Effect of gap suppression on the *ab*-plane conductance spectrum of a normal-metal- $d_{a^2-b^2}$ -wave-superconductor junction

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We study the effect of gap suppression near the surface on the conductance spectra of normal metal- $\{100\}$ and $\{110\}$ d_{a^2} b^2 -wave superconductor junctions using the scattering method. We find that for $\{100\}$ junctions the positions of the maxima of the spectra are not always at the gap maximum of the bulk. The positions depend on the degree of the gap suppression at the interface. For $\{110\}$ junctions, we find that the width of zero-bias conductance peaks (ZBCPs) in the spectra depends on the magnitude of the gap function at the interface of the junction. The ZBCP is absent when the gap function is totally suppressed at the interface. We also find that the shape of the spectra depends on the slope of the order parameter at the interface.

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I. INTRODUCTION

The anisotropy and phase change of $d_{a^2-b^2}$ -wave symmetry can result in pair breaking and thus suppression of the order parameter near the surface. The degree of the suppression depends strongly on the surface orientation. Interpreting the results of the experiments that are sensitive to the surface properties must then be done in a very careful fashion. Tunneling spectroscopy is among these experiments. The conductance spectrum of a normal metal- $d_{a^2-h^2}$ -wave superconductor junction does not always resemble the bulk density of states of the superconductor, as it does for isotropic s-wave superconductors. Instead, it is proportional to the local density of states and, therefore, depends very strongly on the junction orientation. From the calculation in Refs. 2 and 3 for ab-plane junctions away from {100} interface orientations of a $d_{a^2-b^2}$ -wave superconductor, the conductance spectra should contain zero-bias conductance peaks (ZBCPs), which indicate the formation of zero-energy surface-bound states. These bound states result from the scattering of quasiparticles at an interface to a new state with an order parameter of opposite sign, as it is a signature of the $d_{a^2-b^2}$ -wave order parameter.^{4,5} ZBCPs have been observed in many tunneling experiments of high-temperature superconductors. 6-18 However, in some ab-plane tunneling experiments ZBCPs do not always show up (see, for example, Refs. 19-23).

In all the surfaces away from $\{100\}$ surfaces of $d_{a^2-b^2}$ -wave superconductors, the outgoing and incoming quasiparticles experience the order parameter of opposite signs. Assuming no distortion of the order parameter, the existence of zero energy surface bound states is therefore predicted to occur in such surfaces.⁵ However, the assumption that the order parameter is not distorted is not always right. Even for smooth surfaces the $d_{a^2-b^2}$ -wave order parameter can be suppressed due to pair breaking.¹ The degree of suppression depends on the surface orientation, i.e., at $\{110\}$ surfaces the suppression is complete, but there is no suppression at $\{100\}$ surfaces.¹ Surface roughness is predicted to also play a role in the suppression of the order parameter. It causes some suppression in $\{100\}$ surfaces and destroys the total suppression in $\{110\}$ surfaces.²⁴⁻²⁸

In this paper, we investigate the effect of the suppression of the order parameter on the tunneling spectra of $d_{a^2-h^2}$ -wave superconductors using the Blonder-Tinkham-Klapwijk formalism,²⁹ in which one finds the tunneling conductance from the quasiparticle transmission coefficients at the interface. We find that the degree of the suppression affects the position of maxima of the conductance spectra of junctions with {100} interface. Because the conductance spectra of {100} junctions are normally interpreted to be the density of states of the bulk, this would affect the determination of the measured gap maximum. We find that the maximum of the spectra appear at voltage corresponding to the value of the magnitude of the order parameter at the interface. Therefore with any suppression at all, the maxima will appear at an energy smaller than the maximum value of the parameter in the bulk. This result is similar to that from the studies done on the dependence of the surface density of states and/or conductance on surface roughness. 25,27,28 For {110} junctions, we find that the width of ZBCP depends on the magnitude of the order parameter at the interface. If the order parameter is completely suppressed, then the conductance spectra do not contain ZBCPs. This result is different from that found in the previous studies, 1,25,27,28 which obtain the differential conductance from the local density of states.

