Quasiclassical theory of superconductivity near magnetically active interfaces

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We derive boundary conditions that connect the quasiclassical propagators for superconducting metals across magnetically active interfaces. These boundary conditions, combined with the quasiclassical transport theory, determine the structure of the perturbed superconductivity near such an interface, and are essential for a quantitative theory of Josephson tunneling and proximity effects between heavy-fermion superconductors and inhomogeneous structures composed of magnetic and superconducting materials. We discuss some qualitative features of Josephson tunneling between conventional and unconventional superconductors.

I. INTRODUCTION

The discovery of superconductivity in heavy-fermion metals,[1] as well as recent advances in the fabrication of artificial lattices[2] and films of exotic materials, opens new possibilities for studying the interaction and coexistence of superconductivity and magnetism. In this paper we develop the theoretical tools needed to calculate the influence of *magnetically active* interfaces on superconductivity. By "magnetically active" we refer to interfaces which flip the spin of incident electrons either by spin-dependent scattering within the interface, or by a difference in spin-orbit coupling on either side of the interface. We begin by briefly describing some of the recent developments in superconductivity that motivate our theoretical investigations, and then summarize the main elements of the theory.

Superconductivity in the heavy-fermion metals $CeCu_2Si_2$,UBe_{13},UPt_3, etc., is particularly interesting because it is believed to be unconventional.[3] The observed thermodynamic and transport properties deviate qualitatively from the predictions of Bardeen-Cooper-Schrieffer (BCS) theory for *s*-wave (i.e., isotropic) superconductors. The observed power laws for the temperature dependences of the specific heat,[4] ultrasonic attenuation,[5] and nuclear relaxation rate[6] suggest to several authors[4–6] that the superconducting states of these metals are described by a spin-triplet Cooper-pair amplitude that is more like that of superfluid ^{3}He than that of conventional spin-singlet superconductors. However, several of the same authors have since noted that these power laws, and the inference of anisotropic gaps with points or lines of zeroes on the Fermi surface, do not lead to a precise identification of the type of pairing in these superconductors.[7–9]

The hope has been that there would be a single experiment in which a *yes* or *no* result would determine the spin and spatial symmetry of the superconducting order for heavy-fermion materials. In an early paper, Pals *et al.*[10] argue that an ac Josephson effect would serve this purpose. These authors show that Josephson tunneling with frequency 2 $eV/\hbar$ is forbidden between a conventional spin-singlet superconductor and an unconventional spin-triplet superconductor, provided the barrier is nonmagnetic. In particular they argue that if the transfer Hamiltonian,

$$H=\sum_{\mathbf{k},\alpha,\mathbf{q},\beta}\{[t(\mathbf{k},\mathbf{q})]_{\alpha\beta}a^{\dagger}_{\mathbf{k},\alpha}b_{\mathbf{q},\beta}+\mathrm{H.c.}\}\ , \tag{1}$$

where $a^{\dagger}_{\mathbf{k}\alpha}$ ($b^{\dagger}_{\mathbf{q}\beta}$) creates a quasiparticle on the left-hand (right-hand) side of the tunneling barrier is invariant under time-reversal and spin rotations, then the conventional Josephson effect between a singlet and a triplet superconductor does not occur. However, the conclusion of Pals *et al.*[10] does not necessarily hold if spin-orbit coupling is important. Fenton[11] has argued that strong spin-orbit coupling in heavy-fermion materials, combined with spatial variations of the triplet order parameter near the interface, conspire to give a Josephson current even if the interface transmission amplitude is a scalar in spin space. Sauls *et al.* and, independently, Geshkebein and Larkin[12] have shown that spin-orbit scattering of quasiparticles at an interface between singlet and triplet superconductors can lead to Josephson tunneling with the conventional frequency 2 $eV/\hbar$, even if the interface t matrix is symmetric under time reversal. These arguments are of current interest since, for example, Poppe and Schröder[13] and Steglich *et al.*[14] have argued, based on the work of Pals *et al.* that the observation of a dc Josephson current between $CuCu_2Si_2$ and Al of conventional magnitude is evidence that $CeCu_2Si_2$ is a spin-singlet superconductor. Steglich *et al.* also failed to observe Josephson tunneling between UPt_3 and Nb, Al, or UPt_3 as a counter electrode. To date there is no incontrovertible piece of evidence in any heavy-fermion superconductor that forces one to conclude that these exotic superconductors are, in fact, triplet superconductors (or other unconventional superconductors) exhibiting, for instance, the kind of novel spin correlations that are known to exist in superfluid ^{3}He. In the absence of a *smoking gun* to pin down the spin and orbital symmetry of the superconducting order parameters in these materials, it is important to consider theoretically, in some detail, the qualitative and quantitative differences between conventional and unconventional superconductivity near interfaces.

