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Andreev reflection and geometrical resonance effects for a gradual variation of the pair potential near the normal-metal–superconductor interface

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The probability of Andreev reflection is calculated as a function of the energy for quasiparticles that are incident on a normal-metal–superconductor (*N-S*) interface with a gradual variation of the pair potential. These calculations are an extension of the work of Blonder, Tinkham, and Klapwijk [Phys. Rev. B **25**, 4515 (1982)], who assumed a step function for the position dependence of the pair potential. We integrate the Bogoliubov equations numerically in the region in which the pair potential varies with position and apply boundary conditions to find the quantities of interest. This approach is also used to calculate the geometrical resonances in the transmission of a tunnel junction on an *N-S* bilayer. For a steplike variation of the pair potential, the same expression for the transmission is found as with the usual density-of-states approach. Also results are given for a gradual variation of the pair potential at the interface. Both the probability of Andreev reflection and the geometrical resonance effects begin to change if the region in which the pair potential varies with position becomes of the order of the coherence length of the superconductor.

I. INTRODUCTION

In the BCS ground state of a superconductor, electrons with opposite momentum and spin are condensed in Cooper pairs. This is due to an attractive phonon-mediated electron-electron interaction that is larger than the repulsive Coulomb interaction. Below a specific threshold energy, no excited states exist. The quasiparticle states above that threshold are mixtures of electron and hole wave functions. The coupling of these wave functions is described in the Bogoliubov equations via a pair potential Δ. In a normal metal, the pair potential is zero, and there is no energy gap in the excitation spectrum. If an electron in a normal metal is incident on an interface with a superconductor (*N-S* interface), the change in the pair potential causes total or partial Andreev reflection.[1] The electron is then reflected as a hole while a Cooper pair is injected into the superconductor. If the *N-S* interface is not perfect, the electron may also be ordinarily reflected and, if its energy is larger than the energy gap of the superconductor, it may be transmitted as an excitation as well. Blonder, Tinkham, and Klapwijk[2] (BTK) showed that the Bogoliubov equations are very suitable to describe the reflection and transmission of quasiparticles at an *N-S* interface. They assumed that, at the *N-S* interface, Δ increases instantaneously from zero in *N* to a constant value in *S*. Then the solutions of the Bogoliubov equations in *N* and in *S* are simple; the probabilities of reflection and transmission are found by matching the two solutions at the *N-S* interface. Ordinary scattering of quasiparticles at the interface is taken into account via appropriate boundary conditions. The assumption of a step-function for $\Delta(x)$ is valid for the small-area *N-S* junctions in which BTK were primarily interested. In other geometries, for instance, a point contact on an *N-S* bilayer, the Andreev-reflection process induces a correlation between electron and hole states near the interface in *N*. Unless the effective electron-electron interaction in *N* is zero, this means that there is a finite pair potential in *N* (proximity effect[3]). On the other hand, the *N* metal causes a depression of the pair potential in *S* that decays away from the interface.

In this paper, we extend the calculations of BTK to study the effect of a gradual variation of the pair potential near the *N-S* interface on the reflection and transmission coefficients of quasiparticles. Although in principle the position dependence of Δ should be calculated self-consistently,[3,4] we limit ourselves to an assumed $\Delta(x)$ (see Fig. 1). In the region in which $\Delta(x)$ is not constant, the Bogoliubov equations are solved numerically. At the *N-S* interface, a δ-function potential is assumed to represent the scattering of quasiparticles, and we allow a discontinuity of $\Delta(x)$. Like in the calculation of BTK, the δ-function potential is dealt with by means of boundary conditions. At the starting point and at the end point of the integration, the solution is matched to the solutions for zero Δ and for constant Δ in *N* and *S*, respectively. From the coefficients of the latter solutions, the probabilities of reflection and transmission are deduced. The method is described in Sec. II, while in Sec. III results for different choices of $\Delta(x)$ are discussed and compared to the BTK results.

Andreev reflection plays a crucial role in the origin of the geometrical resonance effects that are observed in the

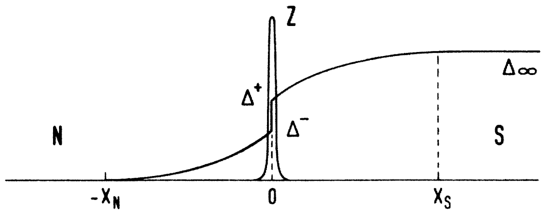

FIG. 1. Position dependence of the pair potential Δ that is assumed in the calculation of the probabilities of reflection and transmission. The parameter Z indicates the scattering potential at the N-S interface.

differential conductance of tunnel junctions on N-S bilayers (for a review, see Ref. 5). The geometry is shown in Fig. 2; the tunnel junction is represented by the δ-function potential at $x=-x_T$. An electron at the tunnel junction in N that moves toward the N-S interface returns to the tunnel junction as a hole. After ordinary reflection at the tunnel barrier and a second Andreev-reflection process, it again returns to the tunnel junction but now as an electron. This electron wave function interferes with the original electron wave function. Depending on the energy of the quasiparticle, the interference will be constructive or destructive, which leads to maxima and minima in the differential conductance versus voltage of the tunnel junction. Usually, the differential conductance is interpreted as reflecting the density of states of excitations in N. Then, the density of states in a thin N slab with on one side an N-S interface and on the other side a perfectly reflecting boundary is calculated by solving the Bogoliubov equations using Green's functions techniques.[5,6] Recently, the calculations have been extended[4] using quasiclassical Green's functions to thick N layers in which the position dependence of the pair potential is no longer steplike. However, BTK have shown that their approach of matching solutions of the Bogoliubov equations can be applied to calculate the differential conductance of an N-S tunnel junction. The transmission of a tunnel junction on an N-S bilayer can be analyzed the same way. If a step function is chosen for $\Delta(x)$, we show that the results of the density-of-states approach and the BTK approach are identical. In Sec. IV, results for different choices of $\Delta(x)$ are given and compared to the result for a step function. The results are similar to those of the density-of-states calculations with a self-consistent $\Delta(x)$.[4]

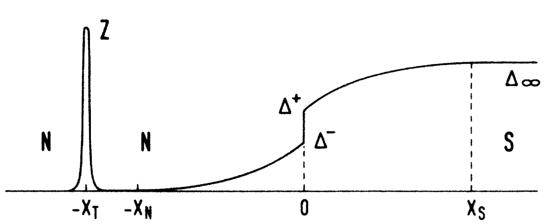

FIG. 2. Position dependence of the pair potential Δ that is assumed in the calculation of the geometrical resonance effects. The parameter Z indicates the tunnel junction.

