Transfer-matrix description of heterostructures involving superconductors and ferromagnets

J. Kopu,[1] M. Eschrig,[1] J. C. Cuevas,[1] and M. Fogelström[2]
[1]*Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany*
[2]*Applied Quantum Physics, MC2, Chalmers, S-41296 Göteborg, Sweden*
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Based on the technique of quasiclassical Green's functions, we construct a theoretical framework for describing heterostructures consisting of superconductors and/or spin-polarized materials. The necessary boundary conditions at the interfaces separating different metals are formulated in terms of hopping amplitudes in a *t*-matrix approximation. The theory is applicable for an interface with arbitrary transmission and exhibiting scattering with arbitrary spin dependence. Also, it can be used in describing both ballistic and diffusive systems. We establish the connection between the standard scattering-matrix approach and the existing boundary conditions, and demonstrate the advantages offered by the *t*-matrix description.

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I. INTRODUCTION

Low-energy (below the superconducting energy gap) electron transport through contacts between a superconductor and a normal metal can be understood in terms of Andreev reflection.[1] In this process, an incident electron from the normal side can enter the superconductor by pairing with another electron with the opposite spin, leaving a reflected hole in the normal metal. The phase-coherent nature of this process results in superconducting correlations being induced in the normal-metal side, referred to as the proximity effect. The important feature of Andreev reflection is that, with singlet superconductors, it involves both spin bands in the normal metal. Therefore, the above simple picture has to be modified when the normal metal is replaced by a ferromagnet with two different Fermi surfaces for the two spins, resulting in new and interesting physical phenomena. In recent years, interplay between superconductivity and ferromagnetism has attracted considerable theoretical[2–5] and experimental[6–9] attention—both out of fundamental scientific interest and in view of the possibility of novel applications and devices. One important consequence of the spin splitting between the two bands in the ferromagnet is that the phase coherence between the particle–hole pair in the clean (dirty) limit is destroyed over a characteristic distance of v_f/h ($\sqrt{D/h}$), where v_f is the Fermi velocity, D the diffusion constant, and h an effective exchange energy which describes the spin splitting. Since this distance is typically very short (of the order of atomic distances), the superconducting correlations induced to the ferromagnetic material are expected to be confined to the immediate vicinity of the separating interface. This raises the question whether, for strong ferromagnets, a mechanism of a different type takes over and dominates the physics of superconductor/ferromagnet (S/F) contacts. One such mechanism, recently under active investigation, is the inducement of spin-triplet correlations: namely, the exchange field only affects correlations of singlet type, i.e., between particles and holes in opposite spin bands. In fact, equal-spin triplet correlations are expected to be created by proximity to a ferromagnet due to the breaking of spin-rotational symmetry. The desire to formulate a theory capable of understanding the detailed nature and the conditions for the formation of these correlations and the corresponding anomalous proximity effect has given the initial motivation for this work.

Problems related to superconducting proximity effect with spin-dependent interfacial scattering are of spatially inhomogeneous nature and, as such, they can only be studied with specialized theoretical tools. Such a tool is provided by the quasiclassical theory of superconductivity.[10,11] This theory is applicable for weakly perturbed superconductors (characteristic length scale of perturbations much larger than Fermi wave length and characteristic frequencies much less than Fermi energy) and can be used in both equilibrium and nonequilibrium situations. It describes quasiparticles with momenta on the Fermi surface moving along straight classical trajectories, the direction of which is given by the corresponding Fermi velocity. A ferromagnetic metal has different Fermi surfaces and, correspondingly, different sets of trajectories for the two spin orientations. In this case, the quasiclassical theory can be used to describe two limiting cases: (i) weak ferromagnetism, where the energy splitting of the two Fermi surfaces and the associated deviation of the Fermi velocities is so small that the two spin trajectories with the same momentum direction are fully coherent, and (ii) strong ferromagnetism, where the splitting is so large that the coherence is lost completely. While the former limiting case has been exhaustively studied in the literature, the latter has only recently received attention.[12] Here we present a theoretical study of the latter possibility. Even in the absence of conventional Andreev reflection processes (which would require coherence between particles and holes in opposite spin bands), interesting and nontrivial physics emerges due to spin-active interfacial scattering. Additional motivation has been provided by the growing interest in a new class of materials, half-metallic ferromagnets.[13–16] In these materials, one spin band is metallic and the other one insulating (100% polarized ferromagnet). Since a half metal has a Fermi surface only for one of the two spin orientations, it is clear that the traditional description for weak ferromagnets is inapplicable, and other methods must be employed.

In Sec. II, we outline the central equations of the quasiclassical theory of superconductivity. Compared with the full microscopic theory, the quasiclassical theory offers consider-

able simplifications when treating spatially inhomogeneous states by reducing the content of (unnecessary) information carried by the Green's functions. However, this leads to nontrivial boundary conditions which have to be formulated at interfaces separating different metals that connect the solutions of the two sides. Such conditions have been derived for nonmagnetic interfaces by Zaitsev,[17] and for magnetic interfaces by Millis *et al.*[18] After a short description of this work in Sec. III, we formulate an alternative but equivalent set of boundary conditions, where the transmission through an interface is parameterized by a hopping amplitude that contains the information of various processes contributing to particle transfer. This approach enables the formulation of boundary conditions in a simple and appealing form. The equivalence to existing methods is demonstrated in Sec. IV. As explained in Sec. V, the advantages of the *t*-matrix formulation are especially evident in studying interfaces that separate two materials with a different structure of the Green's functions and/or a different number of trajectories, such as in the case of a superconductor/strong ferromagnet interface. Finally, in Sec. VI, we apply our theory to study the current through a point contact separating a singlet superconductor from a strong ferromagnet.