Any realistic model for the interface between a heavy-fermion metal and another material will necessarily be magnetically active because of spin-orbit scattering in the heavy-fermion metal. In fact, a transfer Hamiltonian of the form shown in Eq. (1), in which $[t(\mathbf{k},\mathbf{q})]_{\alpha\beta}$ is independent of the spins of the electrons, is probably never a valid representation for the tunneling Hamiltonian if one electrode is a heavy-fermion metal.[12] This is because the quasiparticle states in a heavy-fermion metal are not eigenstates of the spin, but rather are coherent superpositions of "up" and "down" spin states with mixing coefficients determined by the strength of the spin-orbit interaction at the Ce or U sites. The spin-orbit interaction is expected to be strong in the heavy-fermion metals;[3] in consequence, spin-orbit mixing requires a classification of the one-electron states in terms of a two-component pseudospin.[15] Thus, any tunneling Hamiltonian connecting two dissimilar metals must be magnetically active, if for no other reason than to convert a quasiparticle in the pseudospin representation appropriate to the left electrode into a different (in general) pseudospin representation appropriate for the right electrode. If one electrode is a heavy-fermion metal then spin-orbit mixing essentially guarantees that the pseudospin-dependent part of the transfer matrix is the same order of magnitude as the conventional spin-independent amplitude.

Even though spin is not a good quantum number in heavy-fermion metals, Anderson[16] has pointed out that the superconducting order parameters for these metals may be classified as either "singlet" or "triplet," with respect to a two-dimensional pseudospin space, since all the heavy-fermion metals, so far, have inversion symmetry. The argument is simply that if the superconducting order preserves this symmetry, then the gap matrix (order parameter), defined on the Fermi surface, is either even parity (singlet) or odd parity (triplet),

$$\Delta(\hat{\mathbf{p}})=i\sigma_2\Delta_0(\hat{\mathbf{p}})\ \text{(singlet)}\ ,$$

$$\Delta(\hat{\mathbf{p}})=i\boldsymbol{\sigma}\sigma_2\cdot\boldsymbol{\Delta}(\hat{\mathbf{p}})\ \text{(triplet)}\ .$$

The formalism described below is developed, in part, in order to calculate the coupling between conventional superconducting metals and unconventional superconductors, such as heavy-fermion metals.

Another class of systems for which our formalism is directly applicable are *"artificial layered systems"* of magnetic materials (metals or otherwise) and superconductors. Artificial lattices and *"sandwiches"* of Fe and *V* have already proven to be remarkably rich systems in which to study the interaction and coexistence of superconductivity and magnetism.[17] Tunneling studies on layered structures of superconducting aluminum and ferromagnetic EuO (Ref. 18) indicate that these materials behave as a conventional superconductor with an *"internal magnetization"* suggesting the Al electrons spend a great deal of time in the ferromagnetic EuO layer. A quantitative understanding of these layered magnetic-superconducting systems requires a theory that treats specially the boundary conditions on the electronic distribution function and order parameter imposed by a magnetic interface.[19]

Our goal is to derive quasiclassical (QC) equations that are general enough to describe unconventional superconductors in the presence of magnetically active interfaces. The QC theory describes phenomena which vary on scales large compared to the atomic scale; since the interface represents a strong potential, varying in space on the atomic length scale, a QC treatment of electronic propagation in this region is not possible. We treat the interface region separately, eventually replacing it by a boundary condition involving a suitably defined interface scattering matrix connecting the QC propagators on the two sides of the interface.

II. QUASICLASSICAL THEORY OF SUPERCONDUCTIVITY WITH INTERFACES

The quasiclassical (QC) theory of superconductivity is formulated in terms of matrix propagators in Nambu space *(≡spin×particle–hole space)*. These QC propagators $\hat{g}(\hat{\mathbf{p}},\mathbf{R};\epsilon,t)$ carry all the necessary quantum-mechanical information associated with the spin and particle-hole degrees of freedom. At low excitation energies $(k_BT,\ \hbar\omega,\ \gamma H,\ \Delta)\ll E_F$, the wave nature of the electron quasiparticles can be eliminated; this is achieved by integrating over the quasiparticle momentum [or quasiparticle excitation energy $\xi_{\mathbf{p}}=v_F(p-p_F)$],

$$\hat{g}(\hat{\mathbf{p}},\mathbf{R};\epsilon,t)\equiv\frac{1}{a}\int d\xi_{\mathbf{p}}\,\hat{\tau}_3\hat{G}(\mathbf{p},\mathbf{R};\epsilon,t)\ , \tag{2}$$