At an N-S interface, the Cooper pairs of the superconductor leak into the normal metal, so the pair amplitude changes gradually. The pair potential is given by the product of the pair amplitude and the BCS potential that describes the effective electron-electron interaction.[3] If the interaction is repulsive in N, the sign of the pair potential in N is opposite to that in S. As an interesting sidestep, we discuss in Sec. V the influence of $\Delta(x)<0$ in N on the probability of Andreev reflection and on the geometrical resonance effects. In Sec. VI, the conclusions are given.

II. BOGOLIUBOV EQUATIONS

Because in the ground state electrons with opposite momentum and spin are coupled, the elementary excitations of a superconductor are not just single-electron wave functions. An excitation with wave vector k is built up from the creation of an electron with wave vector k and the annihilation of an electron with wave vector $-k$.[7] The latter process can also be interpreted as the creation of a hole excitation with wave vector k. In the Bogoliubov-equation formalism, the excitations are represented by a two-element column vector ψ (we will follow the notation of BTK as much as possible):

$$\psi(x,t)=\begin{bmatrix} f(x,t) \\ g(x,t) \end{bmatrix} .$$

The functions $f(x,t)$ and $g(x,t)$ obey the Bogoliubov equations:

$$i\hbar\frac{\partial f}{\partial t}=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-\mu(x)+V(x)\right]f(x,t)+\Delta(x)g(x,t)\ , \tag{1a}$$

$$i\hbar\frac{\partial g}{\partial t}=-\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-\mu(x)+V(x)\right]g(x,t)+\Delta(x)f(x,t) \tag{1b}$$

in which $\mu(x)$, $\Delta(x)$, and $V(x)$ are the electrochemical potential, the pair potential, and the ordinary potential, respectively. In the normal metal far from the N-S interface $[\Delta(x)=0]$, Eq. (1a) reduces to the Schrödinger equation for electrons. Then Eq. (1b) is the time-reversed Schrödinger equation, which may be interpreted as describing a hole excitation. We have assumed that the potentials vary only in the x direction, the direction normal to the N-S interface. Then the y- and z-dependent parts of the wave function are plane waves and can be disregarded; with k, the x component of the wave vector is meant.

The Bogoliubov equations can be simplified by noting the different length scales in it. Except for a step at the N-S interface, $\mu(x)$ is assumed to be constant. For $V(x)$, a δ function is taken to represent the scattering of quasiparticles at the N-S interface. The effects of the discontinuity of $\mu(x)$ and of the δ-function potential can be combined in a δ-function potential with an effective height.[8] It is accounted for in the boundary conditions of the solutions in N and in S and can therefore be omitted from the differential equation. The wave function oscillates on a scale k_F^{-1}, the inverse Fermi wave vector. As $\Delta(x)$ is much smaller than $\mu(x)=\hbar^2 k_F^2/2m$, the effects of superconductivity on the wave function are limited to small deviations of the wave vector from k_F. For an excitation with energy E, it is therefore convenient to take trial solutions

$$f=\tilde{u}(x)\exp(ik_F x-iEt/\hbar)$$

and

$$g=\tilde{v}(x)\exp(ik_F x-iEt/\hbar)\ ,$$

in which the functions $\tilde{u}(x)$ and $\tilde{v}(x)$ are assumed to vary only on a scale that is much larger than k_F^{-1}. Neglecting higher-order terms, the Bogoliubov equations can be written as:

$$\begin{aligned}\frac{\partial\tilde{u}}{\partial x}&=i(\pi\xi_0\Delta_\infty)^{-1}[E\tilde{u}-\Delta(x)\tilde{v}]\ ,\\ \frac{\partial\tilde{v}}{\partial x}&=-i(\pi\xi_0\Delta_\infty)^{-1}[E\tilde{v}-\Delta(x)\tilde{u}]\ .\end{aligned} \tag{2}$$

The functions $\tilde{u}(x)$ and $\tilde{v}(x)$ vary on the scale of the BCS coherence length

$$\xi_0=\hbar v_F/(\pi\Delta_\infty)=\hbar^2 k_F/(\pi m\Delta_\infty)\ ,$$

which is indeed much larger than k_F^{-1} (Δ_∞ is the value of the pair potential in S far from the interface). If for an excitation with negative wave vector the trial functions

$$f=\tilde{v}(x)\exp(-ik_F x-iEt/\hbar)$$

and

$$g=\tilde{u}(x)\exp(-ik_F x-iEt/\hbar)$$

are chosen, the same equations for $\tilde{u}(x)$ and $\tilde{v}(x)$ are obtained. Thus the general form of the wave function in the region in which $\Delta(x)$ varies with position is

$$\psi=\begin{bmatrix}\tilde{u}_a(x)\\ \tilde{v}_a(x)\end{bmatrix}e^{ik_F x}+\begin{bmatrix}\tilde{v}_b(x)\\ \tilde{u}_b(x)\end{bmatrix}e^{-ik_F x}$$

in which the two sets of functions $(\tilde{u}_{a,b}(x),\tilde{v}_{a,b}(x))$ are solutions of Eq. (2). If $\Delta(x)=\Delta_\infty$ is constant, the solution of Eq. (2) is

$$\begin{bmatrix}\tilde{u}(x)\\ \tilde{v}(x)\end{bmatrix}=\begin{bmatrix}[E\pm(E^2-\Delta_\infty^2)^{1/2}]^{1/2}\\ [E\mp(E^2-\Delta_\infty^2)^{1/2}]^{1/2}\end{bmatrix}e^{\pm i\kappa_S x}$$

with $\kappa_S=(E^2-\Delta_\infty^2)^{1/2}(\pi\xi_0\Delta_\infty)^{-1}$. For later use, we define $\kappa_N=E(\pi\xi_0\Delta_\infty)^{-1}$. The solution is valid for all energies $E>0$ and is not limited to $E>\Delta_\infty$. If the usual BCS coherence factors

$$u_0^2=1-v_0^2=\frac{1}{2}\left[1+\frac{(E^2-\Delta_\infty^2)^{1/2}}{E}\right]$$

are defined also for all $E>0$, the general solution of the Bogoliubov equations for constant $\Delta(x)=\Delta_\infty$ is

$$\begin{aligned}\psi=\alpha\begin{bmatrix}u_0\\ v_0\end{bmatrix}e^{i(k_F+\kappa_S)x}+\beta\begin{bmatrix}v_0\\ u_0\end{bmatrix}e^{-i(k_F-\kappa_S)x}\\ +\gamma\begin{bmatrix}u_0\\ v_0\end{bmatrix}e^{-i(k_F+\kappa_S)x}+\delta\begin{bmatrix}v_0\\ u_0\end{bmatrix}e^{i(k_F-\kappa_S)x}\ .\end{aligned} \tag{3}$$