II. BASIC EQUATIONS OF QUASICLASSICAL THEORY

The quasiclassical theory of superconductivity[10,11] is formulated in terms of quasiclassical Green's functions (or propagators) $\check{g}(\hat{\mathbf{p}},\mathbf{R},\epsilon,t)$ that depend on the spatial coordinate $\mathbf{R}$ and time t and describe quasiparticles with energy ϵ (measured from the chemical potential) and the momentum direction on the Fermi surface $\hat{\mathbf{p}}=\mathbf{p}/p_f$ moving along classical trajectories with direction given by the Fermi velocity $\mathbf{v}_f(\hat{\mathbf{p}})$.[19] The quasiclassical Green's functions are 2×2 matrices in Keldysh space (denoted by a ''check'' accent),

$$\check{g}=\begin{pmatrix}\hat{g}^R & \hat{g}^K\\ 0 & \hat{g}^A\end{pmatrix}, \tag{1}$$

with three nonzero elements (retarded $\hat{g}^R$, advanced $\hat{g}^A$, and Keldysh $\hat{g}^K$). In describing superconductivity, these elements in turn are 4×4 Nambu-Gor'kov matrices in combined particle–hole and spin space (denoted by the hat symbol), for example, the retarded Green's function has the form

$$\hat{g}^R=\begin{pmatrix} g^R_{\uparrow\uparrow} & g^R_{\uparrow\downarrow} & f^R_{\uparrow\uparrow} & f^R_{\uparrow\downarrow}\\ g^R_{\downarrow\uparrow} & g^R_{\downarrow\downarrow} & f^R_{\downarrow\uparrow} & f^R_{\downarrow\downarrow}\\ \tilde{f}^R_{\uparrow\uparrow} & \tilde{f}^R_{\uparrow\downarrow} & \tilde{g}^R_{\uparrow\uparrow} & \tilde{g}^R_{\uparrow\downarrow}\\ \tilde{f}^R_{\downarrow\uparrow} & \tilde{f}^R_{\downarrow\downarrow} & \tilde{g}^R_{\downarrow\uparrow} & \tilde{g}^R_{\downarrow\downarrow}\end{pmatrix}. \tag{2}$$

All these matrix elements are not independent of each other. Indeed, the elements in the lower half of the matrix are related to the ones in the upper half through the conjugation symmetry, e.g.,

$$\tilde{g}^{R,A,K}_{\alpha\beta}(\hat{\mathbf{p}},\mathbf{R},\epsilon,t)=g^{R,A,K}_{\alpha\beta}(-\hat{\mathbf{p}},\mathbf{R},-\epsilon,t)^*. \tag{3}$$

The quasiclassical Green's functions satisfy the Eilenberger transport equation

$$[\epsilon\check{\tau}_3-\check{\Sigma},\check{g}]_\otimes+i\mathbf{v}_f(\hat{\mathbf{p}})\cdot\nabla_{\mathbf{R}}\check{g}=0. \tag{4}$$

Generally speaking, the self-energy $\check{\Sigma}(\hat{\mathbf{p}},\mathbf{R},\epsilon,t)$ includes molecular fields, the superconducting order parameter $\check{\Delta}=\hat{\Delta}\check{1}$, impurity scattering, and external fields. The noncommutative product $\otimes$ combines matrix multiplication with a convolution over the internal variables, and $\check{\tau}_3=\hat{\tau}_3\check{1}$ is a Pauli matrix in particle–hole space. The quasiclassical Green's functions also satisfy a normalization condition

$$\check{g}\otimes\check{g}=-\pi^2\check{1}. \tag{5}$$

In addition to Eqs. (4) and (5), self-consistency equations for different parts of the self-energy have to be provided; e.g., for the (weak-coupling) order parameter the condition reads

$$\hat{\Delta}(\mathbf{R},t)=\lambda\int_{-\epsilon_c}^{\epsilon_c}\frac{d\epsilon}{4\pi i}\langle\hat{f}^K(\hat{\mathbf{p}},\mathbf{R},\epsilon,t)\rangle_{\hat{\mathbf{p}}}, \tag{6}$$

where λ is the strength of the pairing interaction, $\langle\ \rangle_{\hat{\mathbf{p}}}$ denotes averaging over the Fermi surface, and $\hat{f}^K$ is the particle–hole off-diagonal part of the quasiclassical Keldysh Green's function. The cut-off energy ϵ_c is to be eliminated in favor of the transition temperature in the usual manner.

When the quasiclassical Green's function has been determined, physical quantities of interest can be calculated; e.g., the expression for the current density adopts the form

$$\mathbf{j}(\mathbf{R},t)=\int\frac{d\epsilon}{8\pi i}\mathrm{Tr}\langle eN_f\mathbf{v}_f(\hat{\mathbf{p}})\hat{\tau}_3\hat{g}^K(\hat{\mathbf{p}},\mathbf{R},\epsilon,t)\rangle_{\hat{\mathbf{p}}}, \tag{7}$$

where e is the electron charge and N_f is the density of states on the Fermi surface. However, to form a complete theory for studying heterostructures, the above equations must still be supplemented with the boundary conditions connecting the solutions at the separating interfaces. We introduce these conditions in the following section.

III. BOUNDARY CONDITIONS

A. Scattering-matrix approach

Interfaces represent strong perturbations on an atomic length scale and, therefore, fall out of the applicability range of quasiclassical theory. However, as was shown in the pioneering work of Zaitsev,[17] interfaces can be brought within the quasiclassical theory by means of effective boundary conditions that connect trajectories related through interface scattering processes. Later these conditions were generalized for an arbitrary magnetically active interface, i.e., one that scatters quasiparticles differently depending on their spin orientation.[18] The latter case is relevant for studying interfaces with spin-polarized materials such as ferromagnets. The procedure for the derivation of the boundary conditions begins by isolating a region of quasiclassical size $|x|<\delta$ around the interface located at the origin of the perpendicular

coordinate x (δ much larger than the atomic-size range of the strong interface potential but much smaller than the superconducting coherence length ξ). In the half spaces $|x|>\delta$, the solutions for quasiclassical Green's functions can be found by standard methods described in the previous chapter. The solutions for the left (l) and right (r) sides are then matched via a scattering matrix

$$\hat{\mathbf{S}}=\begin{pmatrix} \hat{S}^{ll} & \hat{S}^{lr} \\ \hat{S}^{rl} & \hat{S}^{rr} \end{pmatrix}, \tag{8}$$

the form of which is determined by the detailed microscopic structure of the interface region and on the quasiclassical level has to be treated as a phenomenological parameter of the theory. The crucial simplifying observation is that, since the strong (of the order of the Fermi energy) interface potential dominates the Hamiltonian in the interface region, the scattering matrix (8) corresponds to that of the *normal state*, i.e., does not contain particle–hole mixing. Also, it has no Keldysh space structure.

