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Andreev scattering in anisotropic superconductors

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Three new classes of superconductors have been discovered in the past decade: the organic superconductors, the heavy-fermion superconductors, and the oxide superconductors. All of them show characteristic anomalies that point to the possibility that they are anisotropic superconductors with a directionally dependent (**k**-dependent) gap function that vanishes in points or lines on the Fermi surface. The problem to identify the symmetry type of an anisotropic superconductor has not found a satisfactory solution yet. Although a number of experiments have been proposed that allow one in principle to distinguish between different symmetry types, most of them are ambiguous because they do not couple to the order parameter directly. Here we propose a new experiment: Andreev scattering, i.e., scattering of low-energy normal quasiparticles off the spatially varying order parameter when the quasiparticles approach a normal-metal–superconductor interface from the normal side. The idea is investigated in detail for anisotropic even-parity superconductors. To describe the quasiparticle dynamics, the Bogoliubov–de Gennes equations for anisotropic superconductors are introduced and approximated by the Andreev equations. The nonideality of the interface is taken into account by an interface potential parametrized by a reflection coefficient. This leads to a boundary condition for the Andreev equations at the interface. The pair potential $\Delta(\hat{\mathbf{k}},\mathbf{r})$, i.e., the directionally and space-dependent order parameter that occurs as a scattering potential in the Andreev equations, is determined self-consistently for various nonideal interfaces to *d*-wave superconductors. This is equivalent to solving the proximity effect for interfaces with a finite reflection coefficient, and it is done using the quasiclassical formalism. Once $\Delta(\hat{\mathbf{k}},\mathbf{r})$ has been obtained, the Andreev equations are integrated numerically, and the **k**-dependent Andreev reflection and transmission coefficients as well as the corresponding conductivities are computed. The theory predicts a directional dependence of the conductivities from which the **k** dependence of the order parameter can be reconstructed. For this effect to be a useful tool, new experiments will have to be devised. A double-point-contact experiment is proposed for an experimental realization of the idea.

I. INTRODUCTION

In the past decade, the science of superconductivity has been centered around the discovery of three new classes of superconductors.

(a) *The organic superconductors.* In 1980, Jérome *et al.*[1] discovered the superconducting charge-transfer salt $(TMTSF)_2PF_6$ with a T_c of 1.2 K at 6.5 kbar. In the following years, a variety of other compounds was found; the latest achievement was the synthesis of $(BEDT\text{-}TTF)_2Cu(NCS)_2$ with a T_c of 10.4 K at ambient pressure by Urayama *et al.*[2] The search for organic superconductors had started in 1964 with Little's proposal that one-dimensional conductors might be superconductors at high temperatures, possibly even at room temperature. Although the mechanism of superconductivity in the charge-transfer salts is not completely clear yet, they can not be described by conventional Bardeen-Cooper-Schrieffer (BCS) theory: at least some of the compounds show anomalies characteristic of anisotropic superconductivity.[3]

(b) *The heavy-fermion superconductors* $CeCu_2Si_2$ (Steglich *et al.*[4]), UBe_{13} (Ott *et al.*[5]), and UPt_3 (Stewart *et al.*[6]). Heavy-fermion compounds are characterized by the very high effective masses (of the order of 1000 m_e) of the electrons that are due to hybridization of the almost localized (Ce,U) f electrons with the conduction electrons. The jump in the specific heat at the transition temperature of these systems is proportional to the (very high) normal specific heat, i.e., the heavy electrons are responsible for the superconductivity. The T_c of these compounds is around 1 K, i.e., rather low (although they are "high-temperature superconductors" in the sense that $T_c/T_F \sim 0.1$ is very high), so that applications are not very likely: their understanding is, however, a fundamental test for the many-body theory of metals. The uranium compounds again show anomalous superconducting properties and there are strong hints that they are anisotropic superconductors.

(c) *The Cu-oxide superconductors.* Starting with the discovery of superconductivity above 30 K in $La_{2-x}(Ba,Sr)_xCuO_{4-y}$ by Bednorz and Müller in 1986, the first system to break the "sound barrier" of $T_c = 23$ K for Nb_3Ge established 20 years before, there has been an unprecedented flood of papers and new results on oxide superconductors. The experimental highlights are the new compounds $YBa_2Cu_3O_{7-y}$ with $T_c = 90$ K and the Tl-Ca-Ba-Cu-O system with $T_c = 125$ K. The Cu-oxide superconductors are characterized by two-dimensional CuO planes that are only weakly coupled so that most theories start from two-dimensional models. They show anomalies in the normal state (linear resistivity as a function of temperature between 6 and 600 K) as well as in the superconducting state (e.g., nonexponential specific heat). Again, there are some indications that these materials are anisotropic superconductors.

There are two common themes in all three of these new classes of materials: all of these superconductors are close to magnetic transitions, and in all of them superconductivity is probably caused by a purely electronic mechanism. This is in contrast to the ordinary superconductors that can be described very successfully by the phonon mechanism. Along with the question of the mechanism goes the problem of the symmetry of the order parameter: although the phonon mechanism per se does not exclude anisotropic pairing, all known superconductors described by the phonon mechanism are so-called *s*-wave superconductors, i.e., they have a gap in the excitation spectrum all over the Fermi surface. If superconductivity is caused by an electronic mechanism, however, the order parameter will be *anisotropic* in general, which will imply for us the existence of points or lines of zeroes of the order parameter on the Fermi surface.[7] The spin-fluctuation mechanism,[8] for example, that is responsible at least partially for the pairing interaction in superfluid ^{3}He favors triplet pairing, i.e., Cooper pairs with a total spin $S=1$. The orbital part of the pair wave function has to be of odd parity and will lead to an anisotropic gap [with the exception of the Balian-Werthamer (BW) phase]. To develop a theory for the new materials, it would be of great importance to know exactly which symmetry type a given superconductor belongs to. Unfortunately, progress in this direction has been frustratingly slow: the order parameter cannot be probed directly, it is not a macroscopic observable as, e.g., a magnetization. Hence, theory has to rely on a number of indirect experiments as an input. One tries to infer the type of the order parameter from its influence on various thermodynamic quantities, transport coefficients and the like, but usually these quantities are changed by other mechanisms as well so that it is not easy to find out what the share of the order parameter is. In some cases theory can help to exclude certain possibilities, it is, for example, known that lines of zeroes of the order parameter are not compatible with odd-parity superconductivity (Volovik and Gor'kov,[9] Ueda and Rice,[10] and Blount[11]). For a discussion of various experiments performed and proposed see Refs. 12–25.

Here, we propose a new experiment that offers the advantage of coupling as closely to the order parameter as possible: scattering of quasiparticles that cannot enter a region of a sample because of the existence of a superconducting order parameter. This phenomenon was discovered in 1964 by Andreev[26] and bears the name Andreev scattering.

II. THE ANDREEV EQUATIONS

The weak-coupling formalism of superconductivity is easily generalized to spatially inhomogeneous situations, e.g., sandwiches of different superconductors, normal-metal–superconductor (NS) junctions and the like: the self-consistent pair potential $\Delta(\mathbf{r})$ takes the role of the order parameter Δ, the Bogoliubov quasiparticles are described by wave functions that are two-component spinors fulfilling the Bogoliubov–de Gennes equations, a Schrödinger equation in which $\Delta(\mathbf{r})$ acts as an off-diagonal potential. If a quasiparticle wave packet approaches an inhomogeneity in the pair potential, there is a probability for it to be reflected—as for a wave packet described by the ordinary Schrödinger equation approaching, e.g., a potential step. Analysis of this reflection process[26–28] shows that if the incoming electron has wave vector $\mathbf{k}$ and group velocity $\mathbf{v}_g$, the reflected particle is a hole with (a) wave vector $-\mathbf{k}'\approx\mathbf{k}$ (*missing* particle in $\mathbf{k}'$), (b) positive charge, (c) negative effective mass, and (d) reversed group velocity since

$$\mathbf{v}_g' = -\mathbf{v}_g \ .$$

Property (d) is in contrast to ordinary (specular) reflection in which only the velocity component *perpendicular* to a planar interface is reversed. The difference between Andreev reflection and specular reflection is illustrated in Fig. 1. Properties (a)–(d) were verified experimentally.[29,30]

More general inhomogeneities can be considered if the pair potential has internal structure, i.e., is $\mathbf{k}$ dependent. Examples are quasiparticle scattering at (a) interfaces between the A and B phase of superfluid ^{3}He, where the $\mathbf{k}$ dependence of the order parameter changes its functional form (Yip[31]), (b) order-parameter textures in ^{3}He-A, i.e., gradients in the orientation of the order parameter such that a quasiparticle wave packet moving in a given direction may be subject to a rising local gap in the spectrum (Greaves and Leggett[32]), or (c) rapid phase changes of the order parameter in a current carrying superconducting constriction. We use the name Andreev scattering for all of these.

Our object is to apply Andreev's method to superconductors with an *even-parity anisotropic* ($\mathbf{k}$-dependent) order parameter. The corresponding case of Andreev scattering in an *odd-parity* superconductor leads to additional nice phenomena since the reflected holes may be spin polarized (Kieselmann and Rainer[33]). The theory gets more involved, however, since the interface will act as a magnetic scatterer because of differences in spin-orbit coupling between the normal metal and the superconductor.

Quasiparticles in inhomogeneous anisotropic even-parity superconductors can be described by the Bogoliubov–de Gennes (BdG) equations

$$E^n u^n(\mathbf{x}) = h_0 u^n(\mathbf{x}) + \int d\mathbf{x}'\Delta(\mathbf{x},\mathbf{x}')v^n(\mathbf{x}') \ , \tag{2.1a}$$

$$E^n v^n(\mathbf{x}) = -h_0 v^n(\mathbf{x}) + \int d\mathbf{x}'\Delta^*(\mathbf{x},\mathbf{x}')u^n(\mathbf{x}') \ , \tag{2.1b}$$

FIG. 1. Andreev reflection (right-hand side) and ordinary specular reflection (left-hand side). The arrows give the directions of the group velocity of incoming and outgoing particles.

together with the self-consistency conditions for Δ in terms of u,v:

$$\Delta(\mathbf{x},\mathbf{x}')=-V(\mathbf{x},\mathbf{x}')\langle\psi_\uparrow(\mathbf{x})\psi_\downarrow(\mathbf{x}')\rangle$$
$$=-V(\mathbf{x},\mathbf{x}')\sum_n u^n(\mathbf{x})v^{n*}(\mathbf{x}')[-f(E^n)]$$
$$+v^{n*}(\mathbf{x})u^n(\mathbf{x}')[1-f(E^n)]\ . \qquad (2.2)$$

Here $h_0=-\nabla^2/2m-\mu+U(\mathbf{x})$ is the one-particle Hamiltonian, $V(\mathbf{x},\mathbf{x}')$ is the pairing interaction, and $\Delta(\mathbf{x},\mathbf{x}')$ the pair potential. Note that the dependence on $\mathbf{x},\mathbf{x}'$ cannot be reduced to a dependence on the difference of the two coordinates as in the homogeneous case. The eigenstates are labeled by an index n, and all sums over n run over positive-energy eigenstates.