This is, up to first order in $(k_F\xi_0)^{-1}$, the wave function used by BTK. Far from the interface in N [$\Delta(x)=0$], the general solution is

$$\begin{aligned}\psi=\alpha\begin{bmatrix}1\\ 0\end{bmatrix}e^{i(k_F+\kappa_N)x}+\beta\begin{bmatrix}0\\ 1\end{bmatrix}e^{-i(k_F-\kappa_N)x}\\ +\gamma\begin{bmatrix}1\\ 0\end{bmatrix}e^{-i(k_F+\kappa_N)x}+\delta\begin{bmatrix}0\\ 1\end{bmatrix}e^{i(k_F-\kappa_N)x}\ .\end{aligned} \tag{4}$$

The four terms in Eq. (4) correspond to electrons ($|k|>k_F$) and holes ($|k|<k_F$) moving in positive (α,β) and negative (γ,δ) x direction, respectively.

Although Eq. (2) is a very convenient mathematical formulation of the Bogoliubov equations, it is a physically interesting sidestep to consider a different formulation. We take as a trial solution the wave function given in Eq. (3) but we temporarily define u_0, v_0, and κ_S in terms of the local value of $\Delta(x)$. If this trial solution with the proper time dependence is inserted in the Bogoliubov equations [Eq. (1)], equations for the position dependence of the coefficients α, β, γ, and δ are obtained. Neglecting terms of second order in $(k_F\xi_0)^{-1}$ and expressing u_0 and v_0 in terms of $\Delta(x)$, we find

$$\begin{aligned}\frac{\partial\alpha}{\partial x}&=\frac{\partial\Delta}{\partial x}\left[\frac{\alpha\Delta-\delta E e^{-2i\kappa' x}}{2(E^2-\Delta^2)}+\frac{i\alpha x\Delta}{\pi\xi_0\Delta_\infty(E^2-\Delta^2)^{1/2}}\right]\ ,\\ \frac{\partial\delta}{\partial x}&=\frac{\partial\Delta}{\partial x}\left[\frac{\delta\Delta-\alpha E e^{2i\kappa' x}}{2(E^2-\Delta^2)}-\frac{i\delta x\Delta}{\pi\xi_0\Delta_\infty(E^2-\Delta^2)^{1/2}}\right]\end{aligned} \tag{5}$$

with

$$\kappa'=[E^2-\Delta^2(x)]^{1/2}(\pi\xi_0\Delta_\infty)^{-1}\ .$$

The equations for β and γ are found by replacing α with β and δ with γ. Equation (5) clearly shows the Andreev-reflection process: If Δ varies with position, the coefficients α and δ influence each other. These are the coefficients of an electronlike quasiparticle moving in the positive x direction (α) and a holelike quasiparticle moving in the negative x direction (δ). The two coefficients β and γ also influence each other, but there is no coupling between the two sets of coefficients. Only the potential $V(x)$ gives rise to a coupling between the two sets that correspond to excitations with positive and negative wave vector, respectively. For numerical calculations, Eq. (5) is not very convenient because it contains a singularity at $\Delta(x)=E$. The singularity is limited to the coefficients and is due to the choice of the trial function. The wave function itself shows no singularity. This is confirmed by the fact that the formulation of the Bogoliubov equations in Eq. (2) shows no singularity.

We will analyze the probabilities of reflection and transmission of a quasiparticle incident on an N-S interface that has a geometry as given in Fig. 1. At the interface ($x=0$), the scattering potential $V(x)=Z(\pi\xi_0\Delta_\infty)\delta(x)$ is located, and there is a discontinuity in the pair potential $\Delta^+-\Delta^-$. The parameter Z describes the strength of ordinary scattering at the interface. It contains a contribution of a δ-function potential and a contribution due to the discontinuity of $\mu(x)$ (i.e., of the difference of k_{FN} and k_{FS}). For $x>x_S$ $[\Delta(x)=\Delta_\infty]$ and for $x<-x_N$ $[\Delta(x)=0]$, the solution of the Bogoliubov equations is given by Eqs. (3) and (4), respectively. Like BTK, we are interested in the situation with a single incoming electron wave in N, and we would like to calculate the coefficients of the outgoing reflected electron and hole waves in N and the coefficients of the outgoing transmitted electronlike and holelike waves in S. These coefficients are defined for $x<-x_N$ and $x>x_S$, respectively, and the corresponding wave functions have to be matched via a numerical solution of Eq. (2) in the region $-x_N<x<x_S$. This means, for instance, that there is no incoming hole wave at $x=-x_N$ in N and that there are no incoming waves at $x=x_S$ in S. These boundary conditions are not very suitable for a numerical solution because they apply at two different positions. Therefore we choose the initial values of the coefficients of the outgoing waves at $x=x_S$ and integrate back to $x=-x_N$. If this is done for two independent sets of initial values, the relevant coefficients can be deduced (details are given in the Appendix). The result is the probability currents $A(E)$, $B(E)$, $C(E)$, and $D(E)$ $(A+B+C+D=1)$ that correspond to a quasiparticle with energy E that is incident on the N-S interface. $A(E)$ and $B(E)$ are related to Andreev-reflection and ordinary reflection processes, respectively, while $C(E)$ and $D(E)$ denote transmission without and with change in character (electronlike or holelike) of the quasiparticle.

Geometrical resonances are calculated for the geometry of Fig. 2. The tunnel junction is represented by a (very high) δ-function potential at $x=-x_T$. For simplicity, the δ-function potential at the N-S interface is omitted. The quantity of interest is the transmission of electrical current T, which is given by[2] $T(E)=1-B(E)+A(E)$. This function can be calculated in a similar way as the probability currents for the N-S interface of Fig. 1. Only the boundary conditions have to be adapted because the geometry is different (details are given in the Appendix).

Negative values of $\Delta(x)$ in N can be directly inserted in Eq. (2). In fact, if $(\tilde{u}(x),\tilde{v}(x))$ is a solution of Eq. (2) with $\Delta(x)$, then $(\tilde{u}(x),-\tilde{v}(x))$ is the solution with $-\Delta(x)$. Often the phase of the wave function is not relevant but in the application of boundary conditions it will make a difference. It will therefore be interesting to calculate the probability of Andreev reflection and the geometrical resonance effects also for $\Delta(x)<0$ in N.