The boundary conditions were derived for a smooth (on the scale of ξ) interface, assuming the conservation of momentum $\mathbf{p}_\parallel$ parallel to the interface. In the following, all momentum-dependent quantities should be understood as having the same $\mathbf{p}_\parallel$, unless explicitly stated. In terms of quasiclassical Green's functions they adopt the form[18]

$$(\check{g}^l_{\rm in}-i\pi\check{1})\otimes(\hat{S}^\dagger_{ll}\check{g}^l_{\rm out}\hat{S}_{ll}-\hat{S}^\dagger_{rl}\check{g}^r_{\rm out}\hat{S}_{rl})\otimes(\check{g}^l_{\rm in}+i\pi\check{1})=0, \tag{9a}$$

$$(\check{g}^l_{\rm out}+i\pi\check{1})\otimes(\hat{S}_{ll}\check{g}^l_{\rm in}\hat{S}^\dagger_{ll}-\hat{S}_{lr}\check{g}^r_{\rm in}\hat{S}^\dagger_{lr})\otimes(\check{g}^l_{\rm out}-i\pi\check{1})=0, \tag{9b}$$

$$(\check{g}^r_{\rm in}-i\pi\check{1})\otimes(\hat{S}^\dagger_{rr}\check{g}^r_{\rm out}\hat{S}_{rr}-\hat{S}^\dagger_{lr}\check{g}^l_{\rm out}\hat{S}_{lr})\otimes(\check{g}^r_{\rm in}+i\pi\check{1})=0, \tag{9c}$$

$$(\check{g}^r_{\rm out}+i\pi\check{1})\otimes(\hat{S}_{rr}\check{g}^r_{\rm in}\hat{S}^\dagger_{rr}-\hat{S}_{rl}\check{g}^l_{\rm in}\hat{S}^\dagger_{rl})\otimes(\check{g}^r_{\rm out}-i\pi\check{1})=0, \tag{9d}$$

with $\check{g}_{\rm in}=\check{g}(\hat{\mathbf{p}})$ and $\check{g}_{\rm out}=\check{g}(\bar{\mathbf{p}})$, where $\hat{\mathbf{p}}$ ($\bar{\mathbf{p}}$) is a unit vector along the momentum direction with the perpendicular component directed towards (away from) the interface. The boundary condition consists of four coupled nonlinear equations for the incoming and outgoing matrix propagators on both sides of the interface. Solving this equation system and dealing with the possibility of arriving at unphysical solutions is evidently not a simple task. Progress towards a more convenient form of boundary conditions has been made by Eschrig (nonmagnetic interfaces)[20] and Fogelström (magnetic interfaces).[21] They employed the powerful Riccati parametrization method which allows for a considerably simpler representation of boundary conditions in terms of the Riccati amplitudes.[20,22,23] However, the conditions in Ref. 21 were only derived for the equilibrium (retarded and advanced) propagators. Furthermore, even in equilibrium situations they cannot be used in the published form in the case when the two sides of the interface have a different number of trajectories (i.e., when matrices $\hat{S}_{lr}$ and $\hat{S}_{rl}$ are not invertable). This situation arises in the context of half-metallic materials, where trajectories exist only for one of the spin orientations.

B. Transfer-matrix approach

Due to the abovementioned difficulties we proceed in an alternative but equivalent route.[24,25] This method requires solving for the auxiliary quasiclassical propagators $\check{g}^{l,0}$ and $\check{g}^{r,0}$ for an *impenetrable* interface. They are to be calculated with the self-energies $\check{\Sigma}\{g\}$ determined with the full propagator, and using the simple perfectly-reflecting boundary condition

$$\check{g}^{i,0}_{\rm out}=\hat{S}^i\check{g}^{i,0}_{\rm in}(\hat{S}^i)^\dagger, \tag{10}$$

where $i=l,r$. They also satisfy the normalization condition, $\check{g}^{i,0}\otimes\check{g}^{i,0}=-\pi^2\check{1}$. The impenetrable interface is characterized by two surface scattering matrices, $\hat{S}^l$ and $\hat{S}^r$. Particle conservation requires them to be unitary, $(\hat{S}^i)^\dagger=(\hat{S}^i)^{-1}$. The transmission processes for an interface with arbitrary transparency can be taken into account with a t-matrix formulation. The transfer matrices are determined with effective hopping amplitudes $\hat{\tau}_{lr}$ and $\hat{\tau}_{rl}$ by the following equations:

$$\check{t}^l_{\rm in}=\hat{\tau}_{lr}\check{g}^{r,0}_{\rm out}\hat{\tau}^\dagger_{lr}+\hat{\tau}_{lr}\check{g}^{r,0}_{\rm out}\hat{\tau}^\dagger_{lr}\otimes\check{g}^{l,0}_{\rm in}\otimes\check{t}^l_{\rm in}, \tag{11a}$$

$$\check{t}^r_{\rm in}=\hat{\tau}_{rl}\check{g}^{l,0}_{\rm out}\hat{\tau}^\dagger_{rl}+\hat{\tau}_{rl}\check{g}^{l,0}_{\rm out}\hat{\tau}^\dagger_{rl}\otimes\check{g}^{r,0}_{\rm in}\otimes\check{t}^r_{\rm in}, \tag{11b}$$

with $\hat{\tau}_{rl}=(\hat{\tau}_{lr})^\dagger$ due to particle conservation. The corresponding t matrices for outgoing trajectories are related to the ones for incoming trajectories through the relation

$$\check{t}^i_{\rm out}=\hat{S}^i\check{t}^i_{\rm in}(\hat{S}^i)^\dagger. \tag{12}$$

The t matrix describes the modifications of the decoupled quasiclassical propagators due to virtual hopping processes to the opposite side. Finally, the boundary condition can be expressed in terms of $\check{t}^i$ and $\check{g}^{i,0}$ to read

$$\check{g}^i_{\rm in}=\check{g}^{i,0}_{\rm in}+(\check{g}^{i,0}_{\rm in}+i\pi\check{1})\otimes\check{t}^i_{\rm in}\otimes(\check{g}^{i,0}_{\rm in}-i\pi\check{1}), \tag{13a}$$

$$\check{g}^i_{\rm out}=\check{g}^{i,0}_{\rm out}+(\check{g}^{i,0}_{\rm out}-i\pi\check{1})\otimes\check{t}^i_{\rm out}\otimes(\check{g}^{i,0}_{\rm out}+i\pi\check{1}). \tag{13b}$$