In Sec. II, we briefly describe the model used to represent the junction and method used to calculate tunneling conductance. We then present our results and discussion on {100} and {110} junctions in Sec. III. In Sec. IV, we summarize and comment on possible implications for the interpretation of tunneling experiments.

II. MODEL AND METHOD

We represent our normal metal-superconductor junction with an infinite system, half of which is a normal metal and the other half is a superconductor (see Fig. 1). The junction insulating barrier is represented by a delta function potential with strength H. In our treatment, we ignore the effect of the real Fermi surface. We assume our system is quasi-two-dimensional and use the continuous model to obtain the Fermi surface. The real Fermi surface would provide extra

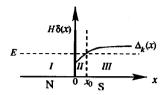


FIG. 1. The normal metal-superconductor junction is represented by an infinite system as shown in this picture. The normal metal fills the x < 0 region, and the superconductor fills the x > 0 region. The insulator layer is represented by a delta function of height H in units of energy per length. The gap function is taken to be zero in the normal metal and to be $\Delta_k(x)$ dependent of x in the superconductor. At energy E, one can divide the system into three regions: I, II, and III.

detailed features in the conductance spectrum.³⁰ Here we concentrate our attention on the ZBCP and the peak which usually occurs at the maximum gap. We do not numerically solve for the spatial dependence of the order parameter (this has been done in other references^{25,27,31,32}), but instead use a phenomenological form to describe it. We allow it to vary in space as

$$\Delta_k(x) = \Delta_{\text{max}}^0 \cos 2(\theta_k - \alpha) + (\Delta_{\text{max}}^b - \Delta_{\text{max}}^0) \cos 2(\theta_k - \alpha) \tanh\left(\frac{x}{\xi_l}\right), \quad (1)$$

where Δ^b_{max} is the maximum magnitude of the order parameter in the bulk, Δ^0_{max} is the maximum magnitude of the order parameter at the interface, θ_k is the angle between the wave vector k and the interface normal vector, α is the angle between the a axis of the superconductor and the interface normal vector, and ξ_l is a length scale characterizing the order parameter suppression. We choose to model the spatial dependence of the order parameter as $tanh(x/\xi_l)$ for simplicity, but we note that this form is qualitatively similar to the result obtained from self-consistent calculations. 25,27 It should also be noted that we do not include any additional component, which may be present when the order parameter is suppressed.²⁶ The additional components are expected to shift the position of the nodes. How far the nodes are moved away from [110] directions depends on how big these components are compared to the dominant d-wave component. In our study, we assume that these components are small enough that the amount, by which the nodes are shifted away from the [110] direction, is small compared to the Fermi wave vector. We, therefore, ignore these components and focus on the effect of the suppression of the order parameter.

The Bogoliubov-de Gennes equations that describe the excitations of the system are

$$\begin{bmatrix} \hat{O}_p + H\delta(x) - \mu & \Delta_k \Theta(x) \\ \Delta_k \Theta(x) & -\hat{O}_p - H\delta(x) + \mu \end{bmatrix} U(\vec{r}) = EU(\vec{r}),$$
(2)

where μ is the chemical potential, $\Theta(x)$ is the Heaviside step function,

$$\hat{O}_p = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right),$$

m is the quasiparticle mass, which we assume to be the same in both metal and superconductor, and $U(\vec{r})$ is a two-component function, which in our case can be written as

$$U(\vec{r}) = \begin{bmatrix} u(\vec{r}) \\ v(\vec{r}) \end{bmatrix} = \begin{bmatrix} u_k(x) \\ v_k(x) \end{bmatrix} e^{i\vec{k}\cdot\vec{r}}.$$
 (3)

The dependence of the amplitudes u_k and v_k on x is due to the fact that the order parameter is x dependent.