III. PROBABILITY OF ANDREEV REFLECTION

Independent of the exact form of $\Delta(x)$, some observations can be made about the values of the probabilities of reflection $A(E)$ and $B(E)$ and of transmission $C(E)$ and $D(E)$ (proofs are given in the Appendix). The probabilities $C(E)$ and $D(E)$ are zero for $E<\Delta_\infty$, while, if $Z=0$, the probabilities B and D are zero for all E. If $\Delta(x)$ changes on a scale that is small compared to ξ_0, the BTK results are reproduced. We calculate the values of the probabilities for the geometry given in Fig. 1. The shape of $\Delta(x)$ is assumed to be parabolic with zero slope at $x=-x_N$ and $x=x_S$. For another shape of $\Delta(x)$, practically the same results are obtained as long as the effective length over which $\Delta(x)$ varies with position and the values of Δ^+ and Δ^- are the same. We take a small δ-function potential at the N-S interface ($Z=0.3$), and we set $2x_N/(\pi\xi_0)=2x_S/(\pi\xi_0)=3$. The probability of Andreev reflection is given in Fig. 3 as a function of energy for three sets of values (Δ^+,Δ^-). The curves for the other probabilities are omitted for clarity. For $E<\Delta_\infty$, $C=D=0$, and $B=1-A$. For $E>\Delta_\infty$, D tends to zero on the same scale as A, while B and C tend to their high-energy values $1-B=C=(1+Z^2)^{-1}$. The results for $A(E)$ are compared to the BTK result (the dashed lines in Fig. 3). The fact that $A\neq0$ for $E>\Delta_\infty$ is a standard result of the quantum mechanics of a sharp potential step. If the potential rises more gradually, A becomes smaller. For $E<\Delta_\infty$, the effects of $\Delta^-\neq0$ and $\Delta^+\neq\Delta_\infty$ are largest for low and higher energies, respectively. In the curve for $\Delta^-=0.4\Delta_\infty$ and $\Delta^+=\Delta_\infty$, the influence of the δ-function potential at $x=0$ is smaller for low quasiparticle energy. This can be understood by realizing that for $E<\Delta(x)$, the functions $\tilde{u}$ and $\tilde{v}$ are exponentially damped, so that the value of the wave function at $x=0$ is small. The maximum of A in the curve for $\Delta^-=0$ and $\Delta^+=0.6\Delta_\infty$ is due to a geometrical resonance effect. For $E>\Delta^+$, it is possible that for a specific energy, the incoming electron wave and the Andreev-reflected hole wave are both zero at $x=0$. Then the δ-function poten-

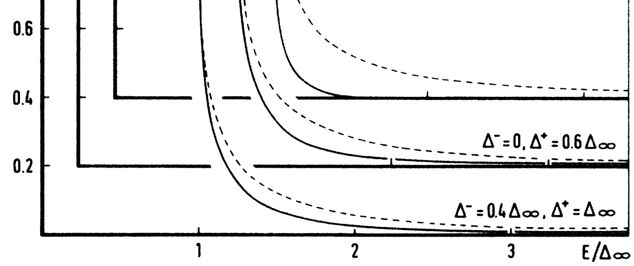

FIG. 3. Energy dependence of the probability of Andreev reflection of a quasiparticle incident on the N-S interface of Fig. 1 for three sets of (Δ^+,Δ^-) values. The parameter $Z=0.3$, while $2x_S/(\pi\xi_0)=2x_N/(\pi\xi_0)=3$. The dashed line is the BTK result for $Z=0.3$.

tial has no influence at all, and A equals unity. In the curve for $\Delta^- = \Delta^+ = 0.5\Delta_\infty$, both effects are present.

IV. GEOMETRICAL RESONANCE EFFECTS

Geometrical resonances occur, for instance, in the geometry of Fig. 2. They are due to interference effects of the wave functions of quasiparticles that feel a pair-potential step on one side of the N slab and an ordinary potential on the other side. The resonances manifest themselves as sharp peaks or as oscillations in the differential conductance (or transmission) of the tunnel junction at $x = -x_T$. The geometrical resonance effects can be calculated in two different ways that correspond to two different interpretations. The usual interpretation is that the differential conductance of the tunnel junction measures the density of states of the excitations in the normal-metal slab backed by a superconductor. The density of states is obtained from the Bogoliubov equations using Green's-functions techniques.[4-6] For $E < \Delta_\infty$, the probability of Andreev reflection is unity, and "bound states" of the quasiparticles are found at specific energy values. For $E > \Delta_\infty$, the density of states shows maxima that are due to "quasibound states." A completely different approach is to calculate the transmission T of electrical current of the complete structure of Fig. 2. Such a calculation has already been done analytically, for arbitrary Z and for a steplike variation of $\Delta(x)$, by Hahn[9] as an extension of the calculations of BTK. In the Appendix, T/T_0 is given in the limit of large Z [$T_0 = (1+Z^2)^{-1}$ is the transmission coefficient of the tunnel junction if no superconductor is present]. This result is identical to the result of the density-of-states approach. The sharp peaks in the transmission for specific energies $E < \Delta_\infty$ are due to the fact that, for those energies, $A = 1$ and $B = 0$, so $T = 2$ independent of the value of Z. This can be understood by realizing that for specific energies it is possible to have a solution of the Bogoliubov equations with an incident electron wave function and an Andreev-reflected hole wave function that both are zero at $x = -x_T$. Such a solution is not influenced by a δ-function potential at that point.

Although the two interpretations are completely different, in the limit of a step-function for $\Delta(x)$ the results are identical. Here, we calculate the transmission of the structure of Fig. 2 in the limit of large Z for

$$2x_N/(\pi\xi_0) = 2x_S/(\pi\xi_0) = 3$$

and

$$2x_T/(\pi\xi_0) = 4 .$$

We omit the δ-function potential at $x = 0$ because the combination of two such potentials leads to oscillations on a very small energy scale due to interference effects of the $\exp(ik_F x)$ parts of the wave functions. This effect makes the numerical calculation much more complicated. Moreover, in a real sample, the thickness is not constant on the scale of k_F^{-1}, so results for several thicknesses have to be averaged, which makes the small-scale oscillations disappear again. To avoid these complications, we limit ourselves to a single δ-function potential

