gap cannot drain off into the superconductor. It is instead reflected at the interface as a hole by transferring a Cooper pair to the superconductor. For a normal-metal–s-wave-superconductor junction, as the interfacial scattering strength is increased, AR is suppressed. For a normal-metal–d-wave-superconductor junction, a hole is fully Andreev reflected through the surface midgap states, regardless of the interfacial scattering strength. Note that the incoming electron and the Andreev reflected hole occupy energy bands with opposite spins. For the case of normal metals, due to the spin degeneracy of energy levels, no spin effects associated with AR occur. However, in a (metallic) ferromagnet, the energy band is spin split. There has been considerable interest in studying the interplay of superconductivity and ferromagnetism in combined structures involving superconducting and ferromagnetic materials. A lot of works have focused on the changes of the critical temperature of the superconductor in s-wave-superconductor–ferromagnet multilayers,[6–9] the Josephson critical current in superconductor-ferromagnet-superconductor junctions,[9–12] and the magnetic coupling in ferromagnet-superconductor-ferromagnet multilayers.[13,14] In an earlier time, the tunneling properties of superconductor junctions with a ferromagnet involved were investigated on the region where AR was unimportant.[15] Recently, the spin splitting effect on the Andreev reflection in ferromagnet–s-wave-superconductor junctions has been explored theoretically[16,17] and experimentally.[18] More recently, the experimental study has been extended to ferromagnet–high-T_c superconductor junctions.[19] However, we have not seen any theoretical work taking into account the unconventional pairing symmetry, which is relevant to the high-T_c superconductor junctions. In this work, we are mainly concerned with the spin-polarized quasiparticle transport in ferromagnet–d-wave-superconductor junctions. We first study a ferromagnet-superconductor junction to show the suppression of AR at the interface by the spin splitting of energy bands in the ferromagnet. We then calculate the differential conductance in a normal-metal–ferromagnet-superconductor junction. Because of the different spin-up and spin-down wave vectors in the ferromagnet, a quantum interference effect manifests itself through the resonance in the subgap conductance. This interference effect is diminished by the barrier scattering at the interface between the ferromagnet and superconductor. Most importantly, the typical behaviors exhibited in the conductance of a d-wave-superconductor junction are, due to the sign change of the order parameter along the $\{110\}$ crystalline direction, significantly different from those of s-wave counterparts, which may explain some related experimental observations.

We adopt the Bogoliubov–de Gennes (BdG) (Ref. 20) approach to ferromagnet-superconductor junctions. Within the Stoner model, the motion of conduction electrons inside the ferromagnet can be described by an effective single-particle Hamiltonian with an exchange interaction. The influence of the magnetization of the ferromagnet on the orbital motion of conduction electrons is neglected since it is much smaller than that via the exchange interaction. In the absence of spin-flip scattering, the spin-dependent (four-component) BdG equations are decoupled into two sets of (two-component) equations, one for the spin-up electron, spin-down hole quasiparticle wave functions $(u_\uparrow, v_\downarrow)$ and the other for $(u_\downarrow, v_\uparrow)$. The equation for $(u_\uparrow, v_\downarrow)$ can be written as

$$[\mathcal{H}_e(\mathbf{r}) - h(\mathbf{r})]u_\uparrow(\mathbf{r}) + \int d\mathbf{r}' \Delta(\mathbf{r},\mathbf{r}') v_\downarrow(\mathbf{r}') = E u_\uparrow(\mathbf{r}), \tag{1a}$$

$$\int d\mathbf{r}' \Delta^*(\mathbf{r},\mathbf{r}') u_\uparrow(\mathbf{r}') - [\mathcal{H}_e^*(\mathbf{r}) + h(\mathbf{r})] v_\downarrow(\mathbf{r}) = E v_\downarrow(\mathbf{r}). \tag{1b}$$