After substituting $U(\vec{r})$ from Eq. (3) into Eq. (2) and referring to \vec{k} as \vec{q} in the normal metal, we obtain the bulk excitation energies for the normal metal as

$$E(\vec{q}) = \pm \, \xi_q = \pm \left[\frac{\hbar^2}{2m} (q_x^2 + q_y^2) - \mu \right],\tag{4}$$

where the plus and minus signs are for electron and hole excitations, respectively. As for the superconductor, as long as u(x) and v(x) vary slowly enough with position, i.e., as long as $(k_F\xi_I)^{-1}$ is much smaller than $|\Delta_k|/E_F$ in our case, we obtain the excitation energies as (to the first-order approximation)

$$E(\vec{k}) = \sqrt{\xi_k^2(x) + \Delta_k^2(x)},\tag{5}$$

where

$$\xi_k(x) = \frac{\hbar^2}{2m} [k_x^2(x) + k_y^2] - \mu.$$
 (6)

Figure 2 shows a plot of the excitation energy of the normal metal (superconductor) as a function of $q_x(k_x)$, the component along the interface normal, at a particular $q_y = k_y$, the component perpendicular to the interface normal. The amplitudes of the excitations, u_k and v_k , of the normal metal are

$$\begin{bmatrix} u_k \\ v_k \end{bmatrix} = \begin{cases} \begin{bmatrix} 1 \\ 0 \end{bmatrix} & \text{for electrons} \\ \begin{bmatrix} 0 \\ 1 \end{bmatrix} & \text{for holes,} \end{cases}$$
 (7)

whereas those of the superconductor, which are, in this case, treated to be position dependent, are

$$\begin{bmatrix} u_k(x) \\ v_k(x) \end{bmatrix} = \frac{1}{\sqrt{|E + \xi_k(x)|^2 + |\Delta_k(x)|^2}} \begin{bmatrix} E + \xi_k(x) \\ \Delta_k(x) \end{bmatrix}.$$
(8)

The wave function in each region is a linear combination of all the appropriate excitations of the same energy and the same momentum of the same component parallel to the surface as follows:

$$U_{I}(\vec{r}) = \left(\begin{bmatrix} 1\\0 \end{bmatrix} e^{iq^{+}x} + a \begin{bmatrix} 0\\1 \end{bmatrix} e^{iq^{-}x} + b \begin{bmatrix} 1\\0 \end{bmatrix} e^{-iq^{+}x} \right) e^{ik_{y}y}, \quad (9)$$

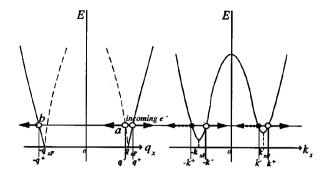


FIG. 2. The plots of two excitation energies as a function of q_x or k_x , the component parallel to the interface normal, at a particular value of $k_{\parallel}=k_y$. The plot on the left is for the excitation energy of the normal metal, and the plot on the right is for the excitation energy of the superconductor. At the same energy, there are four propagating excitations in the superconductor. The wave function of the normal metal is a linear combination of only three excitations represented by the open circles. The wave function in region II of the superconductor is the sum of all four excitations, whereas the wave function in region III is the sum of two outgoing excitations also represented by the open circles. When E is less than the gap, the wave function of the superconductor in each region still takes the same form, only then do all the propagating excitations become decaying excitations, which are not indicated by the arrows in the figure.

$$U_{II}(\vec{r}) = \left(c_{1}^{II}\begin{bmatrix}u_{k^{+}}(x)\\v_{k^{+}}(x)\end{bmatrix}e^{ik^{+}x} + d_{1}^{II}\begin{bmatrix}u_{-k^{-}}(x)\\v_{-k^{-}}(x)\end{bmatrix}e^{-ik^{-}x} + c_{2}^{II}\begin{bmatrix}u_{-k^{+}}(x)\\v_{-k^{+}}(x)\end{bmatrix}e^{-ik^{+}x} + d_{2}^{II}\begin{bmatrix}u_{k^{-}}(x)\\v_{k^{-}}(x)\end{bmatrix}e^{ik^{-}x}\right)e^{ik_{y}y},$$
(10)