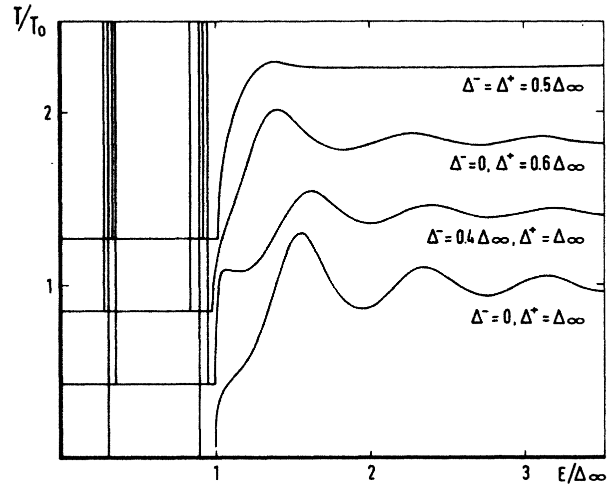

FIG. 4. Energy dependence of the normalized transmission coefficient of the tunnel junction of Fig. 2 for four sets of (Δ^+,Δ^-) values. The vertical lines for $E < \Delta_\infty$ correspond to the singularities of T/T_0. The parameter Z of the tunnel junction is assumed to be infinite, while $2x_S/(\pi\xi_0) = 2x_N/(\pi\xi_0) = 3$ and $2x_T/(\pi\xi_0) = 4$.

at $x = -x_T$. In experiments, the most left N layer in Fig. 2 is often replaced with an S layer because the peak in the density of quasiparticle states in a superconductor reduces the effect of thermal smearing. Because of the tunnel barrier at $x = -x_T$, the geometrical resonance effects are hardly influenced by the nature of the top layer. We take a top N layer because then the calculation is simpler. The results of the calculation for four sets of (Δ^+,Δ^-) values [including a steplike $\Delta(x)$] are given in Fig. 4. For $E \gg \Delta_\infty$, the amplitude of the oscillations scales with the discontinuity $(\Delta^+ - \Delta^-)$ at the interface. For energies only slightly larger than Δ_∞, the amplitude is also influenced by the shift of the maxima. For $E < \Delta_\infty$, the positions of the peaks have shifted too. These energy shifts can be related to phase shifts of the wave function. The shifts to higher energies of the maxima in the curve for $\Delta^- = 0.4\Delta_\infty$ and $\Delta^+ = \Delta_\infty$ are due to the fact that the effective thickness of the N slab is smaller in this case than for a steplike variation of $\Delta(x)$. These results are very similar to the results of the density-of-states calculation with a self-consistent $\Delta(x)$.[4]

V. NEGATIVE PAIR POTENTIAL

In the BCS theory of superconductivity, the effective electron-electron interaction between electrons with opposite momentum and spin is represented by a single potential $-V_{BCS}$. For $V_{BCS} > 0$ (attractive interaction), a superconducting ground state of the electrons is found, while for $V_{BCS} < 0$, $\Delta = 0$ is the only solution. As the effective electron-electron interaction is the sum of an attractive phonon-mediated interaction and the repulsive Coulomb interaction, it may be negative in metals that do not show superconductivity even at very low temperatures. At an N-S interface, the superconductor in general induces a pair amplitude of the electrons in N. If in N $V_{\mathrm{BCS}}<0$, then the pair potential, which is the product of the pair amplitude and V_{BCS}, will be negative. However, N also influences S, and the position dependence of $\Delta(x)$ should in principle be calculated self-consistently. Possibly, the large negative value of Δ^- that we assume in our calculation does not occur in such a self-consistent calculation.

In Fig. 5 results are given for the probability of Andreev reflection and for the geometrical resonance effects for a negative tail of $\Delta(x)$ in N ($\Delta^-=-0.4\Delta_\infty$, $\Delta^+=0.6\Delta_\infty$). Figure 5(b) is very similar to the previous results for positive $\Delta(x)$ in N. The positions of the maxima are shifted somewhat in energy and the amplitude of the oscillations for $E>\Delta_\infty$ scales with the discontinuity in Δ at the interface (and apparently not with the discontinuity of $|\Delta|$ as also might have been expected). The probability of Andreev reflection shown in Fig. 5(a) confirms the observation that the discontinuity of Δ rather than of $|\Delta|$ is important because, for $E>\Delta_\infty$ the curve is almost equal to the BTK result. For $E<\Delta_\infty$ the probability of Andreev reflection differs strongly from the results for positive $\Delta(x)$ in N. The influence of the δ-function potential is enhanced rather than diminished while, for large enough values of Z, A even becomes zero (B then equals 1). This cannot be due to a geometrical resonance effect because in the region beyond the point where $|\Delta(x)|=E$ in N, the functions $\tilde{u}(x)$ and $\tilde{v}(x)$ are not oscillating. Possibly, the contributions to the Andreev-reflected wave due to the decrease of Δ in N and due to the increase of Δ at the interface and in S partly or completely compensate each other.

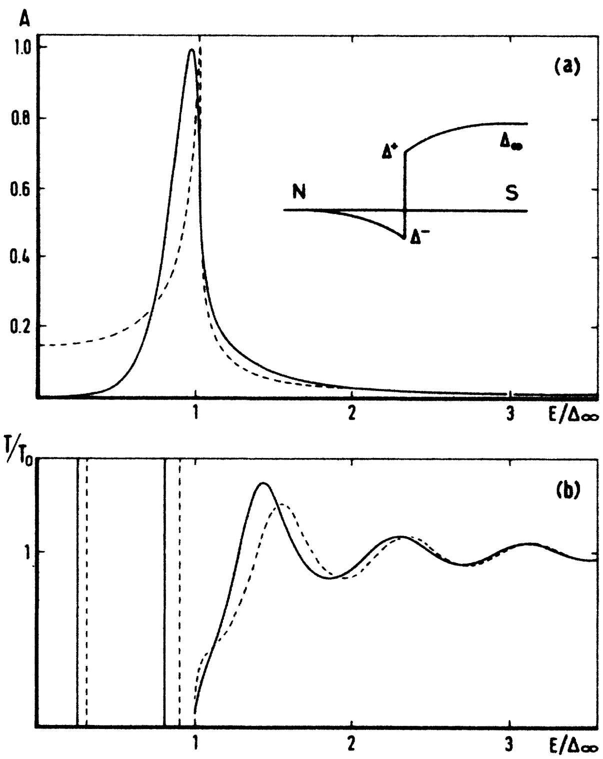

FIG. 5. (a) Energy dependence of the probability of Andreev reflection of a quasiparticle incident on the N-S interface of Fig. 1 for $\Delta^-=-0.4\Delta_\infty$ and $\Delta^+=0.6\Delta_\infty$. The parameter $Z=0.9$, while $2x_S/(\pi\xi_0)=2x_N/(\pi\xi_0)=3$. The dashed line is the BTK result for $Z=0.9$. The inset shows the position dependence of Δ near the interface. (b) Energy dependence of the normalized transmission coefficient of the tunnel junction of Fig. 2 for $\Delta^-=-0.4\Delta_\infty$ and $\Delta^+=0.6\Delta_\infty$. The parameter Z of the tunnel junction is assumed to be infinite, while $2x_S/(\pi\xi_0)=2x_N/(\pi\xi_0)=3$ and $2x_T/(\pi\xi_0)=4$.