Here the excitation energy E is measured relative to the Fermi energy $E_F = \hbar^2 \mathbf{k}_F^2 / 2m_e$ with $\mathbf{k}_F$ the Fermi wave vector, the single-particle Hamiltonian is given by

$$\mathcal{H}_e(\mathbf{r}) = -\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m_e} + V(\mathbf{r}) - E_F \tag{2}$$

with $V(\mathbf{r})$ the usual static potential but without the exchange interaction, and $h(\mathbf{r})$ is the exchange energy which is explicitly given in Eq. (1). $\Delta(\mathbf{r},\mathbf{r}')$ is a non-s-wave pair potential, which not only depends on the center-of-mass coordinates $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2 \equiv (x,y,z)$ but also on the relative coordinates $\mathbf{s} = \mathbf{r} - \mathbf{r}'$, or after a Fourier transform, on the relative wave vector $\mathbf{k}$.[21] In the weak-coupling theory, the pairing only occurs near the Fermi surface, thus only the direction of the Fermi wave vector $\hat{\mathbf{k}}_F = \mathbf{k}_F / k_F$ is a variable. As shown in Fig. 1, we define the interface at $x = 0$ with the region $x < 0$ occupied by the ferromagnet and that with $x > 0$ by the superconductor. We take both the pair potential and the exchange energy as a step function, $\Delta(\mathbf{R},\hat{\mathbf{k}}) = \Delta_0(\hat{\mathbf{k}})\Theta(x)$ and $h(\mathbf{R}) = h_0 \Theta(-x)$, where $\Theta(x)$ is the unit step function. Moreover, to capture the essential interfacial scattering at the interface, a δ-function potential $V(x) = H\delta(x)$ is included. The metallic and tunnel junctions correspond to two limits $H = 0$ and $H \to \infty$, respectively. The BdG equation for $(u_\downarrow, v_\uparrow)$ is obtained by simply changing the sign before $h(\mathbf{r})$ in Eq. (1). If we denote the incident and specularly reflected

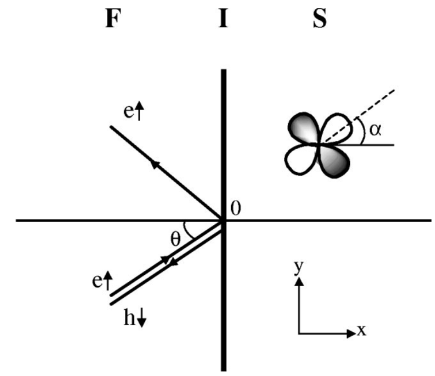

FIG. 1. Schematic geometry of the ferromagnet–d-wave-superconductor junction. The thick solid line represents the interfacial scattering layer. Also shown is the d-wave order parameter profile and the angle α of the crystalline orientation with respect to the interface. The wave vectors are $e:(\pm q_\uparrow, k_y)$ and $h:(q_\downarrow, k_y)$ in the ferromagnet, and $e:(k_e, k_y)$ and $h:(-k_h, k_y)$ in the superconductor, respectively. Andreev reflection: A beam of spin-up electrons incident with angle θ and energy within the gap are normally reflected as spin-up electrons and Andreev reflected as spin-down holes.

wave vectors, respectively, $\mathbf{k}_+ = (k_x, k_y)$ and $\mathbf{k}_- = (-k_x, k_y)$, the pair potential for d-wave superconductivity takes the form

$$\Delta(\mathbf{k}_\pm) = \Delta_0 \cos(2\theta_\pm). \tag{3}$$

Here $\theta_\pm = \theta \mp \alpha$ with θ the incident angle of electron excitations injected from the ferromagnet and α the misorientation angle of the crystalline axis along which the d-wave order parameter reaches the maximum. Both θ and α are measured relative to the positive x axis. The above expression shows that the effective pair potentials experienced by the electronlike and holelike excitations in the superconductor are usually different and can even have opposite signs under appropriate arrangements.