Since the model order parameters we will introduce in (2.1) will be given in the form $\Delta(\mathbf{k},\mathbf{R})$, we have to relate this to $\Delta(\mathbf{x},\mathbf{x}')$: all quantities that depend on $\mathbf{x},\mathbf{x}'$ can be written in terms of center of mass $\mathbf{R}=(\mathbf{x}+\mathbf{x}')/2$ and relative coordinates $\mathbf{r}=\mathbf{x}-\mathbf{x}'$ as well, $\tilde{\Delta}(\mathbf{r},\mathbf{R})\equiv\Delta(\mathbf{x},\mathbf{x}')$. $\Delta(\mathbf{k},\mathbf{R})$ is then given by the Fourier transform of $\tilde{\Delta}(\mathbf{r},\mathbf{R})$ w.r.t. the relative coordinate

$$\Delta(\mathbf{k},\mathbf{R})=\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}\tilde{\Delta}(\mathbf{r},\mathbf{R})\ .$$

Investigation of the BdG equations shows that the eigenfunctions (u^n,v^n) will oscillate on a length scale k_F^{-1}. This is an unwanted and unnecessary difficulty for the numerical integration, since the self-consistent pair potential varies only on a scale much larger, namely ξ_0. This suggests that we introduce new wave functions

$$\begin{pmatrix}\bar{u}\\ \bar{v}\end{pmatrix}=e^{-ik_F\hat{\mathbf{k}}\cdot\mathbf{x}}\begin{pmatrix}u\\ v\end{pmatrix}, \qquad (2.3)$$

i.e., divide out the fast oscillations. Here and in the following we have left out the label n of the eigenfunctions: in the interface problems we are going to study, the pair potential $\Delta(\mathbf{k},\mathbf{r})$ will be homogeneous far away from the interface so that we can label the quasiparticle states by their wave vectors $\mathbf{k}$ in that region. To simplify the notation we will leave out the index $\mathbf{k}$ of u,v. If we retain only terms of lowest order in $(k_F\xi_0)^{-1}$, the substitution of (2.3) in (2.2) leads to the Andreev equations (Kurkijärvi and Rainer[34])

$$E\bar{u}(\mathbf{x})=-iv_F\hat{\mathbf{k}}\cdot\nabla\bar{u}(\mathbf{x})+\Delta(\hat{\mathbf{k}},\mathbf{x})\bar{v}(\mathbf{x})\ , \qquad (2.4a)$$

$$E\bar{v}(\mathbf{x})=+iv_F\hat{\mathbf{k}}\cdot\nabla\bar{v}(\mathbf{x})+\Delta^*(\hat{\mathbf{k}},\mathbf{x})\bar{u}(\mathbf{x})\ . \qquad (2.4b)$$

To show this for the integral operator, we look at

$$\int d\mathbf{x}'\Delta(\mathbf{x},\mathbf{x}')\bar{v}(\mathbf{x}')e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}=\int d\mathbf{r}\tilde{\Delta}(\mathbf{r},\mathbf{x}-r/2)\bar{v}(\mathbf{x}-\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}$$
$$=\Delta(\mathbf{k},\mathbf{x})\bar{v}(\mathbf{x})+\left[\frac{\partial\bar{v}(\mathbf{x})}{\partial\mathbf{x}}-\frac{\bar{v}(\mathbf{x})}{2}\frac{\partial}{\partial\mathbf{x}}\right]\frac{\partial\Delta(\mathbf{k},\mathbf{x})}{\partial\mathbf{k}}+\cdots\ ,$$

where we have assumed that $\bar{v}(\mathbf{x})$ is a slowly varying function as is $\Delta(\mathbf{k},\mathbf{x})$ in the second argument to expand $\bar{v},\Delta$ around $\mathbf{x}$. It is clear that the second term of the sum is down by a factor of $(k_F\xi_0)^{-1}$ w.r.t. the first one. Hence, if we restrict ourselves to terms in lowest order of the small parameter, we are left with (2.4), a first-order differential equation in which $\mathbf{k}$ is a parameter. We will solve (2.4) numerically together with the appropriate boundary conditions. The pair potential $\Delta(\mathbf{k},\mathbf{r})$ is supposed to be an external field, only later will the question of self-consistency be addressed. Since $\Delta(\mathbf{k},\mathbf{r})$ is defined only for k around k_F, we will replace the dependence of $\mathbf{k}$ by one on the direction $\hat{\mathbf{k}}$. The interpretation of $\Delta(\hat{\mathbf{k}},\mathbf{r})$ as an external field does not contradict the principles of quantum mechanics: it is possible because $\mathbf{k}$ and $\mathbf{r}$ may be specified simultaneously in a quasiclassical situation. But the condition for a quasiclassical treatment (slow spatial dependence of external fields on a scale k_F^{-1}) is fulfilled in weak-coupling superconductors, since the scale for spatial variation of the pair potential is given by ξ_0, the coherence length, and $(\xi_0k_F)^{-1}\sim T_c/T_F\ll1$.

From now on we will assume that the interface is lying in the x-y plane and is translationally invariant so that the spatial dependence of $\bar{u},\bar{v}$ and Δ is reduced to a dependence on z. To be specific, the e region $z<0$ will be taken to be the normal side (N) and region $z>0$ will be taken to be the superconducting (S) side of the interface. The Andreev equations (2.4) then take the form

$$E\bar{u}(z)=-iv_F(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})\frac{d}{dz}\bar{u}(z)+\Delta(\hat{\mathbf{k}},z)\bar{v}(z)\ , \qquad (2.5a)$$

$$E\bar{v}(z)=iv_F(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})\frac{d}{dz}\bar{v}(z)+\Delta^*(\hat{\mathbf{k}},z)\bar{u}(z)\ , \qquad (2.5b)$$

where $\hat{\mathbf{z}}$ is a unit vector in the z direction.

The Andreev and normal-reflection coefficients can now be determined by solving Eq. (2.5) for the two-component wave functions

$$\psi_{\hat{\mathbf{k}}}(z)=\begin{pmatrix}\bar{u}(z)\\ \bar{v}(z)\end{pmatrix}$$

with the correct boundary and matching conditions for $z\to\pm\infty$ and $z=0$. The interface couples states with unit vectors $\hat{\mathbf{k}}_N$, $\underline{\hat{\mathbf{k}}}_N$, $\hat{\mathbf{k}}_S$, $\underline{\hat{\mathbf{k}}}_S$ (see Fig. 2). Note that $\hat{\mathbf{k}}_N\neq\hat{\mathbf{k}}_S$ if the metals on both sides of the interface have different Fermi wave vectors. If we assume that $\hat{\mathbf{k}}_N$ gives the direction of the incoming electron, we require that

$$\psi_{\hat{\mathbf{k}}_N}(z\to-\infty)=\begin{pmatrix}1\\0\end{pmatrix}\exp(iE\hat{k}_{Nz}z/v_{F_N})+\begin{pmatrix}0\\ r_A\end{pmatrix}\exp(-iE\hat{k}_{Nz}z/v_{F_N})\ \text{(incoming electron+Andreev reflected holes)}\ , \qquad (2.6a)$$

$$\psi_{\hat{\underline{\mathbf{k}}}_N}(z\to-\infty)=\begin{bmatrix} r_N \\ 0 \end{bmatrix}\exp(iE\hat{\underline{k}}_{Nz}z/v_{F_N})\ \text{(normally reflected electrons , no holes) ,} \tag{2.6b}$$

$$\psi_{\hat{\mathbf{k}}_S}(z\to+\infty)=c_1\begin{bmatrix} E+[E^2-|\Delta(\hat{\mathbf{k}}_S)|^2]^{1/2} \\ \Delta^*(\hat{\mathbf{k}}_S) \end{bmatrix}\exp\{i[E^2-|\Delta(\hat{\mathbf{k}}_S)|^2]^{1/2}\hat{k}_{Sz}z/v_{F_S}\}$$

$$\text{(outgoing electron-like quasiparticles) ,} \tag{2.6c}$$

$$\psi_{\hat{\underline{\mathbf{k}}}_S}(z\to+\infty)=c_2\begin{bmatrix} \Delta(\hat{\underline{\mathbf{k}}}_S) \\ E+[E^2-|\Delta(\hat{\underline{\mathbf{k}}}_S)|^2]^{1/2} \end{bmatrix}\exp\{i[E^2-|\Delta(\hat{\underline{\mathbf{k}}}_S)|^2]^{1/2}\hat{\underline{k}}_{Sz}z/v_{F_S}\}\ \text{(outgoing hole-like quasparticles) .} \tag{2.6d}$$

These forms contain the following boundary conditions at infinity: one incoming electron in direction $\hat{\mathbf{k}}_N$, only outgoing electrons and no holes in direction $\hat{\underline{\mathbf{k}}}_N$. Deep inside the superconductor where $\Delta(\hat{\mathbf{k}})\equiv\Delta(\hat{\mathbf{k}},z\to\infty)$ is spatially homogeneous, the wave functions have to become proportional to the bulk solutions of the Andreev equations: this explains the form of (2.6c) and (2.6d).

For the matching condition at $z=0$ one has to take into account the normal reflection and transmission properties of the interface. They result from interface potentials and mismatch of Fermi velocities and are parametrized by ($\hat{\mathbf{k}}$-dependent) reflection and transmission amplitudes r and t. The reflection coefficient $R=|r|^2$ will be our parameter to describe the nonideality of the interface. It is independent of temperature and has to be distinguished from $R_N=|r_N|^2$, the probability for normal reflection if the right side of the interface is superconducting. With these amplitudes the matching conditions for the two-component wave functions take the form (Shelankov[35])

$$\psi_{\hat{\mathbf{k}}_N}(z=-0)=\frac{1}{t}\psi_{\hat{\mathbf{k}}_S}(z=+0)+\frac{r^*}{t^*}\psi_{\hat{\underline{\mathbf{k}}}_S}(z=+0)\ , \tag{2.7a}$$

$$\psi_{\hat{\underline{\mathbf{k}}}_N}(z=-0)=\frac{r}{t}\psi_{\hat{\mathbf{k}}_S}(z=+0)+\frac{1}{t^*}\psi_{\hat{\underline{\mathbf{k}}}_S}(z=+0)\ . \tag{2.7b}$$

Once we have solved (2.5) with the boundary conditions (2.6) and (2.7), the Andreev reflection coefficient follows

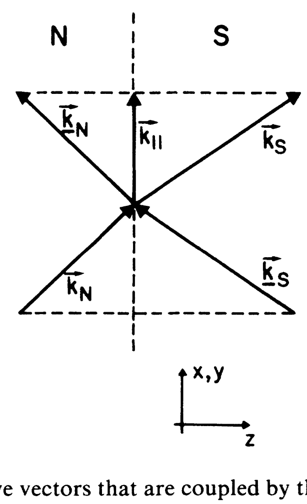

FIG. 2. Wave vectors that are coupled by the interface.

from (2.6a) as $R_A=|r_A|^2$, and the probability for normal reflection from (2.6b) as $R_N=|r_N|^2$. The corresponding transmission coefficients T_1 (ordinary transmission) and T_2 (transmission with change of branch of the excitation spectrum) can be determined from the constants c_1 and c_2 via

$$T_i=\begin{cases} 0 \quad \text{for } E<|\Delta(\hat{\mathbf{k}})| \\ |c_i|^2(\{E+[E^2-|\Delta(\hat{\mathbf{k}})|^2]^{1/2}\}^2-|\Delta(\hat{\mathbf{k}})|^2) \\ \qquad\qquad \text{for } E>|\Delta(\hat{\mathbf{k}})|\ . \end{cases} \tag{2.8}$$

The energy dependence of both R_A and R_N contains information on the superconducting order parameter since $R_A+R_N=1$ for $E<\Delta(\hat{\mathbf{k}})$.