In the t-matrix description, the phenomenological parameters containing the microscopic information of the interface are the surface scattering matrices and the hopping amplitudes. The particle–hole structures of the surface scattering matrix and the hopping amplitude are connected through

$$\hat{S}^i=\begin{pmatrix} S^i & 0 \\ 0 & \tilde{S}^i \end{pmatrix}, \quad \hat{\tau}_{lr}=\begin{pmatrix} \tau_{lr} & 0 \\ 0 & (\tilde{S}^l)^\dagger\tau^*_{lr}(\tilde{S}^r)^\dagger \end{pmatrix}, \tag{14}$$

to ensure the conservation of current. In the general case

$$\tilde{S}(\mathbf{p}_\parallel)=S^{\rm tr}(-\mathbf{p}_\parallel). \tag{15}$$

In this formulation, the boundary problem effectively reduces to calculating the auxiliary Green's functions for perfectly reflecting interfaces. Numerically this is an extremely

simple task, e.g., employing the procedure of Riccati parameterization. Afterwards the boundary Green's functions for the partially transmitting interface can be obtained directly from Eqs. (13), since solving for the necessary t matrices (11) only involves a 4×4 matrix inversion. When contrasted with solving the group of equations (9), the t-matrix approach manifests its usefulness.

IV. RELATION TO OTHER METHODS

The underlying perturbative nature of the t-matrix approach might arise suspicions concerning its applicability when the interface in question has high transparency. The boundary conditions (13) are, however, valid for arbitrary transmission and, in fact, completely equivalent to the corresponding scattering-matrix description (9). The connection between the two approaches is established by the following identification of the full scattering matrix in terms of the surface scattering matrices and hopping amplitudes:

$$\hat{\mathbf{S}}=\begin{pmatrix}\hat{S}_{ll} & \hat{S}_{lr}\\ \hat{S}_{rl} & \hat{S}_{rr}\end{pmatrix}=\begin{pmatrix}\hat{S}_l & 0\\ 0 & \hat{1}\end{pmatrix}\begin{pmatrix}\hat{r} & \hat{d}\\ \hat{d}^\dagger & -\underline{\hat{r}}\end{pmatrix}\begin{pmatrix}\hat{1} & 0\\ 0 & \hat{S}_r\end{pmatrix}, \quad (16)$$

where we have defined

$$\hat{r}=(1+\pi^2\hat{\tau}_{lr}\hat{\tau}_{rl})^{-1}(1-\pi^2\hat{\tau}_{lr}\hat{\tau}_{rl}), \quad (17a)$$

$$\underline{\hat{r}}=(1+\pi^2\hat{\tau}_{rl}\hat{\tau}_{lr})^{-1}(1-\pi^2\hat{\tau}_{rl}\hat{\tau}_{lr}), \quad (17b)$$

and

$$\hat{d}=(1+\pi^2\hat{\tau}_{lr}\hat{\tau}_{rl})^{-1}2\pi\hat{\tau}_{lr}. \quad (17c)$$

The identity (16) serves as a precise definition of the auxiliary matrices $\hat{S}_l$ and $\hat{S}_r$ in terms of the physical parameters of the full scattering matrix. Using Eq. (15), the particle (S_p) and hole (S_h) parts of Eq. (16) can be seen to be related by

$$S_h(\mathbf{p}_\parallel)=\begin{pmatrix}\tilde{S}_l & 0\\ 0 & \tilde{S}_r\end{pmatrix}S_p^*(-\mathbf{p}_\parallel)\begin{pmatrix}\tilde{S}_l & 0\\ 0 & \tilde{S}_r\end{pmatrix}. \quad (18)$$

In particular, if the interface scattering matrix is spin-inactive, Eqs. (9) reduce to those derived by Zaitsev. In the following, we show that the solution of Eqs. (13) in the appropriate limit also solve Zaitsev's boundary conditions for arbitrary transmission of the interface, and in both equilibrium and nonequilibrium situations. On the other hand, in the case of diffusive conductors the boundary conditions of the t-matrix approach are equivalent to the ones derived by Nazarov.[26]

A. Zaitsev's boundary conditions

The boundary conditions of Zaitsev read (we suppress the symbol $\otimes$ and unit matrices for clarity)[17]

$$\check{g}_a^l=\check{g}_a^r=\check{g}_a, \quad (19a)$$

$$\check{g}_a[R(\check{g}_s^+)^2+(\check{g}_s^-)^2]=-i\pi D\check{g}_s^-\check{g}_s^+, \quad (19b)$$

where R (D) is the reflection (transmission) coefficient, $R+D=1$, $\check{g}_a^{l,r}=\pm(\check{g}_{\rm in}^{l,r}-\check{g}_{\rm out}^{l,r})/2$, and $\check{g}_s^{+,-}=(\check{g}_s^r\pm\check{g}_s^l)/2$, with $\check{g}_s^{l,r}=(\check{g}_{\rm in}^{l,r}+\check{g}_{\rm out}^{l,r})/2$. In the corresponding limiting case the surface scattering matrices $\hat{S}^{l,r}$ are unit matrices, the hopping element can be taken as a real number, $\hat{\tau}_{lr}=\tau\hat{1}$, and the boundary conditions in the t-matrix approach are

$$\check{g}_{\rm in}^i=\check{g}^{i,0}+(\check{g}^0+i\pi)\check{t}^i(\check{g}^{i,0}-i\pi), \quad (20a)$$

$$\check{g}_{\rm out}^i=\check{g}^{i,0}+(\check{g}^{i,0}-i\pi)\check{t}^i(\check{g}^{i,0}+i\pi), \quad (20b)$$

with $\check{g}_{\rm in}^{i,0}=\check{g}_{\rm out}^{i,0}=\check{g}^{i,0}$ and $\check{t}_{\rm in}^i=\check{t}_{\rm out}^i=\check{t}^i$. The t-matrix equations now take the form

$$\check{t}^l=(1-\tau^2\check{g}^{r,0}\check{g}^{l,0})^{-1}\tau^2\check{g}^{r,0}, \quad (21a)$$

$$\check{t}^r=(1-\tau^2\check{g}^{l,0}\check{g}^{r,0})^{-1}\tau^2\check{g}^{l,0}. \quad (21b)$$