A beam of incident electrons from the ferromagnet is either normally reflected as electrons at the same spin state or Andreev reflected as holes at the opposite spin state. Using the matching condition of the wave function $\Psi(x) = (u_\uparrow(x), v_\downarrow(x))$,

$$\Psi_{\mathrm{F}}(0) = \Psi_{\mathrm{S}}(0), \tag{4a}$$

$$\left.\frac{d\Psi_{\mathrm{S}}}{dx}\right|_{x=0} - \left.\frac{d\Psi_{\mathrm{F}}}{dx}\right|_{x=0} = \frac{2mH}{\hbar^2} \Psi_{\mathrm{F}}(0), \tag{4b}$$

the Andreev and normal reflection amplitudes, $r_{\downarrow\uparrow}$ and $r_{\uparrow\uparrow}$, are found to be

$$r_{\downarrow\uparrow} = -\frac{2q_\uparrow (v_+/u_+)(k_e + k_h) e^{-i\phi_+}}{\kappa(q_\uparrow - k_h + 2ik_{Fx}z)(q_\downarrow - k_e - 2ik_{Fx}z) - (q_\uparrow + k_e + 2ik_{Fx}z)(q_\downarrow + k_h - 2ik_{Fx}z)}, \tag{5}$$

$$r_{\uparrow\uparrow} = \frac{\kappa(q_\uparrow + k_h - 2ik_{Fx}z)(q_\downarrow - k_e - 2ik_{Fx}z) - (q_\uparrow - k_e - 2ik_{Fx}z)(q_\downarrow + k_h - 2ik_{Fx}z)}{\kappa(q_\uparrow - k_h + 2ik_{Fx}z)(q_\downarrow - k_e - 2ik_{Fx}z) - (q_\uparrow + k_e + 2ik_{Fx}z)(q_\downarrow + k_h - 2ik_{Fx}z)}. \tag{6}$$

Here $z=m_eH/\hbar^2k_{Fx}$ with $k_{Fx}=k_F\cos(\theta)$ represents the strength of interfacial scattering. The wave vectors in the ferromagnet and the superconductor are, respectively,

$$q_{\uparrow,\downarrow}=\left\{\left(\frac{2m_e}{\hbar^2}\right)[E_{Fx}\pm(E+h_0)]\right\}^{1/2} \tag{7}$$

and

$$k_{e,\pm}=k_{Fx}+\left[\left(\frac{m_e}{\hbar^2k_{Fx}}\right)\sqrt{E^2-|\Delta(\mathbf{k}_\pm)|^2}\right], \tag{8a}$$

$$k_{h,\pm}=k_{Fx}-\left[\left(\frac{m_e}{\hbar^2k_{Fx}}\right)\sqrt{E^2-|\Delta(\mathbf{k}_\pm)|^2}\right], \tag{8b}$$

where $E_{Fx}=\hbar^2k_{Fx}^2/2m_e$. The variable κ is given by

$$\kappa=\left(\frac{v_+v_-}{u_+u_-}\right)\exp[-i(\phi_+-\phi_-)], \tag{9}$$

where the BCS coherence factors are

$$u_\pm^2=\frac{1}{2}\left(1+\frac{\sqrt{E^2-|\Delta(\mathbf{k}_\pm)|^2}}{E}\right), \tag{10a}$$

$$v_\pm^2=\frac{1}{2}\left(1-\frac{\sqrt{E^2-|\Delta(\mathbf{k}_\pm)|^2}}{E}\right), \tag{10b}$$

and

$$\phi_\pm=\cos^{-1}\left[\frac{\cos 2(\theta\mp\alpha)}{|\cos 2(\theta\mp\alpha)|}\right]. \tag{11}$$

The reflection amplitudes $r_{\uparrow\downarrow}$ and $r_{\downarrow\downarrow}$ can be obtained by changing the sign before h_0.