where $\hat{G}$ is the one-particle Keldysh Green's function, an 8×8 matrix in which the matrix indices represent the spin and particle-hole degrees of freedom (Nambu indices), and time ordering (labeled by Keldysh indices). For a full explanation of our notation see Serene and Rainer[20] (the factor a, for example, is the quasiparticle renormalization constant). The components of $\hat{g}$ in Keldysh space are simply related to the retarded, advanced, and Keldysh propagators, containing all relevant information on the static and dynamic properties of superconductors. For bulk systems the theory consists of, (1) a transport-like differential equation for the matrix propagator $\hat{g}$,

$$[\epsilon\hat{\tau}_3-\hat{\Delta}-\hat{\sigma},\hat{g}]_{\otimes}+i\mathbf{v}_F\cdot\partial\hat{g}=0\ , \tag{3}$$

(2) an algebraic normalization condition,

$$\hat{g}\otimes\hat{g}=-\pi^2\hat{1}\ , \tag{4}$$

(3) and a set of self-energy equations that determine $\hat{\Delta}$ and $\hat{\sigma}$ as functionals of $\hat{g}$. We use the multiplication symbol $\otimes$, which stands for conventional matrix multiplication and the following operation in the energy and time variables:

$$\hat{f}(\epsilon,t)\otimes\hat{g}(\epsilon,t)=\hat{f}\left[\epsilon-\frac{1}{2i}\frac{\partial}{\partial t_2},t_1\right]\times\hat{g}\left[\epsilon+\frac{1}{2i}\frac{\partial}{\partial t_1},t_2\right]\Bigg|_{t_1=t_2=t'}\ . \tag{5}$$

The symbol $[\hat{f},\hat{g}]_{\otimes}$ denotes the commutator $\hat{f}\otimes\hat{g}-\hat{g}\otimes\hat{f}$.

Interfaces, like that shown in Fig. 1, pose a special problem because they represent a strong perturbation, varying on atomic length scales, that cannot be treated quasiclassically. The goal is to add to the quasiclassical equations for the metals on the left and right half-spaces a boundary condition connecting $\hat{g}^{l}(x\approx 0^{-})$ with $\hat{g}^{r}(x\approx 0^{+})$. This boundary condition has been derived by Zaitsev,[21] and independently by Kieselmann,[22] for translationally invariant, nonmagnetic interfaces. We follow closely Zaitsev's derivation for a nonmagnetic interface, and generalize the boundary condition to include spin-orbit and spin-flip scattering at the interface.

The boundary condition derived below for an idealized translationally invariant interface will also hold locally at any point on a warped interface, provided the interface is smooth on the scale of the coherence length. Translational invariance along the interface implies that Gorkov's equation for the full Green's function $\hat{G}(\mathbf{x},\mathbf{x}')$ (we omit the energy and time variables unless explicitly needed) reduces to a differential equation in the perpendicular coordinate x for the Fourier transform of $\hat{G}(\mathbf{x},\mathbf{x}')$ with respect to the parallel coordinates, which we denote as $\hat{G}(x,x')$. The dependence on the conserved momentum $\mathbf{p}_{\parallel}$ is not explicitly written,

$$\left[\epsilon\hat{\tau}_3-\hat{H}\left[x,\frac{\partial_x}{i}\right]\right]\otimes\hat{\tau}_3\hat{G}(x,x')=\delta(x-x')\hat{1}\ . \tag{6}$$

The "Hamiltonian" H represents the kinetic and potential energies and is discussed in more detail below. Our task is to solve Gorkov's equation accurately in the limit $k_F\xi_0\gg 1$, where k_F is the Fermi wave vector and ξ_0 is the coherence length of the superconducting state. We accomplish this goal in steps. First we solve Eq. (6) in the left (right) half-space, $-\infty<x<-\delta$ $(\delta>x>\infty)$. The distance δ is a cutoff chosen to be large compared to the range of the interface potential but small compared to the superconducting coherence lengths $(k_F^{-1}\ll\delta\ll\xi_0)$. In these half-spaces the Hamiltonian is a smooth function of x on the scale of the coherence length. We can then use any of several standard techniques to derive the QC propagators in these half-space regions. We then solve Gorkov's equation in the interface region by introducing a scattering matrix that connects the solutions for $x\approx-\delta$ to the solutions for $x\approx+\delta$. The scattering matrix is not calculated in our theory; the matrix elements are phenomenological parameters that enter the QC equations via the interface boundary condition. The only information about the scattering matrix that we use is that which is based on the symmetry of the full Hamiltonian, including the interface potential. Following Zaitsev, we than match the half-space solutions $(|x|>\delta)$ with the interface solutions $(|x|<\delta)$ at $x=\pm\delta$, and obtain the solution to Gorkov's equation for all x. The final step is to eliminate the unnecessary quantum-mechanical information in order to obtain a purely QC theory for superconductors in contact with an interface.