We have to choose a model for the $\mathbf{k}$ dependence of r,t: we took the coefficients appropriate to a δ-function potential $V\delta(z)$ for simplicity, i.e.,

$$r=\frac{V}{i(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})-V}\ , \tag{2.9a}$$

$$t=\frac{i(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})}{i(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})-V}\ , \tag{2.9b}$$

where we have used our usual units, $\hbar=v_F=1$ so that, e.g., $i\hbar^2k_z/m=i(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})$. The result for the reflection coefficient is

$$R=|r|^2=\frac{V^2}{V^2+(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})^2}\ . \tag{2.10}$$

The value of R quoted as a parameter for the figures in Secs. V and VI is (2.10) with $\hat{\mathbf{k}}=\hat{\mathbf{z}}$, i.e.,

$$R=\frac{V^2}{V^2+1}\ . \tag{2.11}$$

III. SELF-CONSISTENT DETERMINATION OF THE PAIR POTENTIAL

Andreev[26] used a step function $\Delta(x)=\Delta\Theta(x)$ as a model for the pair potential of a normal-metal–superconductor interface. This would be exact for the case of an s-wave superconductor if the interface had a reflectivity of $R=1$: surfaces are not pair breaking for s-wave superconductors. For finite transmittance, Cooper pairs leak over to the normal side, leading to a decrease of the pair potential as one approaches the interface from the superconducting side and a nonvanishing pair amplitude on the normal side of the interface (proximity effect, see, e.g., Kieselmann[36] and references therein). Since the energy dependence of the Andreev reflection coefficient depends on the shape of the pair potential, we need to determine $\Delta(x)$.

For the case of an unconventional superconductor the situation gets more complicated: reflecting boundaries can be pair breaking in this case so that the pair potential is suppressed at the interface even for ideal reflection.[37] If we use, e.g.,

$$\Delta(\hat{\mathbf{k}})=\Delta_1 k_x k_y + i\Delta_2 k_y k_z$$

for the bulk order parameter, it turns out that Δ_1 and Δ_2 will vary on different length scales as one approaches the interface. Therefore, an accurate determination of the shape of the pair potential is absolutely necessary to study the Andreev reflection problem.

The only tractable formalism for the determination of the self-consistent pair potential is the ELOE (Eilenberger-Larkin-Ovchinnikov-Eliashberg) formalism described, e.g., in Serene and Rainer.[38] It consists in eliminating from the outset the unnecessary quantum-mechanical degrees of freedom, i.e., the fast oscillations of the Gor'kov Green's functions $G(\mathbf{x},\mathbf{x}_2)$. If we transform to relative and center-of-mass coordinates and take the Fourier transform with respect to the relative coordinates, we obtain $G(\mathbf{k},\mathbf{R})$ which, as a function of $|\mathbf{k}|$, is strongly peaked around k_F. Since this structure is not needed in the weak-coupling theory of superconductivity, Eilenberger[39] proposed to get rid of it by integrating over $|\mathbf{k}|$ or rather $\xi=k^2/2m-\mu$. The question was then whether one could obtain a set of equations in which only these modified Green's functions occurred, and Eilenberger showed that Gor'kov's equations could be replaced by a first-order differential equation using $(k_F\xi_0)^{-1}$ as a small parameter (quite similar to the replacement of the BdG equations by the Andreev equations described in Sec. II). We only outline the method here, details can be found in Serene and Rainer,[38] Kieselmann,[36] and Zhang *et al.*[40] The central quantity of the ELOE formalism for *even-parity* superconductors is the 2×2 quasiclassical Green's function $\hat{g}$ that is obtained from the ordinary Gor'kov Green's functions $\hat{G}$ by an integration over the energy variable $\xi=k^2/2m-\mu$. For a homogeneous *s*-wave superconductor, we have, e.g.,

$$\hat{G}=\frac{1}{\epsilon_n^2+\xi^2+|\Delta|^2}\begin{bmatrix}-i\epsilon_n-\xi & \Delta\\ \Delta^* & -i\epsilon_n+\xi\end{bmatrix}, \tag{3.1}$$

and

$$\begin{aligned}\hat{G}&=\int_{-\infty}^{\infty}d\xi\hat{\tau}^3\hat{G}\\ &=\int_{-\infty}^{\infty}d\xi\frac{1}{(\xi-i\Omega)(\xi+i\Omega)}\begin{bmatrix}-i\epsilon_n & \Delta\\ -\Delta^* & +i\epsilon_n\end{bmatrix}\\ &=\left[\frac{-i\pi}{\Omega}\right]\begin{bmatrix}\epsilon_n & +i\Delta\\ -i\Delta^* & -\epsilon_n\end{bmatrix},\end{aligned} \tag{3.2}$$

where the Matsubara frequencies ϵ_n are defined by $\epsilon_n=\pi T(2n-1)$, $\hat{\tau}^i$ are the Pauli matrices and $\Omega=(\epsilon_n^2+|\Delta|^2)^{1/2}$. Unit vectors as well as 2×2 matrices are denoted by a caret. The factor $\hat{\tau}^3$ in the definition of $\hat{g}$ is conventional. Obviously in (3.2) we have $\hat{g}^2=-\pi^2\hat{\tau}^0$ and this normalization condition is fulfilled in the general inhomogeneous case as well. Gor'kov's equations can be transformed to an equation for the quasiclassical Green's function that takes the following form:

$$[i\epsilon_n\hat{\tau}^3-\hat{\Delta}(\hat{\mathbf{k}},z),\hat{g}(\hat{\mathbf{k}},z;\epsilon_n)] + iv_F(\hat{\mathbf{k}}\cdot\hat{\mathbf{z}})\frac{d}{dz}\hat{g}(\hat{\mathbf{k}},z;\epsilon_n)=0\ . \tag{3.3}$$

Here, [,] denotes a commutator and $\hat{\Delta}$ is given by[41]

$$\hat{\Delta}(\hat{\mathbf{k}},z)=\begin{bmatrix}0 & \Delta(\hat{\mathbf{k}},z)\\ -\Delta^*(\hat{\mathbf{k}},z) & 0\end{bmatrix}. \tag{3.4}$$

The self-consistency condition for the pair potential is given by the gap equation

$$\Delta(\mathbf{k},z)=T\sum_{0<\epsilon_n<\omega_c}\int d\Omega_{k'}(4\pi)^{-1}(2l+1)V_l P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')\mathrm{Tr}[\hat{g}(\hat{\mathbf{k}}',z;\epsilon_n)(\hat{\tau}^1-i\hat{\tau}^2)]\ . \tag{3.5}$$

Here, l determines the symmetry type of the order parameter, i.e., $l=0$ for *s*-wave, $l=2$ for *d*-wave superconductivity. P_l is a Legendre polynomial, and V_l denotes the strength of the pairing interaction that depends on the cutoff ω_c. To eliminate V_l from this equation in favor of T_c, we introduce T_c by letting $\Delta\to 0$ in (3.5):

$$\begin{aligned}\frac{1}{V_l}&=\sum_{n=1}^{\omega_c/(2\pi T_c)}\frac{1}{n-0.5}\\ &=\ln\left[\frac{T}{T_c}\right]+\sum_{n=1}^{\omega_c/(2\pi T)}\frac{1}{n-0.5}\ .\end{aligned} \tag{3.6}$$

The inhomogeneity of the interface is encoded in the spatial dependence of V_l and T_c:

$$T_c(z)=\begin{cases}T_{cN} & \text{for } z<0\ ,\\ T_{cS} & \text{for } z>0\ ,\end{cases} \tag{3.7}$$

where T_{cN} and T_{cS} are the bulk transition temperatures of the materials that constitute the left-hand and right-hand sides of the interface. They are input parameters for the calculation of the pair potential $\Delta(\hat{\mathbf{k}},z)$ (that is *not* a step function in the variable z).

Putting (3.6) back into (3.5), we obtain

$$\Delta(\mathbf{k},z)=\frac{T\sum_{n>0}\int d\Omega_{k'}(4\pi)^{-1}(2l+1)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')\mathrm{Tr}[\hat{g}(\hat{\mathbf{k}}',z;\epsilon_n)(\hat{\tau}^1-i\hat{\tau}^2)]}{\ln[T/T_c(z)]+\sum_{n>0}(n-0.5)^{-1}} . \tag{3.8}$$

In the last expression, both numerator and denominator diverge for $\omega_c\to\infty$, but the ratio itself is convergent and does not depend much on the value ω_c chosen so that it is enough to take, e.g., $\omega_c\sim 10T_c$ (Kieselmann[36]).

Equations (3.3) and (3.8) have to be supplemented by a boundary condition at the interface since the quasiclassical equations themselves cannot describe changes at a length scale much shorter than ξ_0, e.g., interface potentials. Whereas the Gor'kov Green's functions are continuous at the interface, the quasiclassical ones, being *envelopes* of the Gor'kov Green's functions, can have discontinuities[17] as shown schematically in Fig. 3.

The boundary condition for $\hat{g}$ has been determined a few years ago by Zaitsev[42] and by Kieselmann:[36] if we assume that the interface has a ($\hat{\mathbf{k}}$-dependent) reflection coefficient R and is specularly reflecting so that the vectors $\hat{\mathbf{k}}_N$, $\hat{\underline{\mathbf{k}}}_N$, $\hat{\mathbf{k}}_S$, $\hat{\underline{\mathbf{k}}}_S$ (see Fig. 2) are coupled, the boundary condition takes the form[17,36,40]

$$\hat{d}_N=\hat{d}_S , \tag{3.9a}$$

$$-i\pi\frac{1-R}{1+R}[\hat{s}_S[1-i\hat{d}_S/(2\pi)],\hat{s}_N]=\hat{d}_S(\hat{s}_S)^2 . \tag{3.9b}$$

Here, [,] denotes a commutator and $\hat{d}_N$ $\hat{s}_N$ are defined by

$$\hat{d}_N=\hat{g}(\hat{\mathbf{k}}_N,-0;\epsilon_n)-\hat{g}(\hat{\underline{\mathbf{k}}}_N,-0;\epsilon_n) , \tag{3.10}$$

$$\hat{s}_N=\hat{g}(\hat{\mathbf{k}}_N,-0;\epsilon_n)+\hat{g}(\hat{\underline{\mathbf{k}}}_N,-0;\epsilon_n) . \tag{3.11}$$

$\hat{d}_S$ and $\hat{s}_S$, respectively, are defined by the same equations with $z=+0$ and $\hat{\mathbf{k}}_N$ replaced by $\hat{\mathbf{k}}_S$. Both $\hat{d}$ and $\hat{s}$ depend on the direction $\hat{\mathbf{k}}$ but we will leave out the argument $\hat{\mathbf{k}}$ to make the notation simpler.