The transport properties of a normal-metal–superconductor junction can be described by the Blonder-Tinkham-Klapwijk (BTK) theory,[22] which expresses the differential conductance in terms of the Andreev and normal reflection probabilities. In contrast to the tunneling Hamiltonian model, which requires an opaque barrier at the interface, the BTK theory can consider the case of an arbitrary barrier strength. Also noticeably, the BTK formalism can be regarded as the earliest version of the Landauer-Büttiker[23] formula applied to the coherent transport through a normal-metal–superconductor structure.[24] We extend the BTK theory to the spin-dependent transport through ferromagnet-superconductor junctions by writing the conductance[16]

$$G_\sigma=\frac{e^2}{h}\left(1+\frac{q_{\bar{\sigma}}}{q_\sigma}|r_{\bar{\sigma}\sigma}|^2-|_{\sigma\sigma}|^2\right), \tag{12}$$

which shows clearly that an incoming electron of spin σ is normally reflected as an electron of the same spin σ and Andreev reflected as a hole of the opposite spin $\bar{\sigma}$. Usually, the conductance for each incident direction is the sum of contributions from both spin directions, $G=G_\uparrow+G_\downarrow$. Considering that the decrease of allowed channel number (i.e., the number of allowed k_y values) with the spin splitting has been well understood,[16] here we are most interested in the transport with both the single incident wave direction and the single spin direction, which can give more detailed information, to understand the spin splitting effect on the subgap conductance in the ferromagnet–d-wave-superconductor junction.

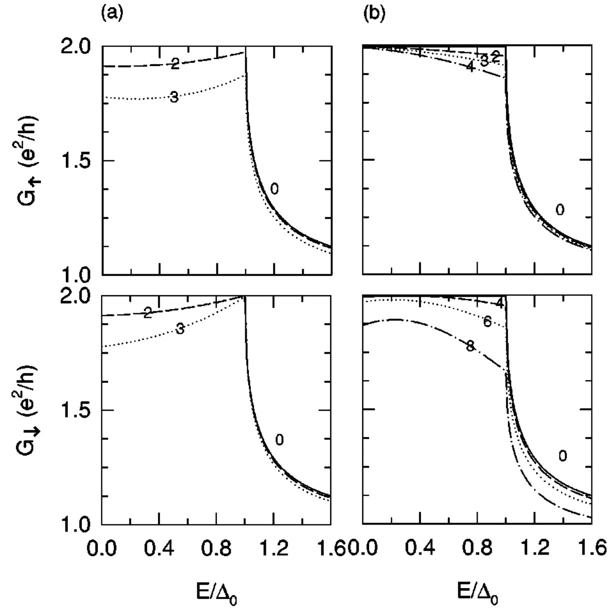

FIG. 2. Conductance versus incident energy E/Δ_0 with various values of h_0/Δ_0 indicated in the figure for a FD (a) and a FS (b) junction. Here $z_0=0$ and $G_{\uparrow,\downarrow}$ are shown in the upper and lower panels, respectively.