$$U_{III}(\vec{r}) = \left(c^{III} \begin{bmatrix} u_{k^{+}}(x) \\ v_{k^{+}}(x) \end{bmatrix} e^{ik^{+}x} + d^{III} \begin{bmatrix} u_{-k^{-}}(x) \\ v_{-k^{-}}(x) \end{bmatrix} e^{-ik^{-}x} \right) e^{ik_{\mu}y},$$
(11)

where q^{\pm} and k^{\pm} (see Fig. 2) satisfy

$$\hbar q^{\pm} = \sqrt{2m(\mu \pm E) - \hbar^2 k_y^2} \tag{12}$$

$$\hbar k^{\pm}(x) = \sqrt{2m(\mu \pm \sqrt{E^2 - \Delta_k^2(x)}) - \hbar^2 k_y^2}$$
 (13)

and a, b, c, and d are appropriate reflection and transmission amplitudes for each region. Note that k^{\pm} are complex when $E < |\Delta_k(x)|$.

Normally the range of the energy E and the energy gap relevant to the tunneling experiments is of order meV, whereas the Fermi energy is of order eV. Therefore, they have little effect on the wave vectors, and we use the following approximations for q^{\pm} and k^{\pm} throughout the calculation:

$$q^+ = q^- = q_{F,x} = q_F \cos \theta_{k,N},$$
 (14)

$$k^{+} = k^{-} = k_{F,x} = k_{F} \cos \theta_{k,S},$$
 (15)

where $q_{F,x}$, $k_{F,x}$ are the magnitudes of the Fermi wave vectors of the normal metal and the superconductor along x axis respectively and θ is the angle between the wave vector and x axis (we assume cylindrical Fermi surface). Using the conservation of the momentum parallel to the surface, we have the following relationship between the two angles:

$$q_{F,v} = q_F \sin \theta_{k,N} = k_{F,v} = k_F \sin \theta_{k,S}. \tag{16}$$

In order to obtain the current across the junction, we need to determine only the Andreev and normal reflection probabilities A(E) and B(E), which are related to the amplitudes a and b through $A=|a|^2(q^-/q^+)$ and $B=|b|^2$. To get a and b, we use the following matching conditions:

$$U_I(x=0) = U_{II}(x=0) \equiv U_0,$$
 (17)

$$2k_F Z U_0 = \left. \frac{\partial U_{II}}{\partial x} \right|_{x=0^+} - \left. \frac{\partial U_{I}}{\partial x} \right|_{x=0^-}, \tag{18}$$

$$U_{II}(x=x_0) = U_{III}(x=x_0),$$
 (19)

$$\frac{\partial U_{III}}{\partial x}\bigg|_{x=x_0} = \frac{\partial U_{II}}{\partial x}\bigg|_{x=x_0},\tag{20}$$

where $Z=mH/(\hbar^2k_F)$ is the parameter that specifies the insulating barrier strength, and the position specifying the boundary of region II and II, x_0 , is

$$x_0 = \xi_l \cdot \left[\frac{E - \Delta_{max}^0 \cos 2(\theta_k - \alpha)}{\Delta_{max}^b - \Delta_{max}^0 \cos 2(\theta_k - \alpha)} \right]$$

for $E \ll \Delta_{max}^b$ (see Fig. 1).

We find the current across the junction as a function of an applied voltage is

$$I_{NS}(V) = \frac{e}{(2\pi)^2} \int d\vec{q} v_{q_x} [1 + A(\vec{q}) - B(\vec{q})]$$

$$\times [f(E_q - eV) - f(E_q)],$$
(21)

where v_{q_x} is the x component of the group velocity of the incoming electron and f(E) is the Fermi-Dirac distribution function. The conductance at zero temperature is, thus,

$$G_{NS}(V) = \frac{dI_{NS}}{dV} = \left\langle \frac{e^2}{h} [1 + A(V, \theta_N) - B(V, \theta_N)] \right\rangle_{k_y}, \quad (22)$$

where the angular bracket refers to the average over k_y . We define our normalized conductance to be

$$G(V) = \frac{G_{NS}(V)}{G_{NS}(\infty)}.$$
 (23)

Because the inequality of the two Fermi vectors has the same effect as increasing the junction barrier, in our calculation we take $q_F = k_F$ for simplicity.