To determine the pair potential one has to choose the input parameters, i.e., $T_c(z)$, the $\hat{\mathbf{k}}$ dependence of the bulk order parameters far away from the interface, and the reflexion coefficient R. Starting the iteration procedure by solving (3.3) for $\Delta(\mathbf{k},z)=\Delta(\hat{\mathbf{k}})$ for *all* $\hat{\mathbf{k}}$ and ϵ_n [taking the *nonlinear* boundary condition (3.9) into account], one obtains the new pair potential by (3.8). The procedure is repeated until self-consistency is achieved.

The solution to this iteration problem has been obtained for various simplified cases. Aschauer *et al.*[17] assumed large reflection coefficients $R\approx 1$ which enabled them to linearize the boundary condition. Nagai and Hara[43] studied an interface between an s-wave and a p-wave superfluid using the boundary condition (3.9), but they used prescribed pair potentials and did not try to solve the self-consistency problem.

None of the mentioned approximations has been used in this work. We solve the system of equations (3.3), (3.8), and (3.9) self-consistently, for temperatures that are *not* close to T_c and for various degrees of nonideality of the interface. It is obvious that this task cannot be performed analytically: some details of the numerical realization of the iteration scheme are given in the Appendix.

IV. DISCUSSION OF VARIOUS PROXIMITY BOUNDARIES

In this section a few examples of the behavior of the pair potential $\Delta(\mathbf{k},z)$ at normal-metal–superconductor interfaces will be given. The superconductors considered are an s-wave superconductor with $\Delta(\mathbf{k})=\Delta_0=$const in the bulk, and two d-wave superconductors with

$$\Delta(k)=\Delta_0(k_x^2-k_y^2)$$

and

$$\Delta(\mathbf{k})=2\Delta_0 k_y(k_x+ik_x) .$$

We choose the transition temperatures of the superconducting and normal sides to be $T_{cS}=1$ and $T_{cN}=10^{-6}$. The pair potentials are evaluated for a temperature of $T=0.1$ and reflection coefficients $R=0.8$, 0.2, and 0.0 are used for the interface. The spatial coordinate z is measured in units of the coherence length of the superconducting side, $\xi_0=v_F/2\Delta_0$, and the pair potential is measured in units of T_{cS}.

The results for the s-wave superconductor are shown in Fig. 4. In Fig. 4(a), the interface is strongly reflecting ($R=0.8$), so the superconductor and the normal conductor are almost decoupled and the pair potential is not depressed. In Fig. 4(b), where $R=0.2$, and in Fig. 4(c), where $R=0.0$, we see an increasing depression of the pair potential in the superconductor. Only in the last

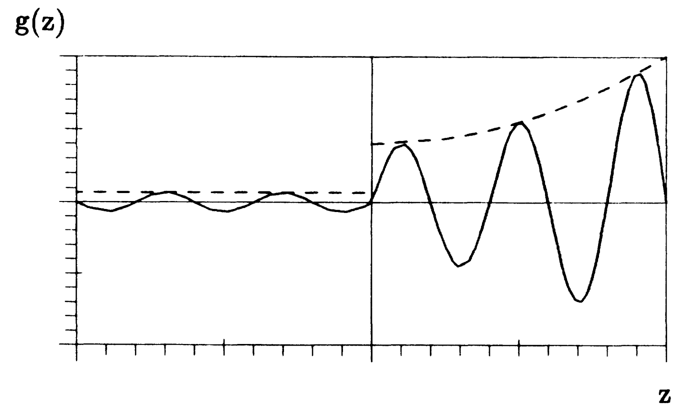

FIG. 3. The envelope of a continuous function may be discontinuous.

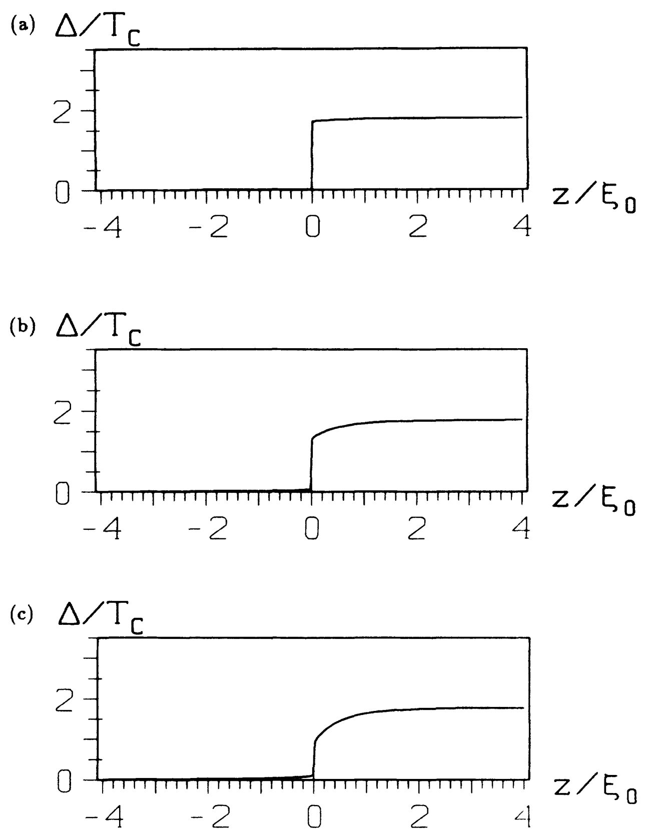

FIG. 4. Pair potential of an s-wave superconductor at an interface. Temperature $T=0.1T_{cS}$. (a) $R=0.8$, (b) $R=0.2$, (c) $R=0.0$.

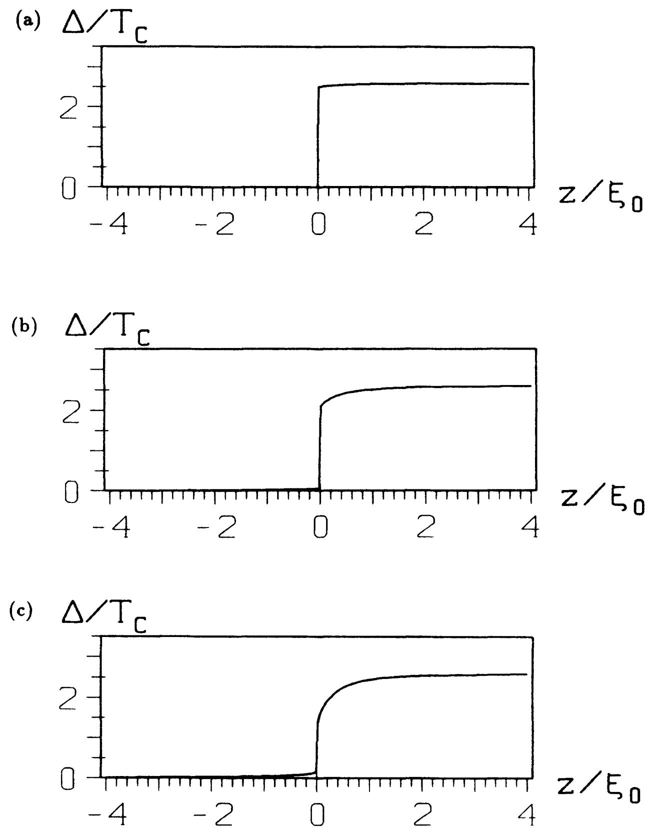

FIG. 5. Same as Fig. 4 for a d-wave superconductor $\Delta(\hat{\mathbf{k}},z)=\Delta(z)(k_x^2-k_y^2)$.

case we see a small pair potential in the normal side as well: this is because we have not plotted the *pair amplitude* $\langle\psi\psi\rangle$ but the *pair potential* $\Delta\sim V\langle\psi\psi\rangle$ that involves the *pairing* interaction V. Since we have assumed a T_{cN} of 10^{-6} which corresponds to a small pairing interaction, the pair potential is negligible on the normal side. It is the pair potential that acts as a scattering potential in the BdG and Andreev equations.

Figure 5 shows the case of the d-wave superconductor

$$\Delta(\hat{\mathbf{k}},z)=\Delta(z)(k_x^2-k_y^2)\ .$$

The spatial dependence of $\Delta(z)$ on z is similar to that of an s-wave pair potential (apart from the ratio Δ_0/T_c that is now given by 2.56 instead of 1.75), since $\Delta(\hat{\mathbf{k}},z)=\Delta(\hat{\underline{\mathbf{k}}},z)$, i.e., quasiparticles are *not* subject to a phase change of the pair potential if they are reflected at the interface. Again, for $R=0.8\simeq 1$ the pair potential stays constant in the superconductor since a reflecting surface in the x-y plane is not pair breaking for this type of d-wave superconductor. The depression of $\Delta(z)$ for $R=0.2$ and 0.0 is similar but not identical to the s-wave case since the directional dependence of the reflection coefficient has different effects in the two cases.

In Fig. 6 we plot a d-wave superconductor with pair potential

$$\Delta(\hat{\mathbf{k}},z)=2\Delta_1(z)k_yk_z+2i\Delta_2(z)k_xk_y\ .$$

Here, the term proportional to Δ_1 of the pair potential changes on reflection, i.e., a reflecting interface is pair breaking since the reflected quasiparticles are subject to a phase change of the pair potential. The self-consistency condition makes the system adjust itself to this adverse condition by depressing the pair potential strongly. Accordingly, Δ_1 and Δ_2 show a very different behavior as a function of R: for $R\approx 0$, both are partially suppressed near the interface due to the proximity effect. For $R>0$, Δ_1 is suppressed further, because of the pair-breaking nature of the interface for this component; Δ_2 rises instead because less Cooper pairs leak over into the normal metal. Finally, for $R\approx 1$, Δ_2 is even enhanced as compared to the bulk value.

The comparison of the two d-wave superconductors clearly proves that the pair potential in unconventional superconductors behaves nontrivially near boundaries and has to be calculated self consistently.

V. REFLECTION COEFFICIENTS AND DIFFERENTIAL CONDUCTIVITIES

Once the self-consistent pair potential of the interface has been calculated, the determination of the Andreev and normal reflection coefficients and the two transmission coefficients (transmission with or without change of branch of the dispersion relation) is reduced to a numeri-

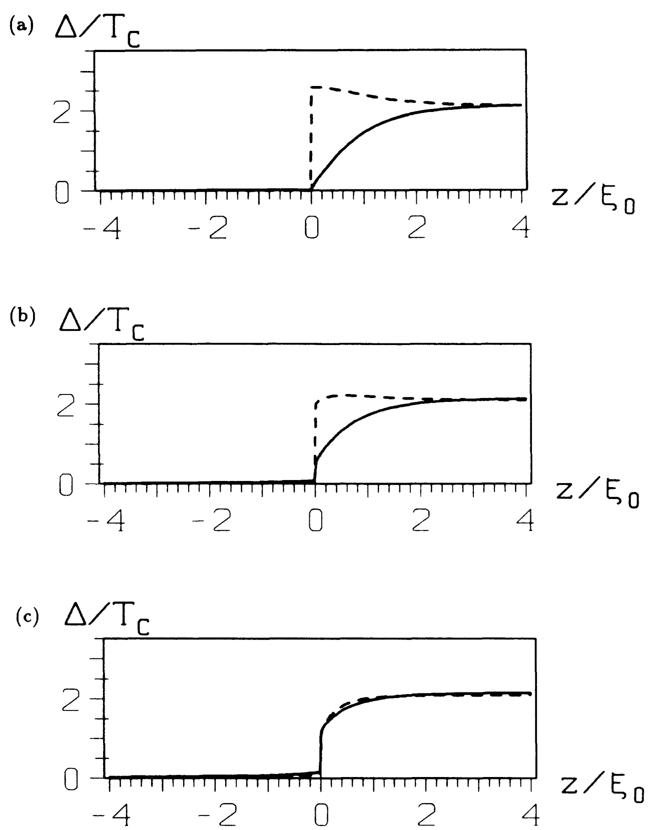

FIG. 6. Same as Fig. 4 for a d-wave superconductor $\Delta(\hat{\mathbf{k}},z)=2\Delta_1(z)k_yk_z+2i\Delta_2(z)k_xk_y$. Solid line: Δ_1. Dashed line: Δ_2.