To study the conductance of a ferromagnet–d-wave-superconductor junction, we typically discuss the arrangement $\alpha=\theta=\pi/4$ [$\alpha=\pi/4$ corresponds to a {110} junction], which gives $\phi_+=0$ while $\phi_-=\pi$. In this case, the energy gaps felt by electrons and holes have the same absolute magnitudes but opposite signs, which is a unique feature of d-wave superconductivity. We refer to this junction as a FD junction. By simply taking $\alpha=\theta=0$ ($\alpha=0$ corresponds to a {100} junction) (thus $\phi_+=\phi_-=0$) so that the gaps experienced by electrons and holes are identical, a ferromagnet–s-wave-superconductor junction (referred to as FS junction) can also be studied. In our following calculations, $\Delta_0/E_F=0.1$ is chosen. In Fig. 2, the conductance G versus the scaled energy E/Δ_0 is plotted for (a) a FD junction and (b) a FS junction with various values of exchange energy h_0/Δ_0 but fixed barrier strength $z_0=m_eH/\hbar^2k_F=0$, and $G_\uparrow$ for the upper panel and $G_\downarrow$ for the lower panel. The conductance $G_\uparrow$ of the FD junction increases slowly with E for a weak exchange interaction, while the conductance of the FS junction decreases monotonically with the incident energy with its maximum located at $E=0$. The conductance $G_\downarrow$ of the FD junction is increased with E in the whole gap range, and a conductance minimum appears at zero energy. Correspondingly, it implies a resistance peak at zero energy. In addition, the larger h_0 is, the larger is the conductance slope within the gap. However, the subgap conductance of the FS junction first increases slightly and then decreases slowly with E. We have studied other arrangements $\theta=\alpha=\pi/6$ (i.e., $\Delta_+=\Delta_0$ and $\Delta_-=-\Delta_0/2$), $\theta=\alpha=5\pi/24$ (i.e., $\Delta_+=\Delta_0$ and $\Delta_-=-\sqrt{3}\Delta_0/2$), and $\theta=\pi/4$ and $\alpha=\pi/6$ (i.e., $\Delta_+=-\Delta_-=\sqrt{3}\Delta_0/2$) and found that the above features qualitatively are unchanged. Therefore, we can conclude that the dramati-

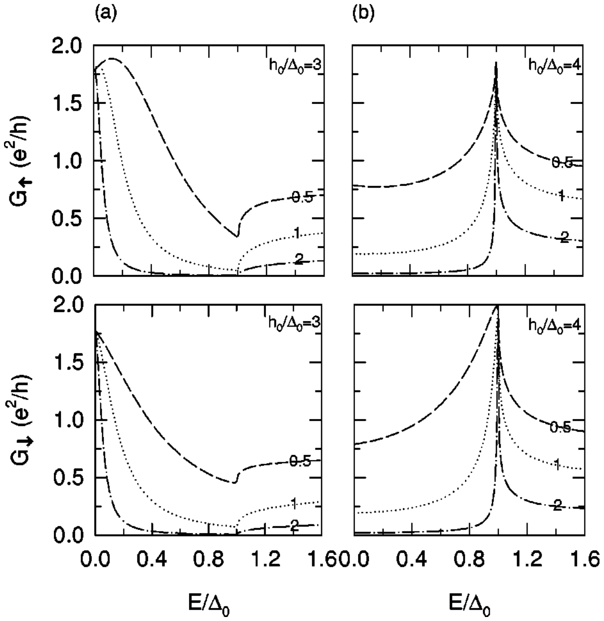

FIG. 3. Conductance versus E/Δ_0 with various values of z_0 for a FD (a) and a FS (b) junction. Here the value of h_0/Δ_0 is shown in each case.

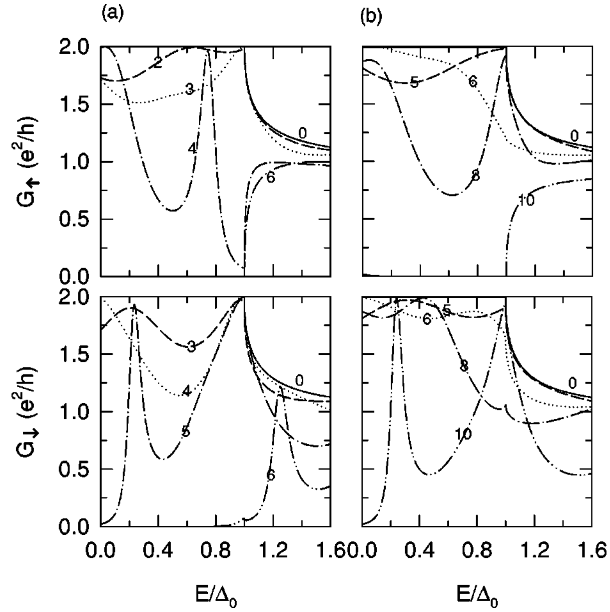

FIG. 4. Conductance versus E/Δ_0 with various values of h_0/Δ_0, for an NFD (a) and an NFS (b) junction. Here $L=2\xi_0$ and $z_0=0$.