From Eqs. (17) we have

$$\check{g}_a^l=i\pi[\check{t}^l,\check{g}^{l,0}], \quad \check{g}_a^r=-i\pi[\check{t}^r,\check{g}^{r,0}], \quad (22)$$

which, using Eq. (18) and the identity

$$(1-\check{a}\check{b})^{-1}\check{a}=\check{a}(1-\check{b}\check{a})^{-1}, \quad (23)$$

immediately gives Eq. (19a). This condition ensures the conservation of current. To show Eq. (19b), we first express it in terms of the quantities $\check{g}_s^{l,r}$ as follows:

$$(1-R)\left[\left(1+\frac{\check{g}_a}{i\pi}\right)\check{g}_s^l\check{g}_s^r-\left(1-\frac{\check{g}_a}{i\pi}\right)\check{g}_s^r\check{g}_s^l\right]$$
$$-2i\pi(R+1)\check{g}_a\left[1-\left(\frac{\check{g}_a}{i\pi}\right)^2\right]=0, \quad (24)$$

where we have used the identity

$$(\check{g}_s^i)^2+(\check{g}_a)^2=-\pi^2, \quad (25)$$

$i=l,r$. Using Eq. (17) we find

$$\check{g}_s^l\check{g}_s^r=\left(1-\frac{\check{g}_a}{i\pi}\right)^2\check{g}_s^{l,0}\check{g}_s^{r,0},$$

$$\check{g}_s^r\check{g}_s^l=\left(1+\frac{\check{g}_a}{i\pi}\right)^2\check{g}_s^{r,0}\check{g}_s^{l,0}, \quad (26)$$

whereby Eq. (24) transforms to

$$\left[1-\left(\frac{\check{g}_a}{i\pi}\right)^2\right]\left\{(1-R)\left[\left(1-\frac{\check{g}_a}{i\pi}\right)\check{g}_s^{l,0}\check{g}_s^{r,0}\right.\right.$$
$$\left.\left.-\left(1+\frac{\check{g}_a}{i\pi}\right)\check{g}_s^{r,0}\check{g}_s^{l,0}\right]-2i\pi(R+1)\check{g}_a\right\}=0. \quad (27)$$

This form exhibits directly the unphysical solutions of Zaitsev's boundary conditions, determined by vanishing of the first square bracket in Eq. (27). The physical solutions are

given by the requirement that the curly bracket of Eq. (27) vanishes. On inserting Eqs. (18) and (19) into this expression and using the identity

$$(1-\check{a})^{-1}\check{a}-(1-\check{b})^{-1}\check{b}=(1-\check{a})^{-1}-(1-\check{b})^{-1}, \quad (28)$$

one arrives at the condition

$$[(1-R)(1+\pi^4\tau^4)-2(R+1)\pi^2\tau^2]\check{g}_a=0, \quad (29)$$

which is identically fulfilled provided that the transmission coefficient in the *t*-matrix description is identified as

$$D=1-R=\frac{4\pi^2\tau^2}{(1+\pi^2\tau^2)^2}. \quad (30)$$

B. Nazarov's boundary conditions

The boundary conditions for diffusive conductors, presented by Nazarov,[26] are formulated in terms of a Keldysh-Nambu matrix current, the Keldysh part of which defines the electric current through the interface. In the *t*-matrix approach, this matrix is proportional to $\check{g}_a$ of Eq. (22) and, therefore, to the quantity

$$\check{I}=[\check{t}^l,\check{g}^{l,0}], \quad (31)$$

determined at the left-hand side of the interface. To simplify the following expressions, we again choose $\hat{\tau}_{lr}=\tau\hat{1}$ and real. Furthermore, in the context of diffusive conductors both the Green's functions and the hopping elements should be regarded as trajectory-averaged quantities, i.e., independent of $\hat{\mathbf{p}}$. Using Eqs. (21a) and (23) we obtain

$$\check{I}=\tau^2\check{g}^r\check{g}^l(\check{1}-\tau^2\check{g}^r\check{g}^l)^{-1}-\tau^2\check{g}^l\check{g}^r(\check{1}-\tau^2\check{g}^l\check{g}^r)^{-1}, \quad (32)$$

where we have dropped the zero from the superscript (all Green's functions are auxiliary ones). Writing the matrix current in the form

$$\begin{aligned}\check{I}=&\tau^2\check{g}^r\check{g}^l(\check{1}-\tau^2\check{g}^l\check{g}^r)(\check{1}-\tau^2\check{g}^l\check{g}^r)^{-1}(\check{1}-\tau^2\check{g}^r\check{g}^l)^{-1}\\&-\tau^2\check{g}^l\check{g}^r(\check{1}-\tau^2\check{g}^l\check{g}^r)^{-1}(\check{1}-\tau^2\check{g}^r\check{g}^l)(\check{1}-\tau^2\check{g}^r\check{g}^l)^{-1},\end{aligned} \quad (33)$$

and exploiting the fact that $\check{g}^l\check{g}^r$ commutes with $\check{g}^r\check{g}^l$, we arrive at

$$\begin{aligned}\check{I}&=-\tau^2[\check{g}^l,\check{g}^r](\check{1}-\tau^2\check{g}^l\check{g}^r)^{-1}(\check{1}-\tau^2\check{g}^r\check{g}^l)^{-1}\\&=-\tau^2[\check{g}^l,\check{g}^r](1-\tau^2\{\check{g}^l,\check{g}^r\}+\pi^4\tau^4)^{-1}.\end{aligned} \quad (34)$$

Finally, using Eq. (30) to identify the transmission coefficient, and defining $\check{G}^{l,r}\equiv\check{g}^{l,r}/(i\pi)$ because of the different convention for normalizing the Green's functions used in Ref. 26, we arrive at

$$\check{I}=\frac{D[\check{G}^l,\check{G}^r]}{4+D(\{\check{G}^l,\check{G}^r\}-2)}, \quad (35)$$

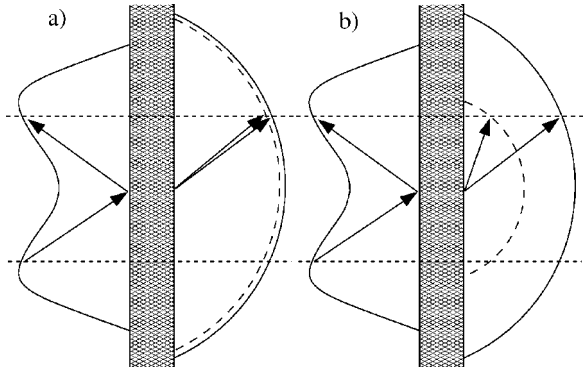

FIG. 1. Two quasiclassical pictures of an interface separating a spin-unpolarized material (left-hand side of the interface) from a ferromagnet (right-hand side): (a) weak ferromagnet with a small splitting of Fermi surfaces for the two spin orientations (indicated by solid and dashed curves) and (b) strong ferromagnet with a large splitting. Incoming trajectory from the left-hand side and corresponding outgoing ones with the same parallel momentum on both sides are indicated by arrows.

which, apart from the prefactor, is the matrix-current expression defining the boundary conditions of Nazarov.