A. Half-space $(|x|>\delta)$ solutions

We introduce Green's functions $\hat{G}^{S}(x,x')$, defined in the half-space, $S=l$ $(x,x'<-\delta)$ or r $(x,x'>+\delta)$, and the model Hamiltonian,

$$\hat{H}=\Theta(x)\hat{H}^{r}+\Theta(-x)\hat{H}^{l}+\hat{V}\ ,$$
$$\hat{H}^{S}\left[x,\frac{\partial_x}{i}\right]=\frac{-1}{2m_S^*}(\partial_x^2-p_{\parallel}^2)-E_F^S+\hat{\Delta}^{S}+\hat{U}^{S}\ , \tag{7}$$

where m_S^* is the quasiparticle effective mass, E_F^S is the Fermi energy, $\hat{V}$ is the interface potential, $\hat{\Delta}^{S}$ is the local

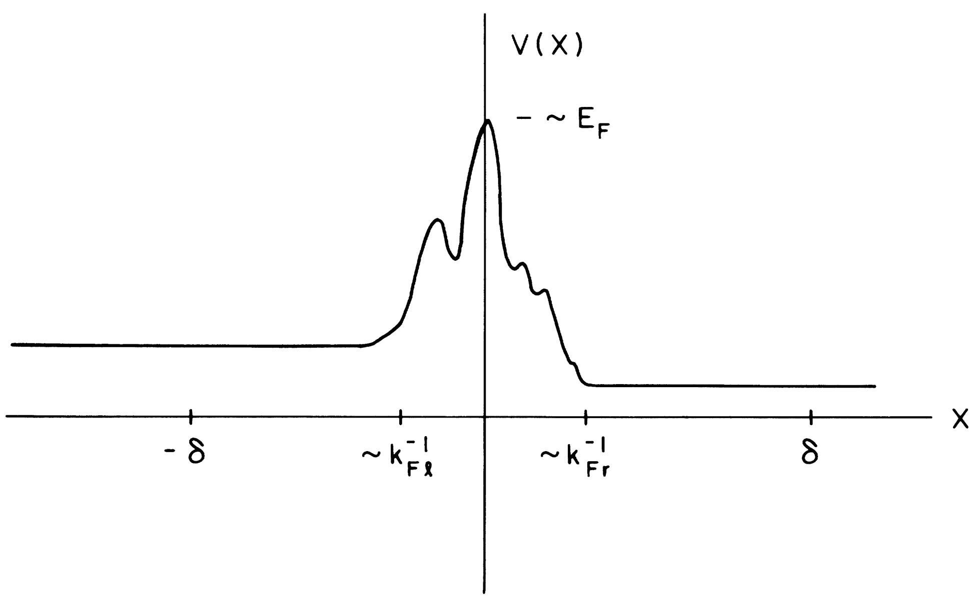

FIG. 1. *Interface potential:* The interface represents a strong potential varying on atomic length scales. δ indicates the arbitrarily chosen cutoff that separates the bulk from the interface.

gap matrix (order parameter), and $\hat{U}^S$ represents the weak external fields ($\hat{U}^S \ll E_F^S$), in the half-space $x \in S$. This model Hamiltonian, with second-order derivatives, is useful for simplifying the derivation of the QC equations, but is not a necessary feature. The smoothness of $\hat{H}[x,(1/i)\partial_x]$ away from the interface [$\hat{\Delta}(x)$ varies smoothly on the scale of ξ_0] suggests the following *ansatz,* due to Zaitsev, for $\hat{G}(x,x')$,

$$\hat{\tau}_3\hat{G}^S(x,x') = \frac{1}{v^S}[\hat{C}^S_{++}(x,x')e^{ip^S(x-x')} + \hat{C}^S_{+-}(x,x')e^{ip^S(x+x')} + \hat{C}^S_{-+}(x,x')e^{ip^S(-x-x')} + \hat{C}^S_{--}(x,x')e^{ip^S(-x+x')}] , \quad (8)$$

representing the four possible combinations of incoming and outgoing waves with momentum p^S in the x direction. Equation (8) can be written compactly in terms of "direction indices," α and β, which specify the momentum direction along the x axis and take values of ± 1,

$$\hat{\tau}_3\hat{G}^S(x,x') = \frac{1}{v^S}\sum_{\alpha,\beta=\pm 1}\hat{C}^S_{\alpha\beta}(x,x')e^{ip^S(\alpha x-\beta x')} . \quad (9)$$

The magnitude of p^S is fixed by the diagonal part of the Hamiltonian,

$$p^S = [2m_S^* E_F^S - (p_\parallel^S)^2]^{1/2} . \quad (10)$$

The prefactors $1/v^S$ in Eq. (8), where v^S are the magnitudes of the x components of the Fermi velocities, are included for convenience; they make the matching conditions in the interface region algebraically simpler. The velocities are given by

$$v^S = p^S/m_S^* . \quad (11)$$

The envelope functions $\hat{C}^S_{\alpha\beta}(x,x')$ are smooth functions on the scale of the coherence length ξ_0^S, except at $x=x'$ where they are discontinuous functions because of the δ function $\delta(x-x')$ in the differential equation [Eq. (6)].