Note that for {100} case, surface roughness causes the suppression of the order parameter, whereas for {110} surfaces, where the suppression is already present even when

they are smooth, roughness alleviates the suppression. We adjust the value of Δ^b_{max} and Δ^0_{max} accordingly. Also, we neglect any possible change due to surface roughness in the component of quasiparticle momentum that is parallel to the interface, i.e., we work in the specular limit. This limit should be valid as long as the characteristic length scale of the surface roughness is much longer than k_F^{-1} .

III. RESULTS AND DISCUSSION

In this section, we present and discuss the results for $\{100\}$ (α =0) and $\{110\}$ (α =45°) orientations. The conductance spectra of junctions for other values of α contain peaks at zero energy and at energies corresponding to the magnitude of the order parameter in the direction parallel to the normal vector of the interface. The effect of gap suppression on the former peaks is similar to that on $\{110\}$ spectra, while the effect on the latter peaks is similar to that on $\{100\}$ spectra. For these reasons, we restrict ourselves to α =0 and α =45°, which together contain all the qualitative behaviors.

A. {100} junctions

According to theoretical results found in Ref. 1 for smooth $\{100\}$ surfaces, $d_{a^2-b^2}$ -wave order parameters are not suppressed near such interfaces. However, suppression does occur near rough $\{100\}$ surfaces. The rougher the surface, the greater the suppression of the order parameter. 24,25,27,33 Figures 3 and 4 display the effect of the suppression on the tunneling conductance spectrum.

Figures 3(a)–3(c) show the plots of the normalized conductance as a function of applied voltage for different junction transparencies Z and different degrees of the suppression $\Delta^0_{max}/\Delta^b_{max}$. In a very transparent junction [Fig. 3(a), where Z=0] the spectrum contains the inverted gap structure of a d-wave superconductor. This peaklike feature is caused by high Andreev reflection probability. As expected in the case where the junction is less transparent and where there is no suppression at all (i.e., $\Delta^0_{max}/\Delta^b_{max}=1$), there is a peak present at voltage corresponding to the maximum value of the order parameter in the bulk. However, in the case where some suppression is present, this feature occurs at voltage corresponding to the value of the order parameter at the interface instead.

In addition to its dependence on the value of the order parameter at the interface, the conductance spectrum depends on the slope of the order parameter at the interface as well. The slope at the surface in this model is proportional to ξ_l^{-1} [see Eq. (1)]. For the junction with $\Delta_{max}^0 \neq 0$, the shape of the spectrum changes with the value of ξ_l as shown in Fig. 4(a); however, the position of the maximum is solely determined by the value of the order parameter at the surface. In the case of total suppression ($\Delta_{max}^0 = 0$), the position of the maximum varies with the slope, as shown in Fig. 4(b). The steeper the slope, the further away from zero voltage the maximum is. Note that for high-temperature superconductors, where $|\Delta_k|/E_F$ is of order 0.1, the case where $k_F\xi_l=1$ is not valid in our model, which requires $(k_F\xi_l)^{-1} \ll |\Delta_k|/E_F$. We include this

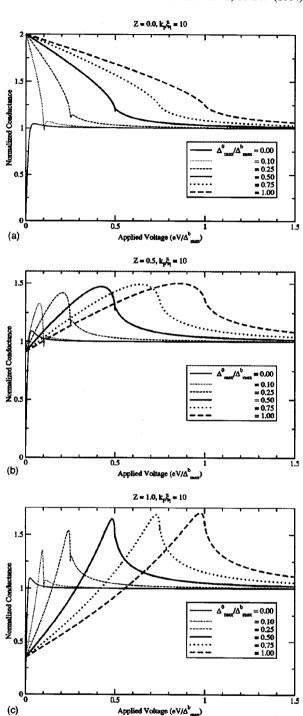


FIG. 3. Normalized conductance spectra of $\{100\}$ junction with different junction transparencies and degrees of suppression of the order parameter. The values of the parameter Z are 0.0, 0.5, and 1.0 in (a), (b), and (c) respectively. $\xi_l=10/k_F$ for all cases. In each graph are the plots of the conductance versus applied voltage for different degrees of the suppression of the order parameter.