V. INTERFACE PROBLEM WITH FERROMAGNETS

A. Weak and strong ferromagnetism

As already mentioned, the quasiclassical theory is formulated in terms of quasiparticles travelling along classical trajectories. Smooth interfaces between different materials introduce coupling between incoming and outgoing trajectories with the same momentum parallel to the interface. A ferromagnet has a different Fermi surface (or, equivalently, set of trajectories) for each of the two possible spin orientations. Consequently, two different limiting cases that allow a quasiclassical description naturally emerge (see Fig. 1). In the first case the exchange energy splitting of the two Fermi surfaces is small enough that the quasiparticle wave packets on the two trajectories corresponding to the same parallel momentum but different spins overlap and, therefore, the two trajectories remain fully coherent in the ferromagnetic region [Fig. 1(a)]. Technically this means that the full 2×2 spin structure of the quasiclassical Green's functions, defined by Eq. (2), is to be retained in the ferromagnetic side of the interface. This case, relevant for weak ferromagnets, has been widely studied in the literature; the standard description simply involves a spin-dependent shift in the quasiparticle energy, effected by the replacement

$$\epsilon\hat{\tau}_3\rightarrow\epsilon\hat{\tau}_3-h\sigma_3\hat{1} \quad (36)$$

in the Eilenberger equation (4). Here h is the exchange-field parameter and σ_3 is a Pauli spin matrix. Other Fermi-surface parameters, i.e., Fermi velocities and the density of states, are assumed identical for the two spin bands in the ferromagnet.

In this article we restrict ourselves to the opposite limiting case of strongly ferromagnetic materials, illustrated in Fig. 1(b). That is, we assume the exchange splitting and the re-

sulting directional deviation of the two spin trajectories sharing the same parallel momentum to be so large that the coherence between them is lost completely. As a consequence, the quasiclassical propagators have no matrix structure in spin space. In particular, conventional Andreev reflection processes are forbidden because electrons and holes in opposite spin bands occupy different trajectories which do not interfere with each other. Trajectories with different spin orientations can only be coupled incoherently, such as e.g. due to elastic spin–flip scattering by magnetic impurities. It should be emphasized that no energy shift of the form (36) should be introduced in this limit; instead, Fermi velocities and the density of states become spin dependent. The reason for this is that the integration over the energy of relative motion (''ξ integration''), employed in the formal process of converting the full two-particle Green's function into quasiclassical ones, is now performed separately around the two different Fermi surfaces. This is in contrast to the case of weak ferromagnets, where the same ξ-integration range is used for both Fermi surfaces simultaneously.

A very interesting special case which falls into the latter category of ferromagnets with strong spin splitting is that of half-metallic materials. In fact, half metals are metallic in one of the spin bands only—the other one is insulating. Such behavior has recently been reported in CrO_2 (Refs. 15,16) and in certain manganite materials.[14] and has attracted considerable attention because of possible applications in the emerging field of spintronics.[27] Since in half metals a Fermi surface only exists for one of the spin orientations, the standard description for weak ferromagnets is obviously inapplicable. However, half metals still allow for a straightforward quasiclassical treatment in the separate-band picture: quasiparticle trajectories simply exist only for one of the spin orientations.

B. Spin mixing

The quasiclassical boundary conditions in the hopping description involve surface scattering matrices $\hat{S}^{l,r}$ that characterize a fully reflecting interface. In the case of a magnetically active interface the most general form of such matrices (for quasiparticles), satisfying the requirement of unitarity, was pointed out by Tokuyasu *et al.*[28] to be

$$S = e^{-i\Phi/2} e^{-i(\theta/2)\hat{\boldsymbol{\mu}}\cdot\boldsymbol{\sigma}}, \tag{37}$$

where $\hat{\boldsymbol{\mu}}$ is a unit vector pointing to the direction of the surface magnetization and $\boldsymbol{\sigma}$ is a vector constructed of Pauli spin matrices. The corresponding scattering matrix for quasiholes follows from Eq. (15). Dropping the irrelevant overall phase factor Φ, the surface scattering matrix is determined by a single parameter, the spin-mixing angle θ. The physics behind spin mixing can be visualized as follows: even for a fully reflecting interface, incident wave functions penetrate a small distance into the forbidden, spin-polarized region. This results in different matching conditions for waves with opposite spin directions and, consequently, different phase shifts for the reflected waves.

The relative phase difference introduced by spin mixing results in interesting nontrivial phenomena at superconductor/ferromagnet interfaces, even in the absence of quantum-mechanical coherence between the two spin bands in the ferromagnet. One such example is the recent prediction of a nonvanishing Josephson current in a heterostructure with a mesoscopic half-metallic piece separating two singlet superconductors—driven by spin-triplet pairing correlations.[12] (This effect requires, in addition to spin mixing, also the presence of spin–flip centers at the interfaces.) However, even though spin mixing is expected to be an intrinsic feature of any spin-active interface, systematic experimental estimations of the typical magnitudes of θ are not yet available. As a guideline for such future experiments, we study in the following chapter the differential conductance of a spin-mixing point contact between a singlet superconductor and a strong ferromagnet—simultaneously offering a view of the *t*-matrix approach at work.