VI. CONCLUSION

We showed that the probabilities of reflection and transmission of a quasiparticle incident on an N-S interface with a gradually changing pair potential can be calculated by numerically solving the Bogoliubov equations near the interface and by applying appropriate boundary conditions. This method can also be applied to find the geometrical resonance effects in the transmission of a tunnel junction on an N-S bilayer. For a steplike variation of the pair potential at the N-S interface, the results of the usual density-of-states calculations are reproduced. Both the probability of Andreev reflection and the geometrical resonance effects begin to change if the region in which the pair potential varies with position becomes of the order of the coherence length of the superconductor. As the pair potential usually varies on this scale, the influence of that variation should be taken into account in a careful comparison of theory and experiment.

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APPENDIX

In order to obtain the probabilities of reflection and transmission of an incoming quasiparticle from the numerical solution of the Bogoliubov equations [Eq. (2)], appropriate boundary conditions have to be applied. The integration is performed from $x=x_S$ to $x=-x_N$ (see Fig. 1) for two independent sets of initial values at $x=x_S$ that only contain outgoing quasiparticles. From the two solutions (denoted with the indices 1 and 2), the probabilities of reflection and transmission of a quasiparticle incident in N can be reconstructed. For $x\geq x_S$ the general solution is given in Eq. (3); we choose the two independent solutions:

$$\psi_1=\begin{bmatrix}u_0\\v_0\end{bmatrix}e^{i(k_F+\kappa_S)x},\qquad \psi_2=\begin{bmatrix}v_0\\u_0\end{bmatrix}e^{-i(k_F-\kappa_S)x}. \tag{A1}$$

For $-x_N\leq x\leq x_S$, the wave function is of the form

$$\psi_j=\begin{bmatrix}\tilde{u}_{aj}(x)\\ \tilde{v}_{aj}(x)\end{bmatrix}e^{ik_Fx}+\begin{bmatrix}\tilde{v}_{bj}(x)\\ \tilde{u}_{bj}(x)\end{bmatrix}e^{-ik_Fx} \tag{A2}$$

in which the four sets of functions $(\tilde{u}_{aj}(x),\tilde{v}_{aj}(x))$ and $(\tilde{u}_{bj}(x),\tilde{v}_{bj}(x))$ $(j=1,2)$ are solutions of Eq. (2). The boundary conditions at $x=x_S$ demand that ψ and $\partial\psi/\partial x$ are continuous. In the latter condition, terms that are proportional to $\partial\tilde{u}/\partial x$, $\partial\tilde{v}/\partial x$, and κ_S may be neglected with respect to terms proportional to k_F (except in the exponent). Then the initial conditions of the numerical integration are

$$\tilde{u}_{a1}(x_S)=\tilde{u}_{b2}(x_S)=u_0e^{i\kappa_Sx_S}\ ,\qquad \tilde{v}_{a1}(x_S)=\tilde{v}_{b2}(x_S)=v_0e^{i\kappa_Sx_S}\ , \tag{A3a}$$

$$\tilde{u}_{b1}(x_S)=\tilde{u}_{a2}(x_S)=0\ ,\qquad \tilde{v}_{b1}(x_S)=\tilde{v}_{a2}(x_S)=0\ . \tag{A3b}$$

Only a single integration of Eq. (2) has to be performed from $x=x_S$ to $x=0$ because two sets of functions are equal to zero (the differential equation is homogeneous), and the other two sets are identical.

The potential $V(x)=Z(\pi\xi_0\Delta_\infty)\delta(x)$ is taken into account via the boundary conditions at $x=0$ (indices $+$ and $-$ indicate the values of the functions for $x\downarrow 0$ and $x\uparrow 0$, respectively):

$$\psi^+=\psi^-\ , \tag{A4a}$$

$$(\partial\psi^+/\partial x)-(\partial\psi^-/\partial x)=2k_FZ\psi^+\ . \tag{A4b}$$

The wave function ψ is given in Eq. (A2). The boundary conditions are simplified by realizing that $\tilde{u}^+_{b2}=\tilde{u}^+_{a1}$, $\tilde{v}^+_{b2}=\tilde{v}^+_{a1}$, and that the other functions are zero. If we again neglect terms proportional to $\partial\tilde{u}/\partial x$ and $\partial\tilde{v}/\partial x$ in Eq. (A4b), we find as initial conditions for the integration for $x\le 0$:

$$\tilde{u}^-_{a1}=(1+iZ)\tilde{u}^+_{a1},\quad \tilde{v}^-_{a1}=(1+iZ)\tilde{v}^+_{a1}\ ,$$

$$\tilde{u}^-_{b1}=-iZ\tilde{v}^+_{a1},\quad \tilde{v}^-_{b1}=-iZ\tilde{u}^+_{a1}\ ,$$

$$\tilde{u}^-_{a2}=iZ\tilde{v}^+_{a1},\quad \tilde{v}^-_{a2}=iZ\tilde{u}^+_{a1}\ ,$$

$$\tilde{u}^-_{b2}=(1-iZ)\tilde{u}^+_{a1},\quad \tilde{v}^-_{b2}=(1-iZ)\tilde{v}^+_{a1}\ .$$

Because the differential equation Eq. (2) is homogeneous, common prefactors of $\tilde{u}$ and $\tilde{v}$ may be split off. This means that for $-x_N\le x\le 0$, the two solutions for the wave function can be written

$$\psi_1=(1+iZ)\begin{bmatrix}\tilde{u}_{a0}(x)\\ \tilde{v}_{a0}(x)\end{bmatrix}e^{ik_Fx}-iZ\begin{bmatrix}\tilde{v}_{b0}(x)\\ \tilde{u}_{b0}(x)\end{bmatrix}e^{-ik_Fx}\ ,$$

$$\psi_2=iZ\begin{bmatrix}\tilde{u}_{b0}(x)\\ \tilde{v}_{b0}(x)\end{bmatrix}e^{ik_Fx}+(1-iZ)\begin{bmatrix}\tilde{v}_{a0}(x)\\ \tilde{u}_{a0}(x)\end{bmatrix}e^{-ik_Fx}\ . \tag{A5}$$

The sets of functions $(\tilde{u}_{a0}(x),\tilde{v}_{a0}(x))$ and $(\tilde{u}_{b0}(x),\tilde{v}_{b0}(x))$ are two solutions of Eq. (2) with initial conditions $\tilde{u}^-_{a0}=\tilde{u}^+_{a1}$, $\tilde{v}^-_{a0}=\tilde{v}^+_{a1}$, and $\tilde{u}^-_{b0}=\tilde{v}^+_{a1}$, $\tilde{v}^-_{b0}=\tilde{u}^+_{a1}$, respectively. In Eq. (A5) it is clear that only if $Z\neq 0$, wave functions with positive and negative wave vector get mixed.