cally different behaviors between the FS and FD junctions are caused by the sign change of the *d*-wave order parameter. Most importantly, our calculation demonstrates that *d*-wave pairing symmetry may be essential to explain the experimental observation of a zero-bias resistance peak in ferromagnet/high-T_c superconductor junctions $La_{2/3}Ba_{1/3}MnO_3/DyBa_2Cu_3O_7$.[19] Common to both the FD and FS junctions, the subgap conductance at a given energy E is suppressed by the exchange interaction due to the suppression of AR.

In Fig. 3, we plot the conductance spectrum for a variety of values of the barrier strength but with fixed exchange energy. For $G_\uparrow$ of the FD junction, when a weak interfacial barrier scattering is introduced, a conductance peak evolves at a finite energy. With the increase of the barrier scattering, the width of the conductance peak becomes narrower, and simultaneously the peak position is shifted to zero energy. This shift of the conductance peak comes from the competition between the constructive interference of electrons and holes at zero energy and the suppression of AR by the ferromagnetic exchange interaction. Therefore, it has a different mechanism than that observed in normal-metal–high-T_c superconductor junctions,[25] which was interpreted by the energy shift of Andreev bound states in a broken-time-reversal-symmetry surface state.[26,27] However, for $G_\downarrow$, we do not see the shift of zero-bias conductance peak (ZBCP) in the presence of exchange interaction in the FD junction. For the FS junction, no pronounced anomalous behaviors show up in conductance.

Now we would like to discuss a new kind of subgap resonance by studying a normal-metal–ferromagnet-superconductor junction. First we give an intuitive description for the phase-coherent transport through this structure. In a normal metal, electrons and holes at energy close to the Fermi energy almost have the same wave vectors. However, when they travel in the ferromagnet, the difference of the wave vectors associated with an electron and a hole is quite large. When the width of the ferromagnet layer is relatively small, it is easier for constructive interference to take place between the electron wave and its Andreev-reflected hole wave than to occur between the electron wave and its normal reflected counterpart. In Fig. 4, the conductance is plotted for various values of exchange energy in (a) a normal-metal–ferromagnet–*d*-wave-(NFD) superconductor junction and (b) a normal-metal–ferromagnet–*s*-wave-(NFS) superconductor junction in the absence of the interfacial barrier scattering $(z_0=0)$. The width of the ferromagnet layer is $L=2\xi_0$, where $\xi_0=\hbar v_F/2\Delta_0$ is the superconducting coherence length. For the small exchange interaction, the conductance weakly oscillates as a function of the energy in both cases. As the exchange interaction is intermediately strong, a very sharp conductance peak can show up in both junctions. In addition, if the exchange energy is so large as to exceed the kinetic energy of the Andreev-reflected holes, the hole waves become exponentially damped along the positive *x* direction. Then there is no interference between the electron and hole waves. In particular, due to the dramatical suppression of AR, there is no conduction through the structure within the energy gap. The theoretical motivation for putting the ferromagnet in contact with an additional normal metal is to make the scattering approach well defined for the strong exchange interaction. Figure 5 shows the effect of an interfacial scattering between the ferromagnet and the superconductor on the NFD and NFS structure with the other parameters the same as those in Fig. 4. As the interfacial scattering is increased, a zero-bias conductance peak appears and becomes sharper in the NFD junction, but there is no such ZBCP appearing in the NFS junction. Of particular interest, we find that the subgap resonant conductance peak occurring in both junctions is suppressed by the interfacial scattering but with its position unchanged. Physically, this behavior demonstrates convincingly that the ZBCP is due to electron and hole coherence at the surface of the *d*-wave superconductor, while the subgap resonance comes from the interference of