One derives quasiclassical differential equations from Gorkov's equation for the functions $\hat{C}^S_{\alpha\beta}(x,x')$ by performing Andreev's gradient expansion to retain only the leading order derivatives of the slowly varying envelope functions. For any function $\hat{f}(x)e^{\pm ip^S x}$, where $\hat{f}(x)$ varies on the scale $\xi_0^S \gg p^{S^{-1}}$,

$$\hat{H}\left[x,\frac{1}{i}\partial_x\right]\otimes\hat{f}(x)e^{\pm ip^S x} \approx e^{\pm ip^S x}[\hat{H}(x,\pm p^S) \mp iv^S\partial_x]\otimes\hat{f}(x) . \quad (12)$$

One immediately obtains the QC differential equations (for $x \neq x'$) for the envelope functions,

$$[\epsilon\hat{\tau}_3 - \hat{H}(x,\alpha p^S) + i\alpha v^S\partial_x]\otimes\hat{C}^S_{\alpha\beta}(x,x') = 0 . \quad (13)$$

The equivalent differential equation in the variable x' is (for $x \neq x'$),

$$\hat{C}^S_{\alpha\beta}(x,x')\otimes[\epsilon\hat{\tau}_3 - \hat{H}(x',\beta p^S) - i\beta v^S\partial_{x'}] = 0 . \quad (14)$$

The discontinuity of $\hat{C}^S_{\alpha\beta}(x,x')$ at $x=x'$ is obtained by integrating Gorkov's equation about $x \approx x'$,

$$\partial_x\hat{G}^S(x,x')\,|_{x=x'+0} - \partial_x\hat{G}^S(x,x')\,|_{x=x'-0} = 2m_S^*\hat{1} , \quad (15)$$

and combining Eq. (15) with the continuity condition,

$$\hat{G}^S(x'+0,x') = \hat{G}^S(x'-0,x') . \quad (16)$$

The resulting discontinuities in the envelope functions are

$$\hat{C}_{\alpha\beta}(x'+0,x') - \hat{C}_{\alpha\beta}(x'-0,x') = -i\alpha , \quad (17)$$

and imply δ functions in the QC differential equations [13 and 14],

$$[\epsilon\hat{\tau}_3 - \hat{H}(x,\alpha p^S) + i\alpha v^S\partial_x]\otimes\hat{C}^S_{\alpha\beta}(x,x') = v^S\delta_{\alpha\beta}\delta(x-x')\hat{1} , \quad (18)$$

$$\hat{C}^S_{\alpha\beta}(x,x')\otimes[\epsilon\hat{\tau}_3 - \hat{H}(x',\beta p^S) - i\beta v^S\partial_{x'}] = v^S\delta_{\alpha\beta}\delta(x-x')\hat{1} . \quad (19)$$

These equations for the envelope functions still contain considerably more quantum-mechanical information than is necessary. In particular, the QC propagator we seek is a continuous function of one variable x. We can reduce the amount of information by defining envelope functions of one variable,

$$\hat{C}^S_{\alpha\beta}(x) = \hat{C}^S_{\alpha\beta}(x,x+0) , \quad (20)$$

which are related to the QC propagators as shown below. From Eqs. (18) and (19) for the envelope functions we obtain homogeneous differential equations for $\hat{C}^S_{\alpha\beta}(x)$,

$$\partial_x\hat{C}^S_{\alpha\beta}(x) = \frac{-1}{i\alpha v^S}[\epsilon\hat{\tau}_3 - \hat{H}(x,\alpha p^S)]\otimes\hat{C}^S_{\alpha\beta}(x) + \frac{1}{i\beta v^S}\hat{C}^S_{\alpha\beta}(x)\otimes[\epsilon\hat{\tau}_3 - \hat{H}(x,\beta p^S)] , \quad (21)$$

which yield for $\alpha=\beta$,

$$[\epsilon\hat{\tau}_3 - \hat{H}(x,\alpha p^S), \hat{C}^S_{\alpha\alpha}(x)]_\otimes + i\alpha v^S\partial_x\hat{C}^S_{\alpha\alpha}(x) = 0 , \quad (22)$$

and for $\alpha \neq \beta$,

$$\{\epsilon\hat{\tau}_3 - \hat{H}(x,\alpha p^S)\}\otimes\hat{C}^S_{\alpha\beta}(x) + \hat{C}^S_{\alpha\beta}(x)\otimes\{\epsilon\hat{\tau}_3 - \hat{H}(x,-\alpha p^S)\} + i\alpha v^S\partial_x\hat{C}^S_{\alpha\beta}(x) = 0 . \quad (23)$$