VI. S/F POINT CONTACT WITH SPIN MIXING

We consider a point contact with arbitrary transmission separating a conventional singlet superconductor and a strong ferromagnetic material. The small (compared with the coherence length of the superconductor) dimensions of the contact and, consequently, the small size of the current flowing through it does not appreciably affect the state of the coupled half-spaces from that corresponding to zero transmission. This offers a simplification by relieving us from the necessity of calculating the superconducting order parameter self-consistently. According to Eq. (7), the current, calculated at the interface on the ferromagnetic side, adopts the form

$$j = \sum_{\alpha} \int \frac{d\epsilon}{8\pi i} \langle e N_f^{\alpha} v_f^{\alpha} \cos\phi \, \mathrm{Tr}[\hat{\tau}_3(\hat{g}_{\mathrm{in}}^K - \hat{g}_{\mathrm{out}}^K)] \rangle_+^{\alpha}, \tag{38}$$

where $\alpha = \uparrow, \downarrow$ labels the spin band of the ferromagnet, each with its own density of states N_f^{α} and the Fermi velocity v_f^{α}. For simplicity, the Fermi surfaces are assumed cylindrical and the interface specularly reflecting, the generalizations are straightforward. The impact angle ϕ determines the angle between the trajectory and the current direction. The angular averaging is to be taken over trajectories with $\cos\phi \geqslant 0$. The two spin bands in the ferromagnet give two separate contributions to the current. From Eqs. (13) follows

$$\hat{g}_{\mathrm{in}}^K - \hat{g}_{\mathrm{out}}^K = 2\pi i [\check{t}, \check{g}^0]^K, \tag{39}$$

where the *t* matrix and the auxiliary Green's function $\check{g}^0$ (for a perfectly reflecting interface) are to be evaluated on the ferromagnetic side where the latter has the simple form $\hat{g}^{R,0} = -\hat{g}^{A,0} = -i\pi\hat{\tau}_3$, and $\hat{g}^{K,0} = \hat{g}^{R,0}\hat{F} - \hat{F}\hat{g}^{A,0}$, with

$$\hat{F} \equiv \begin{pmatrix} F_e & 0 \\ 0 & F_h \end{pmatrix} = \begin{pmatrix} \tanh\left(\dfrac{\epsilon - eV}{2T}\right) & 0 \\ 0 & \tanh\left(\dfrac{\epsilon + eV}{2T}\right) \end{pmatrix}, \tag{40}$$

where V is the voltage over the contact and T is the temperature. We choose the electrical potential to be zero on the superconducting side of the interface. Writing out the commutator (39), Eq. (38) reads

$$j=\sum_{\alpha}\frac{i\pi eN_f^{\alpha}v_f^{\alpha}}{2}\int d\epsilon\langle\cos\phi\,\mathrm{Tr}[\hat{t}^K-(\hat{t}^R\hat{F}-\hat{F}\hat{t}^A)]\rangle_+^{\alpha}. \tag{41}$$

Using now Eq. (11), the relation $\hat{t}^A=\hat{\tau}_3(\hat{t}^R)^{\dagger}\hat{\tau}_3$, and the properties of the trace, we find

$$j=\sum_{\alpha}\pi eN_f^{\alpha}v_f^{\alpha}\int d\epsilon\,\mathrm{Im}\langle\cos\phi\,\mathrm{Tr}[(\hat{N}^R)^{\dagger}\hat{v}^R\hat{N}^R(\hat{F}-F_0)]\rangle_+^{\alpha}, \tag{42}$$

where we have defined an effective interface potential $\hat{v}^R=\hat{\tau}\hat{g}^S\hat{\tau}^{\dagger}$, with $\hat{g}^S=\hat{g}^{R,0}_{\mathrm{out}}$ the auxiliary Green's function on the superconducting side of the interface, $\hat{N}^R=(1+i\pi\hat{\tau}_3\hat{v}^R)^{-1}$, and $F_0=\tanh(\epsilon/2T)$. We assume that the interface does not flip the spin, i.e., hopping processes from an incoming trajectory in the ferromagnet to an outgoing trajectory on the superconducting side are without loss of generality determined by two real numbers, $\hat{\tau}_{\alpha}=\tau_{\alpha}\hat{1}$, for the two possible spin orientations. In this case Eq. (42) gives

$$j=\sum_{\alpha}eN_f^{\alpha}v_f^{\alpha}\int d\epsilon\left\langle\cos\phi\frac{2\pi\tau_{\alpha}^2\,\mathrm{Im}\,g^S_{\alpha\alpha}}{|1+i\pi\tau_{\alpha}^2g^S_{\alpha\alpha}|^2}\right\rangle_+^{\alpha}(F_e-F_0), \tag{43}$$

where $g^S_{\uparrow\uparrow}$ ($g^S_{\downarrow\downarrow}$) is the 1,1 (2,2) element of the full 4×4 auxiliary Green's function at the interface on the superconducting side. In the presence of spin mixing (described by the spin-mixing angle θ) this has the form

$$g^S_{\uparrow\uparrow}=\pi\frac{\epsilon\cos\frac{\theta}{2}+\Omega\sin\frac{\theta}{2}}{\epsilon\sin\frac{\theta}{2}-\Omega\cos\frac{\theta}{2}}, \tag{44}$$

where $\Omega\equiv\sqrt{\Delta^2-\epsilon^2}$, Δ is the magnitude of the bulk order parameter, and $g^S_{\downarrow\downarrow}$ can be obtained by replacing $\theta\rightarrow-\theta$. Inserting Eq. (44) into Eq. (43) we obtain

$$j=\sum_{\alpha}eN_f^{\alpha}v_f^{\alpha}\int d\epsilon\langle\cos\phi j_{\epsilon}^{\alpha}\rangle_+^{\alpha}(F_e-F_0), \tag{45}$$

with

$$j_{\epsilon}^{\uparrow}=\frac{2\pi^2\tau_{\uparrow}^2\epsilon\,\mathrm{Im}\,\Omega}{\left|\epsilon\left(\sin\frac{\theta}{2}+i\pi^2\tau_{\uparrow}^2\cos\frac{\theta}{2}\right)-\Omega\left(\cos\frac{\theta}{2}-i\pi^2\tau_{\uparrow}^2\sin\frac{\theta}{2}\right)\right|^2}, \tag{46}$$

and $j_{\epsilon}^{\downarrow}$ follows from $\tau_{\uparrow}\rightarrow\tau_{\downarrow}$ and $\theta\rightarrow-\theta$. For subgap energies, $|\epsilon|\leqslant\Delta$, j_{ϵ}^{α} vanishes because Ω is real. This simply reflects the fact that the contribution from Andreev reflection processes vanishes in quasiclassical approximation due to the lack of coherence between spin-up and spin-down bands on the ferromagnetic side. Introducing the normal-state transmission and reflection coefficients with Eq. (30), Eq. (46) can be written for $|\epsilon|\geqslant\Delta$ as

$$j_{\epsilon}^{\alpha}=\frac{-2D^{\alpha}\sqrt{1-\left(\frac{\Delta}{\epsilon}\right)^2}}{\left[1-\sqrt{R^{\alpha}}+(1+\sqrt{R^{\alpha}})\sqrt{1-\left(\frac{\Delta}{\epsilon}\right)^2}\right]^2+4\sqrt{R^{\alpha}}\left(\frac{\Delta}{\epsilon}\right)^2\sin^2\frac{\theta}{2}}. \tag{47}$$