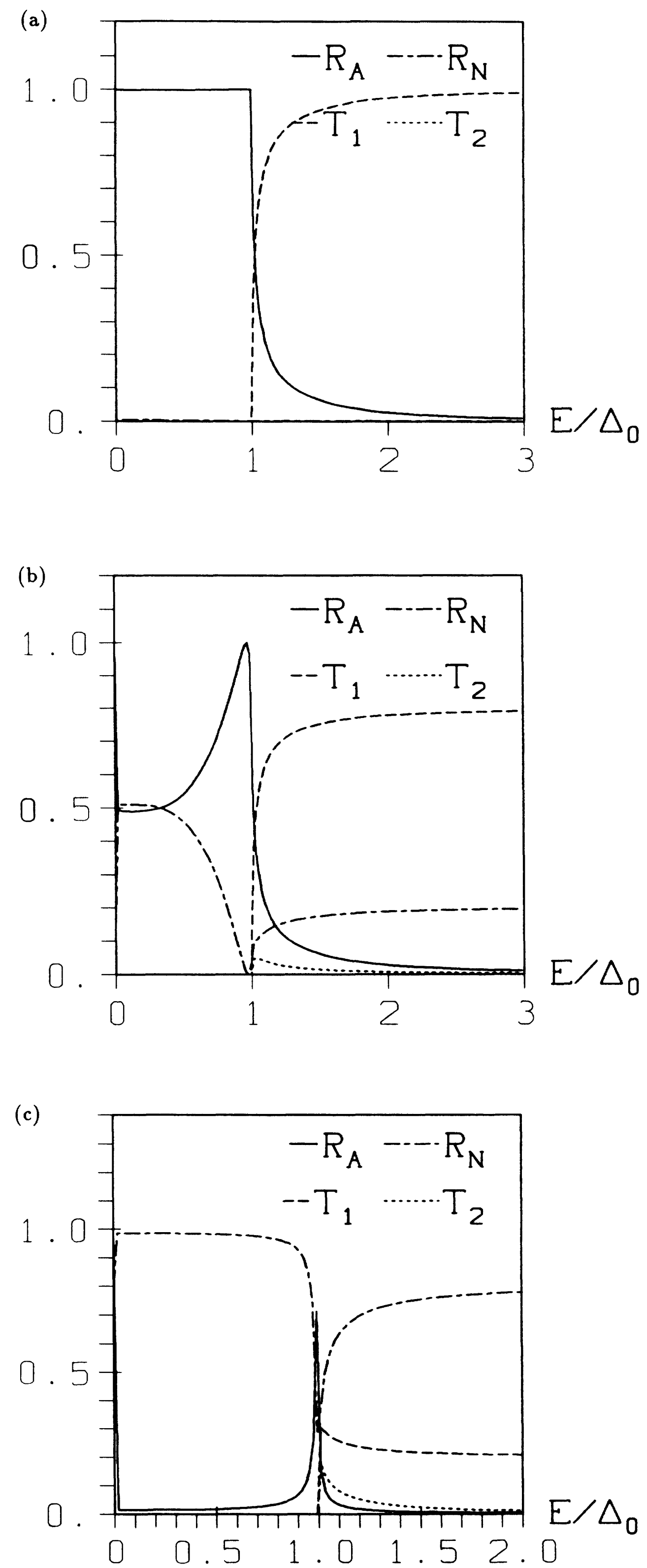

FIG. 7. Reflection and transmission coefficients for an interface of a normal conductor and an s-wave superconductor. Different parameter values for the nonideality of the interface are chosen: (a) $R=0$, (b) $R=0.2$, (c) $R=0.8$. Note the different energy scale in (c).

cal integration of Andreev's equation (2.5) with the boundary and matching conditions (2.6) and (2.7).

These reflection and transmission coefficients have also been calculated for s-wave superconductors by Blonder *et al.*[44] who treated a nonideal interface by introducing a normal potential $V(x)=v\delta(x)$ but approximated the pair potential $\Delta(x)$ by a step function. Similarly, van Son *et al.*[45] looked at smoothly varying but arbitrarily chosen pair potentials and used both the intrinsic reflection coefficient R and the shape of the pair potential as parameters which is not consistent. In our self-consistent treatment, however, R determines the shape of $\Delta(x)$ so that the two cannot be chosen independently.

As a first example, we plot the Andreev reflection coefficient for an s-wave superconductor as a reference. In Fig. 7, we show the Andreev and normal reflection coefficients R_A and R_N and the transmission coefficients without and with branch change, T_1 and T_2 for different values of the intrinsic reflection coefficient R.[46] For $R=0$ in Fig. 7(a), we obtain Andreev's well-known result that $R_A=1$ for $E<\Delta_0$. The pair potential for this situation that we have plotted in Fig. 4(c) does not quite show the shape of a step function so that the *site* at which the incoming particle is reflected will vary with energy. This does not affect R_A, however. The behavior of R_A for

$E > \Delta_0$ will be changed slightly as compared to Andreev's result

$$R_A = \{E/\Delta_0 - [(E/\Delta_0)^2 - 1]^{1/2}\}^2$$

because the pair potential varies smoother around the threshold than a step function.

For $R = 0.2$ in Fig. 7(b), R_A is less than 1 for $E < \Delta_0$ because of a sizable contribution of the normal reflection (remember that $R_A + R_N = 1$ for $E < \Delta_0$). R_N is more than double the value of R for $E = 0$ but vanishes for $E \to \Delta_0$. Anomalous transmission is only present very near the threshold and its size is negligible for $E > 1.5\Delta_0$. In Fig. 7(c) we consider $R = 0.8$ at which R_A is reduced to a narrow spike around $E = \Delta_0$ and a corresponding dip in R_N. The feature that $R_A = 1$ at the bulk gap energy $\Delta(\hat{\mathbf{k}}, z \to \infty)$ even for high interface reflection parameters R for which $R_A < 1$ at $E < \Delta_0$ is important and will occur again and again; it was found by earlier workers as well[44] and can be attributed to the behavior of $\Delta(z)$ at large z: $\Delta(z) \to \Delta_0$ for $z \to \infty$ in our model. That means that for

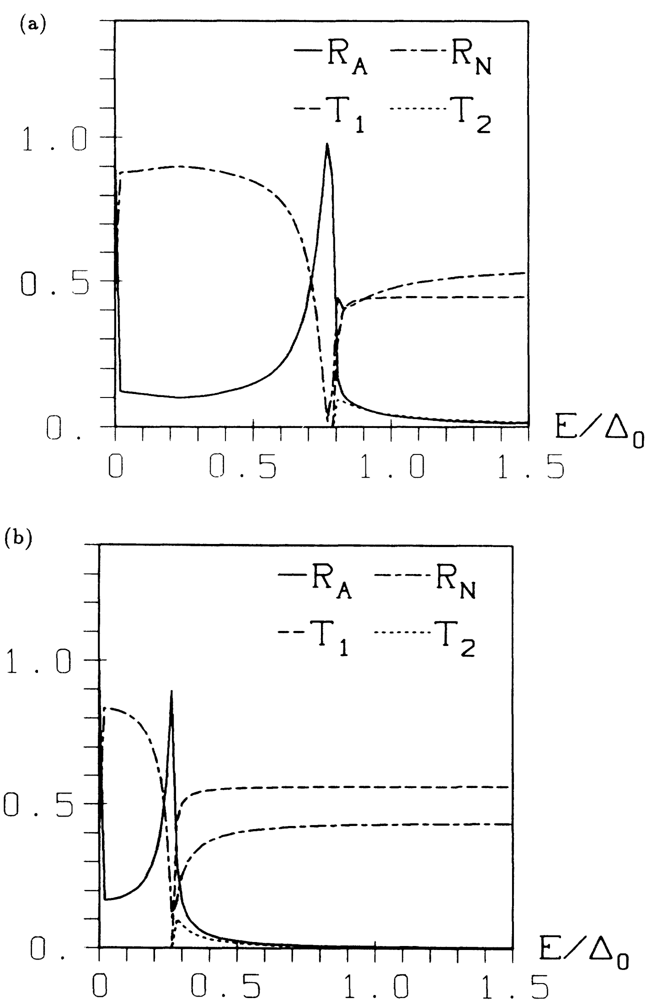

FIG. 8. Reflection and transmission coefficients for an interface of a normal conductor and a d-wave superconductor $\Delta(\hat{\mathbf{k}}) = \Delta(k_x^2 - k_y^2)$. $R = 0.2$. Different $\hat{\mathbf{k}}$ vectors for the incoming electron are chosen: (a) $\hat{\mathbf{k}} = (0, 0.9, 0.45)$, (b) $\hat{\mathbf{k}} = (0.45, 0.7, 0.6)$.

an electron with wave vector $\mathbf{k}$ there is a peak in $R_A(E)$ and a corresponding dip in $R_N(E)$ at $E = \Delta(\hat{\mathbf{k}}, z \to \infty)$.

Now we want to look at anisotropic superconductors. Since the direction of the incoming electron $\hat{\mathbf{k}}$ is a parameter in the Andreev equations, the reflection coefficients depend on energy E and direction $\hat{\mathbf{k}}$.

In Fig. 8 we look at a d-wave superconductor with $\Delta(\hat{\mathbf{k}}) = \Delta(k_x^2 - k_y^2)$ and take $R = 0.2$ for the intrinsic interface reflection. The spatial dependence of the pair potential for this case was shown in Fig. 5(b). The results resemble the s-wave case but now depend on the wave vector of the incoming electron: for $\hat{\mathbf{k}} = (0, 0.9, 0.45)$ shown in Fig. 8(a), we get the usual resonance at the bulk gap value $E = \Delta_0 k_y^2 \approx 0.8\Delta_0$ whereas for $\hat{\mathbf{k}} = (0.45, 0.7, 0.6)$ shown in Fig. 8(b) the resonance peak is shifted down to lower energies.

It is this directional dependence of the Andreev reflection coefficient that we have been looking for: the anisotropy in the interface reflection and transmission coefficients.