Equation (22) is recognized as the QC transport equation, and we conclude that the diagonal amplitudes $\hat{C}^S_{\alpha\alpha}(x)$ are simply related to the QC propagators $\hat{g}^S(\hat{\mathbf{p}},x)$ and $\hat{g}^S(\hat{\underline{\mathbf{p}}},x)$, where $\hat{\mathbf{p}}$ and its reflected partner $\hat{\underline{\mathbf{p}}}$ are unit vectors along the directions of $\mathbf{p} = \mathbf{p}_\parallel + p^S\hat{x}$ and $\underline{\mathbf{p}} = \mathbf{p}_\parallel - p^S\hat{x}$. The off-diagonal amplitudes $\hat{C}_{+-}$ and $\hat{C}_{-+}$ are *drone* amplitudes, which are useful in deriving the interface boundary condition (see below), but will eventually be discarded since they carry no physical information in the limit $k_f\xi_0 \gg 1$.

The precise connection between the amplitudes $\hat{C}_{\alpha\alpha}(x)$ ($\alpha=\pm$) and the QC propagators is obtained by explicitly integrating Eq. (8) with respect to ξ_p,

$$\hat{g}^S(\hat{\mathbf{p}},x)=\pi[2\hat{C}^S_{++}(x)-i\hat{1}] , \quad \hat{g}^S(\underline{\hat{\mathbf{p}}},x)=\pi[2\hat{C}^S_{--}(x)+i\hat{1}] , \tag{24}$$

for $\hat{\mathbf{p}}\cdot\hat{\mathbf{x}}>0$. The complete set of equations governing the QC propagators in the smooth half-spaces is obtained by deriving normalization conditions for the function $\hat{C}^S_{\alpha\beta}(x)$. Starting from Eqs. (18) and (19) for the full envelope functions, we follow Shelankov[23] to derive the normalization conditions for the one-variable envelope functions. The technique is to define auxiliary functions,

$$\hat{a}^S_\gamma(y)\equiv\hat{C}^S_{\alpha\gamma}(x,y)\otimes\hat{C}^S_{\gamma\beta}(y,x') , \tag{25}$$

that are functions of y with (x,x') and direction indices as parameters (note that there is no summation on γ). Using Eqs. (18) and (19) we obtain the following differential equation for the auxiliary function:

$$i\gamma\partial_y\hat{a}_\gamma(y)=[-\delta_{\alpha\gamma}\delta(x-y)+\delta_{\gamma\beta}\delta(y-x')]\hat{C}^S_{\alpha\beta}(x,x') . \tag{26}$$

Integrating this equation with the boundary conditions,

$$\hat{a}^l_\gamma(y)=0, \quad y\to-\infty , \qquad \hat{a}^r_\gamma(y)=0, \quad y\to+\infty , \tag{27}$$

gives $\hat{a}^S_\gamma(y)$ in terms of $\hat{C}_{\alpha\beta}(x,x')$,

$$\begin{aligned} i\gamma\hat{a}^l_\gamma(y)&=[-\delta_{\alpha\gamma}\Theta(y-x) +\delta_{\beta\gamma}\Theta(y-x')]\hat{C}^l_{\alpha\beta}(x,x') , \\ i\gamma\hat{a}^r_\gamma(y)&=[\delta_{\alpha\gamma}\Theta(x-y) -\delta_{\beta\gamma}\Theta(x'-y)]\hat{C}^r_{\alpha\beta}(x,x') . \end{aligned} \tag{28}$$

Finally, taking the limit $x'\to x+0$ with $x<y<x'$ we obtain the required normalization conditions,

$$\hat{C}^l_{\alpha\gamma}(x)\otimes\hat{C}^l_{\gamma\beta}(x)=i\alpha\delta_{\alpha\gamma}\hat{C}^l_{\alpha\beta}(x) , \tag{29}$$

$$\hat{C}^r_{\alpha\gamma}(x)\otimes\hat{C}^r_{\gamma\beta}(x)=i\beta\delta_{\gamma\beta}\hat{C}^r_{\alpha\beta}(x) . \tag{30}$$

The multiplication rules for the diagonal (in direction space) envelope functions $\hat{C}^S_{\alpha\alpha}(x)$ imply Eilenberger's normalization condition [Eq. (4)].