For $x\le -x_N$, the general solution for the wave function is in principle given by Eq. (4). The solutions ψ_1 and ψ_2 we started with in Eq. (A1), correspond to a single outgoing electronlike quasiparticle and to a single outgoing holelike quasiparticle, respectively. Such solutions have to correspond in N to mixtures of incoming electron and hole wave functions with their respective reflected waves. Therefore, for $x\le -x_N$, the wave function is written as

$$\begin{aligned}\psi_j=\nu_j&\left[\begin{bmatrix}1\\0\end{bmatrix}e^{i(k_F+\kappa_N)x}+a_e\begin{bmatrix}0\\1\end{bmatrix}e^{i(k_F-\kappa_N)x}+b_e\begin{bmatrix}1\\0\end{bmatrix}e^{-i(k_F+\kappa_N)x}\right]\\&+\eta_j\left[\begin{bmatrix}0\\1\end{bmatrix}e^{-i(k_F-\kappa_N)x}+a_h\begin{bmatrix}1\\0\end{bmatrix}e^{-i(k_F+\kappa_N)x}+b_h\begin{bmatrix}0\\1\end{bmatrix}e^{i(k_F-\kappa_N)x}\right]\ .\end{aligned} \tag{A6}$$

The coefficients a_e and b_e are the amplitudes of the Andreev-reflected wave and the ordinarily reflected wave, respectively, for an incident electron wave with amplitude 1. The coefficients a_h and b_h are in magnitude equal to a_e and b_e, respectively, but may differ in the phase factor. By applying the boundary conditions at $x=-x_N$ (namely, continuity of ψ and of $\partial\psi/\partial x$), the coefficients $a_{e,h}$ and $b_{e,h}$ can be expressed in the solutions of the numerical integration

$$\tilde{u}_{a0}(-x_N)=\tilde{u}_a,\quad \tilde{v}_{a0}(-x_N)=\tilde{v}_a\ ,$$

$$\tilde{u}_{b0}(-x_N)=\tilde{u}_b,\quad \tilde{v}_{b0}(-x_N)=\tilde{v}_b\ .$$

The result is

$$a_e=\frac{(1+Z^2)\tilde{u}_a\tilde{v}_a-Z^2\tilde{u}_b\tilde{v}_b}{(1+Z^2)\tilde{u}^2_a-Z^2\tilde{u}^2_b}e^{-2i\kappa_Nx_N}\ ,\qquad b_e=\frac{iZ(1-iZ)(\tilde{u}_b\tilde{v}_a-\tilde{u}_a\tilde{v}_b)}{(1+Z^2)\tilde{u}^2_a-Z^2\tilde{u}^2_b}e^{-2i\kappa_Nx_N}\ , \tag{A7}$$

while $a_h=a_e$ and $b_h=-b_e(1+iZ)/(1-iZ)$. The amplitudes of the transmitted waves corresponding to a single incident electron wave (c_e and d_e) or corresponding to a single incident hole wave (c_h and d_h) can be deduced by writing for $x\ge x_S$:

$$\psi_j=v_j\left[c_e\begin{bmatrix}u_0\\v_0\end{bmatrix}e^{i(k_F+\kappa_S)x}+d_e\begin{bmatrix}v_0\\u_0\end{bmatrix}e^{-i(k_F-\kappa_S)x}\right]+\eta_j\left[c_h\begin{bmatrix}v_0\\u_0\end{bmatrix}e^{-i(k_F-\kappa_S)x}+d_h\begin{bmatrix}u_0\\v_0\end{bmatrix}e^{i(k_F+\kappa_S)x}\right]\ .$$

These ψ_j should be equal to the wave functions we started with in Eq. (A1). The coefficients ν_j and η_j are known from the foregoing calculation, so the amplitudes $c_{e,h}$ and $d_{e,h}$ can be determined:

$$c_e=\frac{(1-iZ)\tilde{u}_a}{(1+Z^2)\tilde{u}_a^2-Z^2\tilde{u}_b^2}e^{-i\kappa_N x_N},$$
$$d_e=\frac{iZ\tilde{u}_b}{(1+Z^2)\tilde{u}_a^2-Z^2\tilde{u}_b^2}e^{-i\kappa_N x_N}, \quad \text{(A8)}$$

while $c_h=c_e(1+iZ)/(1-iZ)$ and $d_h=-d_e$. Following BTK, we define probability currents A, B, C, and D for the various wave-function components. These are given by

$$A=|a_{e,h}|^2,\quad B=|b_{e,h}|^2,$$
$$C=|c_{e,h}|^2(|u_0|^2-|v_0|^2),$$
$$D=|d_{e,h}|^2(|u_0|^2-|v_0|^2).$$

If the region near the N-S interface in which $\Delta(x)$ is not constant is much smaller than ξ_0, the integration of Eq. (2) over this region hardly changes $\tilde{u}$ and $\tilde{v}$. It can easily be shown that then $\tilde{u}_a=\tilde{v}_b=u_0\exp(i\kappa_S x_S)$ and $\tilde{v}_a=\tilde{u}_b=v_0\exp(i\kappa_S x_S)$. As $\kappa_S x_S$ and $\kappa_N x_N$ are very small in this limit, Eqs. (A7) and (A8) reduce to the BTK results. So deviations from the BTK results are only to be expected if $\Delta(x)$ varies on the scale of ξ_0. Two observations of BTK can be shown to hold also for this more general situation. First, if $Z=0$, there is no ordinary reflection and no transmission with change of character of the quasiparticle ($B=D=0$). Secondly, if $E<\Delta_\infty$, u_0 and v_0 are complex conjugates, so $C=D=0$. If also $Z=0$, $B=0$, and A necessarily equals 1. This also follows from the calculation because the initial values of $\tilde{u}$ and $\tilde{v}$ are complex conjugates [note that for $E<\Delta_\infty$, κ_S in Eq. (A3a) is imaginary]. Then during integration of Eq. (2), the functions remain complex conjugate and, for $Z=0$, $A=|(\tilde{v}_a/\tilde{u}_a)\exp(-2i\kappa_N x_N)|^2=1$.