Reflection and transmission coefficients for various $\hat{\mathbf{k}}$ directions for

$$\Delta(\hat{\mathbf{k}}) = 2\Delta_1 k_z k_y + 2i\Delta_2 k_y k_x \ , \tag{5.1}$$

the third case we want to investigate, are shown in Fig. 9. Again we have chosen $R = 0.2$. The shape of $\Delta_1(z)$ and $\Delta_2(z)$ has been shown in Fig. 6(b), and an incoming electron with wave vector $\mathbf{k}$ is subject to a linear combination of these two pair potential with weight factors given in (5.1). For $z \to \infty$, $\Delta_1(z), \Delta_2(z) \to \Delta_0$.

For $\hat{\mathbf{k}} = (0, 0.9, 0.45)$ shown in Fig. 9(a), there is no contribution of Δ_2, the resulting pair potential rises smoothly, leading to a rather different shape of $R_A(E)$ than shown in Figs. 8 and 9. Rotating $\hat{\mathbf{k}}$ to $\hat{\mathbf{k}} = (0.1, 0.9, 0.4)$ in Fig. 9(b), the steplike Δ_2 component that is present now shows up in a second resonance peak at $E = 0.2\Delta_0$, i.e., at $2\Delta_0 k_y k_x$. The other resonance peak at the total bulk gap value $E \approx 0.8\Delta_0$ is a very narrow structure that is barely visible in this plot. For $\hat{\mathbf{k}} = (0.3, 0.8, 0.5)$ shown in Fig. 9(c), the second resonance peak is shifted to higher energies with the rising Δ_2 component.

If we lower $|k_y|$ instead, that is to choose, e.g., $\hat{\mathbf{k}} = (0.8, 0.1, 0.6)$ as in Fig. 9(d), all these structures are scaled down to lower energies, and for $k_y = 0$, no Andreev reflection is observed.

The reflection coefficients cannot be measured directly in an experiment, rather one measures the differential conductivity of a point-contact or a double-point-constant device. We use the simplest possible theory to relate reflection coefficients and currents, i.e., we assume that the electron distribution functions in the normal metal and the superconductor are given by shifted Fermi functions if we apply a voltage at the interface. Thus,

$$I \sim \int_{-\infty}^{\infty} dE [f(E - eV) - f(E)] \mathcal{T}(E)$$
$$= \frac{1}{2} \int_0^{\infty} dE \left[\tanh\left[\frac{E + eV}{2T}\right] - \tanh\left[\frac{E - eV}{2T}\right] \right] \mathcal{T}(E) \ . \tag{5.2}$$

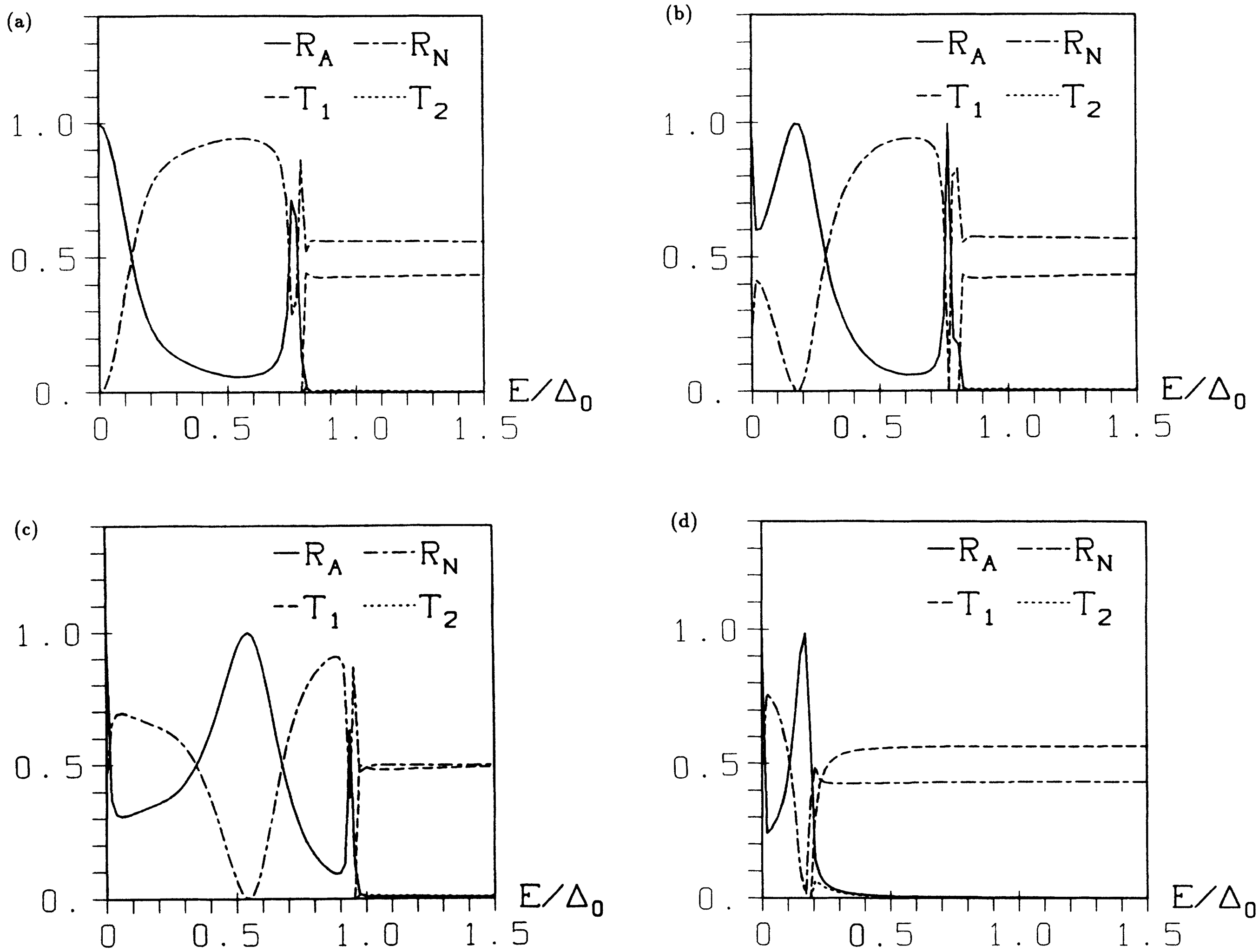

FIG. 9. Reflection and transmission coefficients for an interface of a normal conductor and a d-wave superconductor $\Delta(\hat{\mathbf{k}})=2\Delta_1 k_z k_y+2i\Delta_2 k_y k_x$. $R=0.2$. Different $\hat{\mathbf{k}}$ vectors for the incoming electron are chosen: (a) $\hat{\mathbf{k}}=(0,0.9,0.45)$, (b) $\hat{\mathbf{k}}=(0.1,0.9,0.4)$, (c) $\hat{\mathbf{k}}=(0.3,0.8,0.5)$, (d) $\hat{\mathbf{k}}=(0.8,0.1,0.6)$.

Here, f is the Fermi function and V the voltage across the interface region, $\mathcal{T}(E)$ is an expression that depends on the experimental situation we are looking at:

$$\mathcal{T}(E)=1+R_A(E)-R_N(E) \tag{5.3a}$$

if we are interested in the total current through the interface. Note that Andreev reflection increases the current since the reflected holes carry positive charge. If we collect the reflected holes with a second point contact and ask for their current,

$$\mathcal{T}(E)=R_A(E)\ , \tag{5.3b}$$

and if we collect the normally reflected electrons,

$$\mathcal{T}(E)=R_N(E)\ . \tag{5.3c}$$

The peak observed in $R_A(E)$ at $E=\Delta(\hat{\mathbf{k}},z\to\infty)$ leads to a peak in the differential conductivity dI/dV as well. In Fig. 10 the currents and differential conductivities as a function of voltage (measured in units of Δ_0/e) are shown for the pair potential plotted in Fig. 5(b), and the reflection and transmission coefficients plotted in Fig. 8, i.e., a d-wave order parameter $\Delta(\mathbf{k})\sim k_x^2-k_y^2$ and $R=0.2$. In Fig. 10(a), the direction is $\hat{\mathbf{k}}=(0,0.9,0.45)$ and in Fig. 10(b), $\hat{\mathbf{k}}=(0.45,0.7,0.6)$. The temperature is $T=0.01T_c$. We assume that only the reflected holes are picked up by a second point contact, i.e., we take (5.3b) as a definition of $\mathcal{T}(E)$.

The basic result is that the peak in $R_A(E)$ gets translated into a peak in the differential conductivity dI/dV that appears at the same energy. The anisotropy of the Andreev reflection coefficient leads to a corresponding anisotropy of the differential conductivity, hence, we have obtained a possibility to map out the anisotropy of the spectrum.

In Fig. 10(c) we have used the same parameters as in Fig. 10(a) but the temperature has now been fixed to $T=0.1T_c$. The structures in the differential conductivity

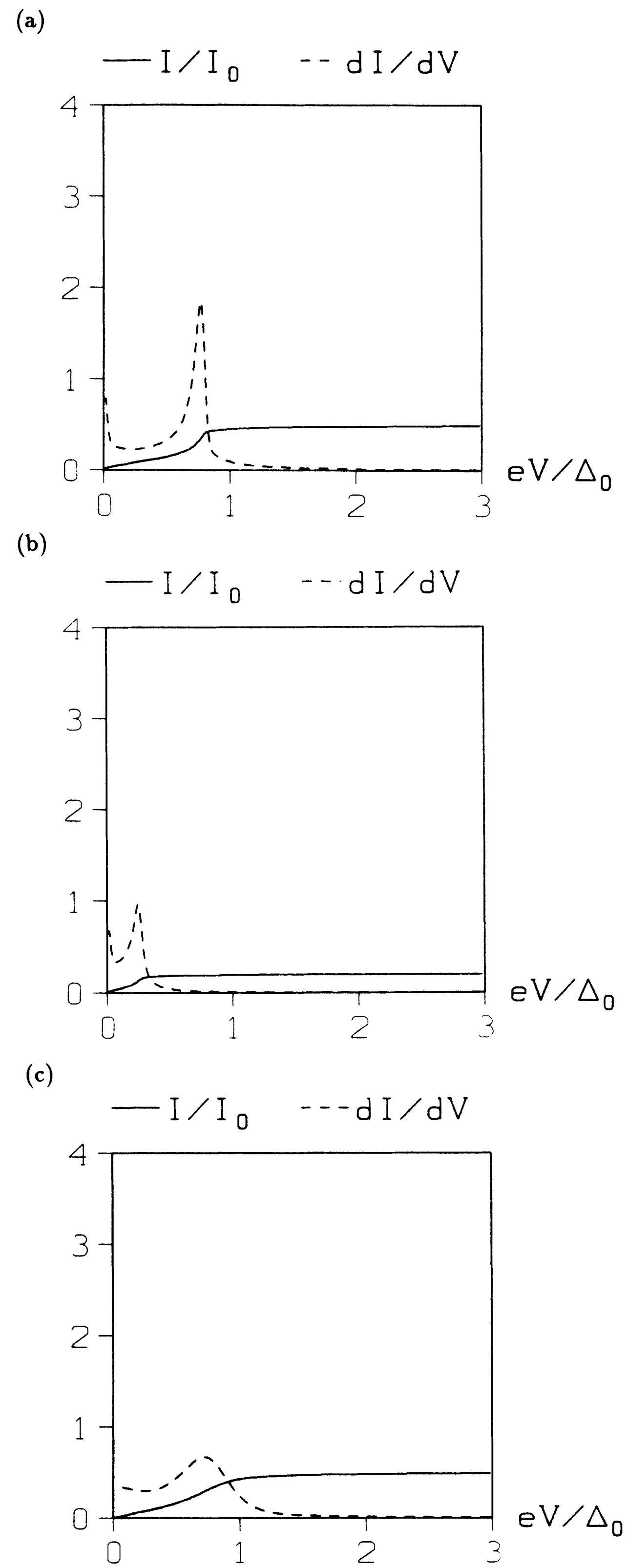

FIG. 10. Current (solid line) and differential conductivity (dashed line) as a function of voltage for an interface to a d-wave superconductor with $\Delta \sim k_x^2 - k_y^2$. The reflection and transmission coefficients for this case have been shown in Fig. 8. $T = 0.01T_c$. (a) $\hat{\mathbf{k}} = (0,0.9,0.45)$. (b) $\hat{\mathbf{k}} = (0.45,0.7,0.6)$. (c) Same as (a) but $T = 0.1T_c$.

are very much smeared out so that $0.1T_c$ would not be low enough a temperature in an experiment.