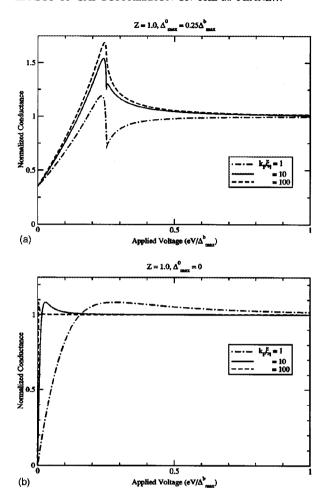


FIG. 4. Normalized conductance spectra of $\{100\}$ junctions with different degrees of the suppression and ξ_l (the range, over which the order parameter is recovered to its bulk value). The values of the suppression $\Delta_{max}^0/\Delta_{max}^b$ are 0.25 and 0.00 in (a) and (b), respectively. The junction transparency for all cases is Z=1.0. In each graph are the plots of the conductance versus applied voltage for different ξ_l .

case for reference to give some idea of the limiting behavior of our model.

These results indicate that the {100} tunneling spectrum is sensitive to the properties of the order parameter at the interface instead of in the bulk. In particular, the shape of the spectrum depends on both the slope and the value of the order parameter at the interface. The magnitude of the order parameter detected by this technique should then be considered with caution. If the order parameter is suppressed to some degree (which occurs when the surface is not smooth), the position of the maximum will provide the magnitude of the order parameter at the interface, which is smaller than what it should be in the bulk. Only in some special circumstances in which the value of the order parameter may be higher at the surface than in the bulk, ³¹ will the value of the order parameter obtained from the tunneling experiment be higher than that in the bulk.

B. {110} junctions

For $\{110\}$ junctions of a $d_{a^2-b^2}$ -wave superconductor, the order parameter suffers a total suppression at smooth surfaces. The degree of the suppression is decreased when the surfaces are rougher. ^{24,25,27,33} The suppression affects the zero-bias conductance peak in the conductance spectrum.

Figure 5 shows the conductance spectra of {110} junctions with different degrees of suppression and junction transparencies. Like in {100} junctions, when the order parameter is totally suppressed, the conductance spectrum does not contain a peak at zero voltage no matter how transparent the junction is. When the order parameter is partially suppressed, which would be the case for any {110} junctions with some roughness, the conductance spectrum in the tunneling limit contains a zero-bias conductance peak. The height of the peak does not depend on the degree of the suppression of the order parameter, whereas its width does.

Also as in $\{100\}$ junctions, the conductance spectra with total suppression as shown in Fig. 6(a) depends on the slope of the order parameter at the surface ξ_I^{-1} . On the contrary, for junctions with partial suppression the conductance spectra are not strongly dependent on the value of ξ_I . In this case, the height and width of zero-bias conductance peak remain the same, as shown in Fig. 6(b). As in $\{100\}$ case, we include the case where $k_F\xi_I=1$ for reference to show the limiting behavior of our model.

The absence of a zero-bias conductance peak in the conductance spectrum of $\{110\}$ junction implies there are no zero-energy bound sates. This result can be seen by considering the condition for which the zero-energy surface bound states in superconductors occur. It is that, at the surface, the order parameter of the quasiparticle with positive $v_k = \partial E/\partial k_x$ has opposite sign to that of the quasiparticle with negative v_k .^{4,5} In the case where the order parameter is totally suppressed, this condition is not satisfied.