To calculate the geometrical resonance effects, the foregoing discussion has to be adapted only slightly. The geometry is given in Fig. 2. The tunnel junction is represented by a δ-function potential with very large Z at $x=-x_T$, while at the N-S interface no barrier is assumed to be present to avoid interference effects due to the $\exp(ik_F x)$ parts of the wave functions. The quantity to be calculated is the transmission coefficient T of the whole geometry. That will be very low but it should be scaled with $T_0=(1+Z^2)^{-1}$ the transmission coefficient if no superconductor is present. If the charge current is evaluated at $x<-x_T$ in N, T is given by $T=1-B+A$. Because there is no δ-function potential at the N-S interface, the two solutions given by Eq. (A2) can be evaluated all the way to $x=-x_N$. The result is two numbers $\tilde{u}_{a1}(-x_N)=\tilde{u}_{b2}(-x_N)=\tilde{u}_a$ and $\tilde{v}_{a1}(-x_N)=\tilde{v}_{b2}(-x_N)=\tilde{v}_a$; the other four functions are identically zero. For $-x_T\le x\le -x_N$, the solutions are given by Eq. (4) with the coefficients being determined by the boundary conditions at $x=-x_N$:

$$\psi_1=\tilde{u}_a e^{i\kappa_N x_N}\begin{bmatrix}1\\0\end{bmatrix}e^{i(k_F+\kappa_N)x}+\tilde{v}_a e^{-i\kappa_N x_N}\begin{bmatrix}0\\1\end{bmatrix}e^{i(k_F-\kappa_N)x},$$

$$\psi_2=\tilde{u}_a e^{i\kappa_N x_N}\begin{bmatrix}0\\1\end{bmatrix}e^{-i(k_F-\kappa_N)x}+\tilde{v}_a e^{-i\kappa_N x_N}\begin{bmatrix}1\\0\end{bmatrix}e^{-i(k_F+\kappa_N)x}.$$

Now, for $x\le -x_T$, the wave functions of Eq. (A6) are chosen and, at $x=x_T$, they are matched to the above solutions using the boundary conditions of Eq. (A4). The results for the coefficients $a_{e,h}$ and $b_{e,h}$ are

$$a_e=\frac{\tilde{u}_a\tilde{v}_a e^{-2i\kappa_N x_N}}{\tilde{u}_a^2+Z^2(\tilde{u}_a^2-\tilde{v}_a^2e^{4i\kappa_N(x_T-x_N)})},$$
$$b_e=\frac{-iZ(1-iZ)(\tilde{u}_a^2-\tilde{v}_a^2e^{4i\kappa_N(x_T-x_N)})}{\tilde{u}_a^2+Z^2(\tilde{u}_a^2-\tilde{v}_a^2e^{4i\kappa_N(x_T-x_N)})}\times e^{-2i(k_F+\kappa_N)x_T}, \quad \text{(A9)}$$

while $a_h=a_e$ and

$$b_h=-b_e\exp(4ik_F x_T)(1+iZ)/(1-iZ).$$

In the limit of very large Z, the normalized transmission coefficient T/T_0 of the tunnel junction is given by

$$\frac{T}{T_0}=1+2\,\mathrm{Re}\left[\frac{\tilde{v}_a^2e^{4i\kappa_N(x_T-x_N)}}{\tilde{u}_a^2-\tilde{v}_a^2e^{4i\kappa_N(x_T-x_N)}}\right]$$
$$=\mathrm{Re}\left[\frac{\tilde{u}_a^2e^{-2i\kappa_N(x_T-x_N)}+\tilde{v}_a^2e^{2i\kappa_N(x_T-x_N)}}{\tilde{u}_a^2e^{-2i\kappa_N(x_T-x_N)}-\tilde{v}_a^2e^{2i\kappa_N(x_T-x_N)}}\right]. \quad \text{(A10)}$$

The latter expression for T/T_0 is most suitable to discuss the energy range $E<\Delta_\infty$. As has been discussed before, for those energies, $\tilde{u}_a$ and $\tilde{v}_a$ are complex conjugates. Then the numerator is real while the denominator is purely imaginary. This means that T/T_0 equals zero except if the denominator is zero, which is the case if the phase factors obey

$$\tan[2\kappa_N(x_T-x_N)]=\mathrm{Im}(\tilde{u}_a^2)/\mathrm{Re}(\tilde{u}_a^2). \quad \text{(A11)}$$

For specific values of the energy of the quasiparticles, this condition may be fulfilled and T/T_0 diverges. From Eq. (A9) it follows that, for these energies, $B=0$ and $A=1$, so $T=2$ independent of the height of the tunnel barrier. This can be understood by realizing that, for specific values of the phase of the coefficient a_e, it will be possible to have an incident electron wave function and an Andreev-reflected hole wave function that both are zero at $x=-x_T$. Such a wave function is not influenced by the presence of a δ-function potential at that point (note that there is no δ-function potential at the N-S interface).

If at the N-S interface the pair potential $\Delta(x)$ varies only on a scale that is much smaller than ξ_0, no numeric integration has to be performed. The solution is then given by $\tilde{u}_a=u_0$ and $\tilde{v}_a=v_0$, while $\kappa_N x_N=\kappa_S x_S=0$. Most other calculations of geometrical resonance effects assume such a steplike variation of $\Delta(x)$. The condition for the peaks of T/T_0 for $E<\Delta_\infty$, Eq. (A11), then is

$$\tan(2\kappa_N x_T)=\frac{(\Delta_\infty^2-E^2)^{1/2}}{E} .$$

This is exactly the condition that has already been found by de Gennes and Saint-James.[10] The expression for T/T_0, Eq. (A10), reduces to

$$\frac{T}{T_0}=1+2\,\mathrm{Re}\left[\frac{v_0^2 e^{4i\kappa_N x_T}}{u_0^2-v_0^2 e^{4i\kappa_N x_T}}\right] .$$

This expression has also been obtained by calculating the density of states of the normal-metal slab using Green's functions to solve the Bogoliubov equations.[4–6] So in the limit of a steplike variation of $\Delta(x)$, the two methods yield identical results.

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