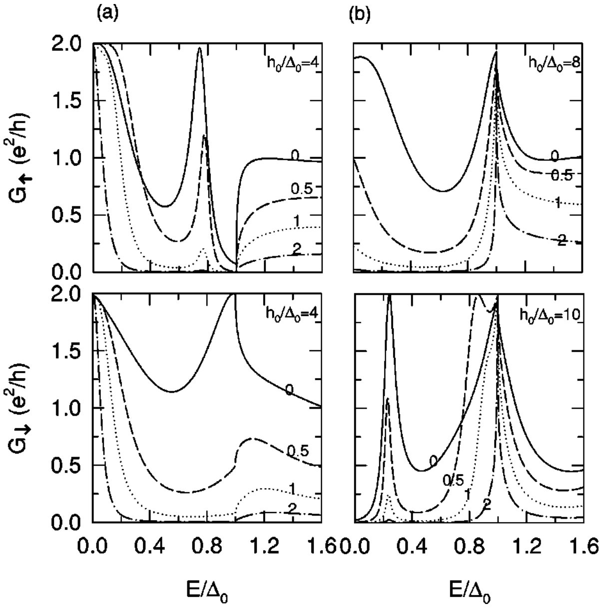

FIG. 5. Conductance versus E/Δ_0 with various values of z_0 for an NFD (a) and an NFS (b) junction. Here $L=2\xi_0$ and the value of h_0/Δ_0 is shown in each case.

electrons and holes in the ferromagnetic layer. As the interfacial scattering is strong, the probability for holes to be created by AR becomes smaller. Thus the corresponding interference in the ferromagnetic layer is suppressed.

We believe the above phenomena can be experimentally accessible. The scanning tunneling spectroscopy is best suitable for exploring the directionality of transmission.[31] For a point contact junction, an average should be taken over incident directions.[19] We find that the ZBCP is robust against the average. However, the subgap resonant behavior is very sensitive to the incident direction because the resonant condition is difficult to satisfy for the different absolute magnitude of the effective energy gaps experienced by electrons and holes.

Finally we would like to point out that since the pair potential in the superconductor is taken as a step function, the proximity effect is neglected. The self-consistent calculations have shown[28–30] that the order parameter is suppressed near the low transparent interface for some crystalline orientation of the d-wave superconductor. At low temperatures, the suppression region is at a distance ξ_0 from the interface. Based on the quasiclassical analysis,[28,29] it was found that in addition to the zero-energy bound state as a consequence of the sign change of the order parameter, a nonzero-energy bound state can also exist for some special incident momentum and crystalline orientation, due to the depletion of the order parameter. However, the results from an extended Hubbard model did not find this feature.[30] In our case with $\alpha=\theta=\pi/4$, if we assume that the order parameter is suppressed to zero with the region L from the interface, the existence of at least one nonzero-energy bound state should satisfy the condition $\pi\xi_0/2L \geqslant \sqrt{2}$.[4] Since $L\approx\xi_0$, the nonzero-energy bound state may not exist in our case. Therefore, as done in many other works (e.g., Refs. 2–4), it is a reasonable approximation to use the step function for the order parameter. However, to give a more rigorous and systematic study, a self-consistent calculation is still useful, which goes beyond the present work.

In conclusion, we have found that the subgap conductance behavior of a ferromagnet–d-wave-superconductor junction is qualitatively different from a nonmagnetic junction, due to the modification of AR by the exchange interaction in the ferromagnet, and can also be dramatically different from those of the ferromagnet–s-wave junction because of the sign change of the d-wave order parameter. For a ballistic FD junction, under appropriate conditions, a zero-bias conductance minimum could be achieved, which is lacking in a FS junction. In addition, a conductance maximum at finite bias could be evolved by interfacial scattering. For an NFD junction, conductance resonances are predicted because electron and hole wave vectors disperse greatly in the ferromagnet.

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