Equations (22), (29), (30), and (24) for the functions $\hat{C}^S_{\alpha\alpha}(x)$ give a complete QC description of the smooth half-space regions $|x|>\delta$. The *drone* amplitudes $\hat{C}^S_{+-}(x)$ and $\hat{C}^S_{-+}(x)$ are unnecessary at the QC level; these functions, which represent interference between incoming and outgoing waves, play an important role in the interface region where a QC solution is not possible. In particular, they force the boundary condition connecting the QC envelope functions to be nonlinear.

B. Interface solution ($|x|<\delta$)

In the interface region, $-\delta<x<\delta$, the dominant terms in Gor'kov's equation come from the large ($>E_F$) interface potential. As in the nonmagnetic case we can then neglect the order parameter $\hat{\Delta}(x)$, the weak external perturbations $\hat{U}^s$, and the small excitation energy, $\epsilon\hat{\tau}_3$; we are then left with

$$\hat{H}_{\text{normal}}\left[x,\frac{1}{i}\partial_x\right]\otimes\hat{\tau}_3\hat{G}(x,x')=\delta(x-x')\hat{1} , \tag{31}$$

$$\hat{\tau}_3\hat{G}(x,x')\otimes\hat{H}_{\text{normal}}\left[x',\frac{-1}{i}\partial_{x'}\right]=\delta(x-x')\hat{1} . \tag{32}$$

The Hamiltonian is just the normal-state Hamiltonian including the interface potential $\hat{V}(x)$, which is diagonal in particle-hole space, but not necessarily diagonal in spin space. In fact we are particularly interested in spin-active interfaces. In Keldysh space $\hat{H}_{\text{normal}}$ is proportional to the unit matrix, while in particle-hole space $\hat{H}_{\text{normal}}$ has the simple representation,

$$\hat{H}_{\text{normal}}=H_{\text{normal}}\left[x,\frac{1}{i}\partial_x\right]\frac{(\hat{1}+\hat{\tau}_3)}{2} +H_{\text{normal}}\left[x,\frac{1}{i}\partial_x\right]^*\frac{(\hat{1}-\hat{\tau}_3)}{2} , \tag{33}$$

where H_{normal} is an operator in spin space.

We want to construct solutions in the interface that match the solutions we have for the smooth half-spaces, which we represent by the envelope expansion of Eq. (8). Since we are ultimately interested only in the connection between the QC amplitudes $\hat{C}^l_{\alpha\beta}(x=-\delta)$ with $\hat{C}^r_{\alpha\beta}(x=+\delta)$, we need only solve the Gor'kov equation for the case $x'>x$, in which case we can solve the simpler equation

$$\hat{H}_{\text{normal}}\left[x,\frac{1}{i}\partial_x\right]\otimes\hat{\tau}_3\hat{G}(x,x')=0 . \tag{34}$$

in order to obtain the desired boundary condition connecting $\hat{C}^l_{\alpha\beta}(0^-)$ with $\hat{C}^r_{\alpha\beta}(0^+)$ [since the envelope functions are smooth on the scale of ξ^S_0 we set $\hat{C}^l(-\delta)\sim\hat{C}^l(0-)$ and $\hat{C}^r(+\delta)\sim\hat{C}^r(0+)$], it is useful to study the solutions of Schrödinger's equation at the Fermi surface,

$$\hat{H}_{\text{normal}}\left[x,\frac{1}{i}\partial_x\right]\vec{\phi}(x)=0 , \tag{35}$$

where $\vec{\phi}(x)$ is a four-component spinor in Nambu space (the Keldysh index is irrelevant and will be dropped unless explicitly needed). The general solution of (35) in the regions $x\approx\pm\delta$, where the potential is flat, is

$$\vec{\phi}(x)=\frac{1}{(v^l)^{1/2}}\sum_{\alpha=\pm1}\vec{\phi}^l_\alpha e^{\alpha i p^l x}; \quad x\approx-\delta \tag{36}$$

and

$$\vec{\phi}(x)=\frac{1}{(v^r)^{1/2}}\sum_{\alpha=\pm1}\vec{\phi}^r_\alpha e^{\alpha i p^r x}; \quad x\approx+\delta . \tag{37}$$

The coefficients $\vec{\phi}^l_\alpha$ and $\vec{\phi}^r_\alpha$ are constant Nambu vectors, which are constrained only by the condition that Eqs. (36) and (37) represent the same solution of Eq. (35). This leads to a linear relation among the coefficients $\vec{\phi}^l_{+1},\vec{\phi}^l_{-1},\vec{\phi}^r_{+1},\vec{\phi}^r_{-1}$, which can be expressed in terms of an *interface transfer matrix*,[25] $\hat{M}_{\alpha\beta}$,

$$\vec{\phi}^{\,l}_{\alpha}=\sum_{\beta=\pm1}\hat{M}_{\alpha\beta}\vec{\phi}^{\,r}_{\beta}\ . \tag{38}$$