In Fig. 11 we present the currents and differential conductivities for the pair potential depicted in Fig. 6(b) and the reflection and transmission coefficients plotted in Fig. 9, i.e., for a d-wave superconductor with $\Delta(\mathbf{k}) \sim k_y(k_z + ik_x)$. This time the definition (5.3a) has been chosen for $\mathcal{T}(E)$ which is correct for a (hypothetical) one-point-contact device with directional sensitivity (as might be obtained by etching out structures from the superconducting part of the interface so that only electrons emitted in a particular direction would be Andreev reflected). Here the normalization of the differential conductivity has been chosen such that dI/dV tends to 1 for $eV/\Delta_0 > 1$. The interpretation of the peaks below the threshold remains the same as before, i.e., they correspond to the peaks in the Andreev reflection coefficient $R_A(E)$ and are shifted to lower energies if the gap in the direction looked at is lower.

VI. FEASIBILITY OF AN ANDREEV EXPERIMENT

All experiments supposed to study Andreev scattering have to fulfill a number of general conditions (Benistant[47] and Hoevers[48]).

(a) The normal part of the interface has to be a good single crystal and temperatures have to be low enough such that the mean free path of the electron/holes is of the order of the thickness of the crystal. Any additional scattering would weaken the signal at the collecting point contact and make an interpretation more difficult.

(b) Point contacts have to be used for the injection of electrons into the normal part of the sample: any voltage drop has to occur at the point contact such that the electrons are moving field free and ballistically in the normal metal.

For an experiment trying to exploit the considerations in Sec. V, one would have to be able to measure the reflectivity of the interface for electrons of a given direction only. Previous Andreev scattering experiments do not fulfill this condition: they were done either with one-point contact as is Fig. 12 or with two-point contacts and a magnetic field parallel to the interface as in Fig. 13.

In the one-point-contact experiment shown in Fig. 12 (Benistant *et al.*[49] and Hoevers *et al.*[50]), the reflected holes follow the paths of the injected electrons in the opposite directions. They show up in the differential conductivity of the contact because they increase the current for $T < T_c$. This type of experiment does not need any additional focusing of the reflected holes, but we do not gain information about the $\hat{\mathbf{k}}$ dependence of the reflection coefficient either because it is averaged out. The only possibility we can think of is to remove parts of the superconducting side of the interface. In this way, only the electrons emitted in certain directions would be Andreev reflected, but to change the direction looked at, one would have to take a different sample. Sample differences would make it difficult to compare the results and to extract an angular dependence.

The two-point-contact experiments (Bozhko *et al.*[29]

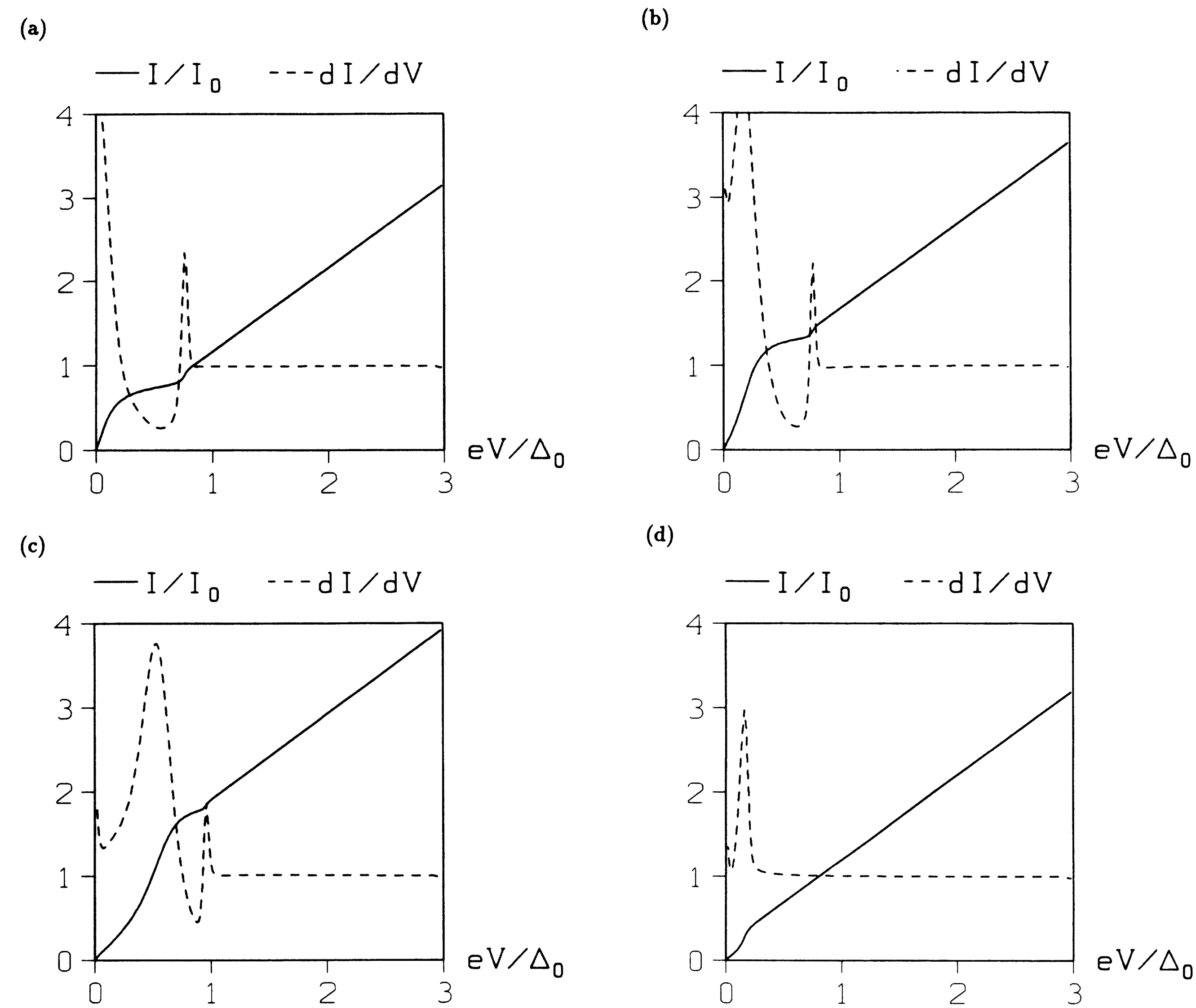

FIG. 11. Current (solid line) and differential conductivity (dashed line) as a function of voltage for an interface to a d-wave superconductor with $\Delta \sim k_y(k_z+ik_x)$. The reflection and transmission coefficients for this case have been shown in Fig. 9. $T=0.01T_c$. (a) $\hat{\mathbf{k}}=(0,0.9,0.45)$. (b) $\hat{\mathbf{k}}=(0.1,0.9,0.4)$. (c) $\hat{\mathbf{k}}=(0.3,0.8,0.5)$. (d) $\hat{\mathbf{k}}=(0.8,0.1,0.6)$.

and Benistant *et al.*[30]) use a homogeneous magnetic field parallel to the interface to deflect the reflected holes from the path of the incoming electrons. The configuration used by Benistant *et al.* is shown in Fig. 13. The magnetic field has a very important second purpose: it focuses the reflected holes onto a second point contact. Without this focusing the signal at the second point contact would be much too small to be detected. This focusing arises

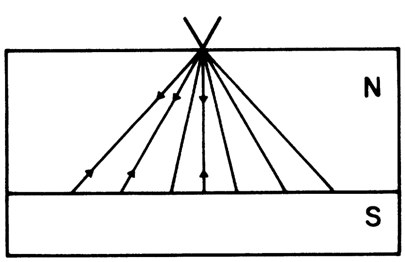

FIG. 12. Andreev reflection in the one-point-contact experiment.

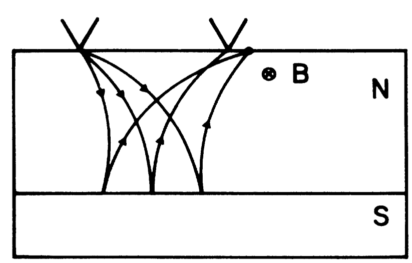

FIG. 13. Two-point-contact configuration used by Benistant *et al.* (Ref. 30).

because all the reflected holes arrive again at the upper surface of the sample at a distance $d > d_0$ from the injecting point contact.

Hence, we obtain focusing of holes *at* the minimum distance d_0 so that this is the distance one should choose between the two point contacts.

Moving the second point contact around the first one (or rather using several point contacts in different lattice directions) and looking at the differential conductivity as a function of the applied voltage, it would indeed be possible to study the $\hat{\mathbf{k}}$ dependence of the Andreev reflection coefficient and hence to deduce $\Delta(\hat{\mathbf{k}})$. The beautiful two-point-contact experiments described above show that this technique works in the case of conventional superconductors like lead, so that one should not expect unsurmountable difficulties in applying it to an interface with an anisotropic superconductor.

There is one difficulty, however: on analysis of the focusing by a homogeneous magnetic field parallel to the interface, it turns out that all the holes that are focused at the minimal distance d_0 emerge from the interface in the *normal* direction, hence, they cannot be used to probe the $\hat{\mathbf{k}}$ dependence of the order parameter. Another collmination technique for the reflected electrons/holes is needed: there are some indications that an inhomogeneous field could do the job, but one needs high-field gradients and correspondingly high fields that would destroy superconductivity at least in part of the sample.

An alternative experiment would be to concentrate not on the reflected but on the *transmitted* quasiparticles. Suppose we put some detector for quasiparticles on the side of the superconductor opposite to the normal conductor (let us call it the right-hand side). The quasiparticles with wave vector $\hat{\mathbf{k}}$ injected by the point contact will then traverse the normal conductor, enter the superconductor, and reach the detector on the right-hand side of the superconductor if their kinetic energy E is larger than $\Delta(\hat{\mathbf{k}})$. If, on the other hand, $E < \Delta(\hat{\mathbf{k}})$, the quasiparticle will be Andreev reflected at the interface so that no quasiparticles can be detected on the right-hand side of the superconductor. This does not means that *nothing* enters the superconductor. A Cooper pair will be transmitted, so that the net result in a stationary situation would be supercurrents in certain $\hat{\mathbf{k}}$ directions and quasiparticle currents in other directions. A tunnel junction is a possible detector that might be used to distinguish between the two kinds of currents since its current-voltage characteristic would resemble that of a *NIN* tunnel junction (*N*: normal metal, *I*: insulator) for incident quasiparticle currents. For an incident supercurrent, however, one expects the current-voltage characteristic of a *NIS* tunnel junction (*S*: superconductor). Accordingly, an array of tunnel junctions on the right-hand side of the superconductor could be used to map out the $\mathbf{k}$ dependence of the order parameter by looking at the current-voltage characteristics of the tunnel junctions in different locations.