The differential conductance $G=\partial j/\partial V$ for $|eV|\geqslant\Delta$ can now be obtained by differentiation, and at $T=0$ adopts the form

$$G=-\sum_{\alpha}2e^2N_f^{\alpha}v_f^{\alpha}\langle\cos\phi j_{\epsilon}^{\alpha}(\epsilon=eV)\rangle_+^{\alpha}. \tag{48}$$

In particular, for a half metal with a conducting spin-up band and a reflection coefficient $R^{\uparrow}=R$ independent of impact angle ϕ, the conductance (normalized to the normal-state value G_N) reads

$$\frac{G}{G_N}=\frac{4\sqrt{1-\left(\frac{\Delta}{eV}\right)^2}}{\left[1-\sqrt{R}+(1+\sqrt{R})\sqrt{1-\left(\frac{\Delta}{eV}\right)^2}\right]^2+4\sqrt{R}\left(\frac{\Delta}{eV}\right)^2\sin^2\frac{\theta}{2}}, \tag{49}$$

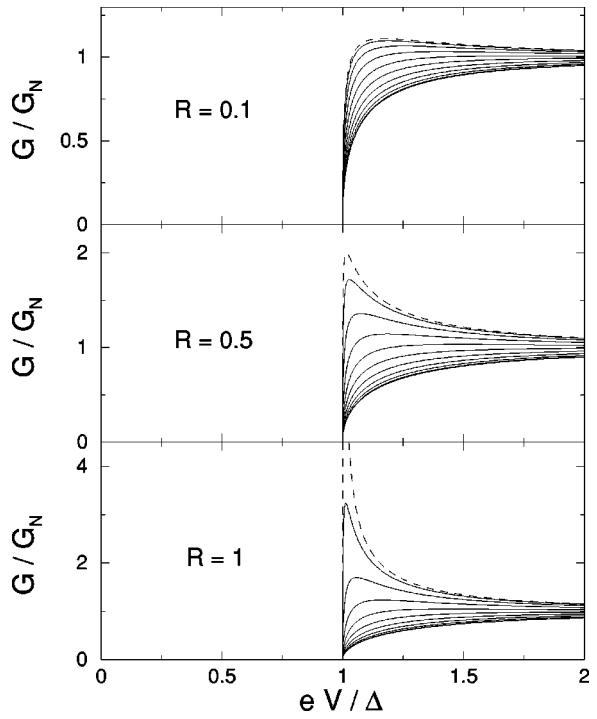

FIG. 2. The normalized conductance G/G_N as a function of eV/Δ for $R=0.1$ (top figure), $R=0.5$ (middle), and $R=1$ (bottom). The different curves in each figure correspond, from top to bottom, to different values of the spin-mixing angle ranging from $\theta=0$ (dashed curve) to $\theta=\pi$ in intervals of $\pi/10$.

when $|eV|\geqslant\Delta$. The contribution due to a finite spin-mixing angle θ has the effect of broadening the conductance features near the gap edge. This is demonstrated in Fig. 2 which shows the normalized conductance as a function of the spin-mixing angle for three different reflection coefficients of the contact. In particular, the characteristic BCS square-root singularity for a tunnel-limit ($R\rightarrow 1$) contact is removed. On the other hand, for perfectly transmitting interfaces, $R\rightarrow 0$, spin mixing has no effect. As an additional detail, the maximum of Eq. (49), attained at $eV/\Delta=(1+\sqrt{R})/2R^{1/4}$ when $\theta=0$, is shifted towards higher voltages when $\theta>0$, vanishing altogether if $\theta\geqslant\pi/2$.

VII. CONCLUSIONS

We have presented a quasiclassical theory which is suited for detailed studies of heterostructures consisting of a wide variety of materials: superconductors (both conventional and unconventional), normal metals, and both weak and strong ferromagnets. The most crucial part of this description is the treatment of boundary conditions at interfaces separating different materials. These conditions are formulated in terms of hopping amplitudes, containing the information of allowed transmission processes, and the corresponding t matrices. Compared with the traditional scattering-matrix approach, the t matrix approach provides clear advantages for studying spin-active interfaces, or interfaces which connect materials with different numbers of trajectories or with different internal structures of their Green's functions. A particular example are strong ferromagnets of which the half-metallic materials form a special case. In connection with such materials, nontrivial physics arises due to spin-dependent interfacial scattering processes. The crucial parameter controlling the details of these effects is the degree of spin mixing. At present, there have been no attempts to determine experimentally the magnitude of this parameter at a spin-active interface. To provide a guideline for such studies, and to demonstrate the t-matrix approach, we have calculated the differential conductance for a superconductor/half metal point contact. In the tunneling limit of such contacts, the conductance depends strongly on spin mixing, and should provide an effective means of determining the importance of the new physics related to spin-active interfaces.

Finally, it is also worth stressing that the transfer-matrix formalism presented in this work is also well suited for calculating time-dependent properties such as the current–voltage characteristics or as current fluctuations in junctions with arbitrary transmission and bias voltage.[25,29,30] Additionally, as we have shown in Ref. 25 for nonmagnetic situations, our approach can be straightforwardly generalized to deal with junctions of unconventional superconductors. In this sense, we can for instance address the issue of the interplay between interface Andreev bound states[31] and the spin polarized current in ferromagnet/d-wave superconductors contacts, which has attracted a lot of attention in the last years.[32–34]

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