These findings indicate that tunneling spectroscopy is very sensitive to the surface properties. Where the features occur in the conductance spectrum not only depends very much on the junction orientation, but also the value of the order parameter at the interface, not in the bulk. This means the information we extract from the tunneling data must be carefully interpreted.

IV. CONCLUSIONS

We have examined the effect of the suppression of the order parameter on the ab plane tunneling conductance spectra of a normal metal- $d_{a^2-b^2}$ -wave superconductor junction. We find the conductance spectrum depends strongly on the properties of the order parameter at the surface; that is, the position and shape of the main features in the conductance spectrum depend on both the slope and value of the order parameter at the surface. In particular, the maximum of the conductance spectrum of $\{100\}$ junctions occurs at the voltage corresponding to the value of the order parameter at the surface. The slope of the order parameter only affects the shape, but not the position of the maximum of the spectrum in the case where the suppression is not complete. The slope affects the position of the maximum more when the order

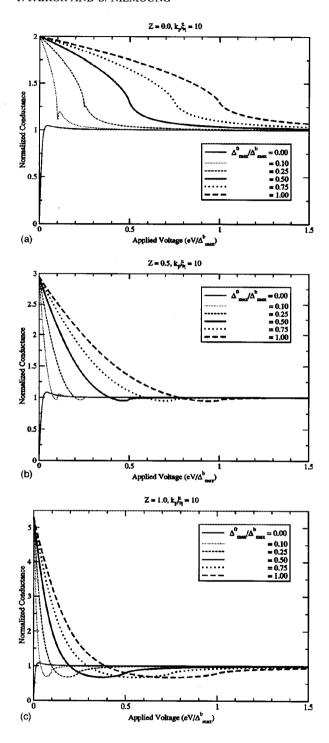


FIG. 5. Normalized conductance spectra of $\{110\}$ junctions with different junctions transparencies and degrees of suppression of the order parameter. The values of the parameter Z are 0.0, 0.5, and 1.0 in (a), (b), and (c), respectively. $\xi_I = 10/k_F$ for all cases. In each graph are the plots of the conductance versus applied voltage for different degrees of the suppression of the order parameter.

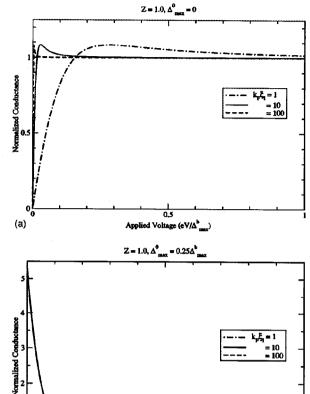


FIG. 6. Normalized conductance spectra of $\{110\}$ junctions with different degrees of the suppression and ξ_l (the range, over which the order parameter is recovered to its bulk value). The values of the suppression $\Delta^0_{max}/\Delta^b_{max}$ are 0.00 and 0.25 in (a) and (b), respectively. The junction transparency for all cases is Z=1.0. In each graph are the plots of the conductance versus applied voltage for different ξ_l .

0.5

Applied Voltage (eV/Δ^b_{max})

parameter is totally suppressed. However, in real {100} surfaces the total suppression is unlikely to occur because even though roughness suppresses the order parameter, the suppression reaches its maximal limit around 40% of the bulk value. 25,27

For the {110} junctions, we find that the width of ZBCP depends on the value of the order parameter at the surface. If the order parameter is totally suppressed at the surface, ZBCP will be absent. Like {100} junctions, the slope of the order parameter at the surface affects the spectrum more when the total suppression occurs. However, unlike {100} junctions, the complete suppression is likely to occur when the junction is relatively smooth enough for specular reflection to dominate.

In experiments, whether or not the suppression will play a role depends on two length scales: ξ_l , which is related to the slope of the suppressed order parameter at the surface

(b)

(and in our model is also the distance over which the order parameter recovers to its bulk value) and the depth of the sample to which the tunneling experiments probe. Our results apply to the case in which the former length exceeds the latter, and the effect of the order parameter suppression will be important.

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