A point that has been raised by Anderson[51] in connection with the Andreev scattering experiments done on silver/Y-Ba-Cu-O junctions is the question of what really causes the Andreev scattering of the incoming normal quasiparticle: is it the order parameter of Y-Ba-Cu-O or rather some proximity-induced order parameter in the silver? If the induced order parameter is of the same type as the order parameter of the superconductor, there is no problem since it is not important to know exactly where the incoming quasiparticle has been reflected. If, on the other hand, the induced order parameter is of a different type, we argue as follows: it is the pair potential $\Delta(\hat{\mathbf{k}},z)$ that enters the Bogoliubov–de Gennes equations and causes a scattering of incoming particle into outgoing hole states. Since the pair potential contains the pairing interaction, $\Delta \sim V\langle\psi\psi\rangle$, it is small if the pairing interaction V is small although the induced pair amplitude $\langle\psi\psi\rangle$ may not be small. Now, if one takes silver for the normal side of the interface, the pairing interaction is very small since it is estimated that the T_c of bulk silver is less than 10^{-9} K (Mota[52])—hence, the induced pair potential can only influence incoming electrons at a very low energy but not modify the Andreev scattering at energies of the order of the pair potential of the superconductor.

Up to now, we have not talked about *odd-parity* superconductors since there are additional theoretical and experimental difficulties in this case: as was mentioned in Sec. II, a triplet superconductor will lead to new phenomena involving the spin of the Andreev reflected hole (Kieselmann and Rainer[3]). If we take the equivalent of the A_1 phase of superfluid ^{3}He as a superconductor, the Cooper pairs will be characterized by spin projections $S_z = \pm 1$, and one spin projection will dominate, e.g., $S_z = +1$. Hence, if an unpolarized beam of electrons is injected towards the interface, most of the reflected holes will have a spin projection $S_z = -1$ (missing electrons with $S_z = +1$). To detect the spin polarization of the reflected holes may be possible by using a point contact made from a half-metallic ferromagnet. These materials like NiMnSb, CrO_2, or Fe_3O_4 have a partially filled band and a Fermi surface for spin-up electrons, whereas the spin-down population fills a band and has a gap at the Fermi energy (de Groot *et al.*[53]). Hence, a point contact made of such a material would accept the holes only if they were polarized correctly. Point contacts made of half-metallic ferromagnetics were proposed by Hoevers[48] who was interested in spin-polarized Andreev reflection involving two reflection events at an ordinary *s*-wave superconductor, but to use these materials to distinguish between even- and odd-parity superconductors is suggested here for the first time. Unfortunately, there seem to be material problems which make it very difficult to produce point contacts out of the half-metallic ferromagnetics known at present.[48]

Another problem concerns the interpretation of such an experiment. If one wants to look at spin-polarized Andreev scattering, one has to worry about magnetic scattering at the interface caused by differences in spin-orbit coupling of the two sides of the interface. The boundary condition (3.9) used to calculate the self-consistent pair potential would have to be replaced by a more complicated condition recently found by Millis *et al.*,[16] and more free parameters would have to be introduced to characterize the nonideality of the interface.

VII. CONCLUSION

In conclusion, we have computed the Andreev and normal reflection coefficients of a nonideal NS interface for the case of an anisotropic superconductor by solving the Andreev equations. The pair potential $\Delta(\mathbf{k},z)$ that occurs in the Andreev equations had to be determined self-consistently because of its nontrivial behavior near interfaces: interfaces are pair breaking for non-s-wave superconductors. The result is that the reflection coefficients strongly depend on the direction of the incoming electron: it was shown, that, as a consequence, the differential conductivity is directionally dependent such as to yield enough information to allow the determination of the type of the superconducting order parameter.

Although the experimental question how to obtain the scattering data has not been answered satisfactorily yet, a generalized two-point-contact experiment can be used in principle to look at the $\hat{\mathbf{k}}$ dependence of the Andreev and normal reflection coefficients. The problem of electron collimation (by other means than a homogeneous magnetic field parallel to the interface) remains to be solved. Experiments using one point contact, on the other hand, need no extra focusing, but up to now there are only inelegant ways of making them sensitive to electrons that are emitted and collected in particular directions, e.g., etching out part of the superconductor.

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APPENDIX: NUMERICAL SOLUTION OF THE SELF-CONSISTENCY PROBLEM

For practical calculations it is convenient to expand the quasiclassical Green's function and all the 2×2 matrices that occur in the boundary condition (3.9) in Pauli matrices, i.e., $\hat{g}=\mathbf{g}\cdot\tau$, etc. There is no $\hat{\tau}^0$ component in $\hat{g}$ because it has to fulfill the normalization condition $\hat{g}^2=-\pi^2$. Doing this, the quasiclassical equation (3.3) takes the form

$$\frac{d}{dz}\mathbf{g}(z)=\frac{2}{k_z v_F}\begin{bmatrix} 0 & i\epsilon_n & i\Delta_R(z) \\ -i\epsilon_n & 0 & -i\Delta_I(z) \\ -i\Delta_R(z) & i\Delta_I(z) & 0 \end{bmatrix}, \tag{A1}$$

where Δ_R and Δ_I are the real and imaginary parts of the pair potential, the self-consistency condition reads

$$\Delta(\mathbf{k},z)=\frac{2T\sum_{n>0}\int d\Omega_{k'}(4\pi)^{-1}(2l+1)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')[g_1(\hat{\mathbf{k}}',z;\epsilon_n)-ig_2(\hat{\mathbf{k}}',z;\epsilon_n)]}{\ln[T/T_c(z)]+\sum_{n>0}(n-0.5)^{-1}} \tag{A2}$$

and the boundary condition becomes[54]

$$\mathbf{d}_S=\mathbf{d}_N\ , \tag{A3}$$

$$\alpha[2\pi\mathbf{s}_N\times\mathbf{s}_S-\mathbf{d}_S(\mathbf{s}_N\cdot\mathbf{s}_S)]+\mathbf{d}_S(\mathbf{s}_S)^2=0\ , \tag{A4}$$

where $\alpha=(1-R)/(1+R)$. Since the pair potential will be constant and equal to its bulk value far away from the interface, we have to know the solutions of (A1) for constant Δ. There is one constant solution,

$$\mathbf{g}_{\text{const}}(z)=\frac{-i\pi}{E_n}\begin{bmatrix} -\Delta_I \\ -\Delta_R \\ \epsilon_n \end{bmatrix}, \tag{A5}$$

where $E_n=(\epsilon_n^2+|\Delta|^2)^{1/2}$, and two exponentially increasing and decreasing solutions

$$\mathbf{g}_i(z)=\begin{bmatrix} -\Delta_R E_n+i\Delta_I\epsilon_n \\ \Delta_I E_n+i\Delta_R\epsilon_n \\ i(\Delta_R^2+\Delta_I^2) \end{bmatrix}\exp\left[\frac{2E_n z}{v_F k_z}\right],$$

$$\mathbf{g}_d(z)=\begin{bmatrix} \Delta_R E_n+i\Delta_I\epsilon_n \\ -\Delta_I E_n+i\Delta_R\epsilon_n \\ i(\Delta_R^2+\Delta_I^2) \end{bmatrix}\exp\left[-\frac{2E_n z}{v_F k_z}\right]. \tag{A6}$$

Now to solve (A1) with (A3) and (A4), we have to take appropriate linear combinations of (A5) and (A6) as an ansatz for the solutions far away from the interface where the system is homogeneous and then determine the coefficients in this ansatz by an integration of the quasiclassical equation.

As an example, consider the solution in direction $\hat{\mathbf{k}}_S$ (see Fig. 2) and choose a point $z_0>0$ far away from the interface, i.e., $z_0/\xi_0\gg1$. Here the system is homogeneous so that we can use the following initial value for the integration of the quasiclassical equation:

$$\begin{aligned} \mathbf{g}(z_0)&=\mathbf{g}_{\text{const}}(z_0)+a_S\mathbf{g}_d(z_0)\ , \\ \mathbf{g}(-z_0)&=\mathbf{g}_{\text{const}}(-z_0)+a_N\mathbf{g}_d(-z_0)\ . \end{aligned} \tag{A7}$$

Here we have left out the arguments $\hat{\mathbf{k}}_S,\hat{\mathbf{k}}_N$. The exponentially rising solution $\mathbf{g}_i(z)$ cannot contribute to (A7) since the quasiclassical Green's function has to be bounded for $z\rightarrow\infty$. Integration of the quasiclassical equation leads to

$$\mathbf{g}(0+)=U(0,z_0)\mathbf{g}_{\text{const}}(z_0)+a_S U(0,z_0)\mathbf{g}_d(z_0)\ , \tag{A8}$$

$$\mathbf{g}(0-)=U(0,-z_0)\mathbf{g}_{\text{const}}(-z_0)+a_N U(0,-z_0)\mathbf{g}_d(-z_0)\ ,$$

since we are dealing with a linear differential equation. The symbol $U(z,z_0)$ is used to denote the evolution operator for the differential equation (A1). Repeating this procedure for the other directions involved, $\hat{\mathbf{k}}_S$, $\hat{\mathbf{k}}_N$, $\hat{\mathbf{k}}_N$ (see Fig. 2), we can now calculate $\mathbf{d}_N$, $\mathbf{d}_S$, $\mathbf{s}_N$, $\mathbf{s}_S$ and put them in the first part of the boundary condition (A3) to obtain a linear relation between the coefficients a_S and a_N that we have introduced in the initial value.

The second part of the boundary condition then takes the form of a polynomial of third degree with coefficients c_n and variable a_S:

$$\sum_{n=0}^{3} c_n a_S^n = 0 \ . \tag{A9}$$

The zeroes of this polynomial can be found easily. At this point the nonuniqueness problem[38] of the quasiclassical theory rears its head: the correct zero has to be chosen by a physical argument, i.e., adiabatic continuation from some known case, e.g., $R=0$ or 1.

Numerical integration of the differential equation (A1) was performed with a Runge-Kutta algorithm using the multiplication trick of Thuneberg *et al.*:[55] it is used to obtain the equivalent of the constant solution (A5) in the inhomogeneous case. Simple numerical integration starting at (A5) will not do because of the presence of the exponentially rising solutions (A6) that will dominate any numerical integration scheme. The multiplication trick uses the fact that the product of the exponentially increasing and decreasing solutions (written in matrix notation) just yields the constant solution.

The numerical integration over the unit sphere needed in the self-consistency condition (A2) was done with the Romberg algorithm using a small number of interpolation points since the evaluation of the integrand (the solution of a boundary value problem) is expensive in computation time.

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