The Nambu matrices $\hat{M}_{++}$, $\hat{M}_{+-}$, etc., are diagonal in the particle-hole subspace because the interface Hamiltonian does not mix particle and hole solutions. The $\hat{M}$ matrices in general depend on the incoming momentum $\mathbf{p}$, the unit normal to the interface and the interface magnetization, among other variables. We make explicit these dependences only when necessary. The hole solutions are constructed by simply taking the complex conjugate of the particle solutions. This then implies

$$\hat{M}_{\alpha\beta}=\frac{M_{\alpha\beta}(\hat{1}+\hat{\tau}_3)}{2}+\frac{\tilde{M}_{\alpha\beta}(\hat{1}-\hat{\tau}_3)}{2}\ , \tag{39}$$

with the transfer matrix $\tilde{M}_{\alpha\beta}$ related to $M_{\alpha\beta}$ by

$$\begin{bmatrix}\tilde{M}_{++}(\mathbf{p}_{\parallel}) & \tilde{M}_{+-}(\mathbf{p}_{\parallel})\\ \tilde{M}_{-+}(\mathbf{p}_{\parallel}) & \tilde{M}_{--}(\mathbf{p}_{\parallel})\end{bmatrix} =\begin{bmatrix}M^*_{--}(-\mathbf{p}_{\parallel}) & M^*_{-+}(-\mathbf{p}_{\parallel})\\ M^*_{+-}(-\mathbf{p}_{\parallel}) & M^*_{++}(-\mathbf{p}_{\parallel})\end{bmatrix}\ . \tag{40}$$

Note that conjugation interchanges the direction indices and inverts $\mathbf{p}_{\parallel}$, and that the coefficients M_{++}, etc., are 2×2 matrices in spin space.

The columns of the Green's function, $\hat{\tau}_3\hat{G}(x,x')$, in the interface region, fulfill the Schrödinger equation (35), and the rows of $\hat{\tau}_3\hat{G}$ fulfill the adjoint equation,

$$\overleftarrow{\phi}(x')\hat{H}_{\text{normal}}\left[x',-\frac{\partial_{x'}}{i}\right]=0\ , \tag{41}$$

where $\overleftarrow{\phi}$ denotes the transposed spinor in Nambu space. The adjoint of (38) gives,

$$\overleftarrow{\phi}^{\,l}_{\alpha}=\sum_{\beta=\pm1}\overleftarrow{\phi}^{\,r}_{\beta}\hat{M}^{+}_{\beta\alpha}\ , \tag{42}$$

and we then conclude that the expansion coefficients of $\hat{G}$; i.e., the envelope functions $\hat{C}^{\,l}_{\alpha\beta}(0^-)$ and $\hat{C}^{\,r}_{\alpha\beta}(0^+)$ are connected by

$$\hat{C}^{\,l}_{\alpha\beta}(0^-)=\sum_{\mu,\nu}\hat{M}_{\alpha\mu}\hat{C}^{\,r}_{\mu\nu}(0^+)\hat{M}^{+}_{\nu\beta}\ . \tag{43}$$

This boundary condition supplements the equations for $\hat{C}^{\,S}_{\alpha\beta}(x)$ [Eqs. (22) and (23)].

C. Symmetries of the scattering matrix

The transfer matrix $M_{\alpha\beta}$ must reflect the symmetry of the interface potential. In the following we discuss the restrictions on $M_{\alpha\beta}$ imposed by symmetries of the interface Hamiltonian. It is convenient for this purpose to drop the direction indices $(\alpha\beta)$ in favor of a compact matrix notation. We denote by M a 4×4 matrix acting on spin and direction indices, and introduce a set of Pauli matrices in direction space, $(\gamma_1,\gamma_2,\gamma_3)$, in addition to the usual Pauli matrices in spin space $(\sigma_1,\sigma_2,\sigma_3)$.

We require the interface potential to conserve particle current. From the continuity equation expressing conservation of probability we have for the two-component particlelike spinors[26] (and similarly for the holelike spinors),

$$\phi^{l\dagger}_{+}\phi^{l}_{+}-\phi^{l\dagger}_{-}\phi^{l}_{-}=\phi^{r\dagger}_{+}\phi^{r}_{+}-\phi^{r\dagger}_{-}\phi^{r}_{-}\ , \tag{44}$$

which implies the condition,

$$M^{+}\gamma_3 M=\gamma_3\ . \tag{45}$$

This condition is equivalent to the unitarity condition that is imposed on the scattering S matrix, which connects the "incoming" amplitudes with the "outgoing" amplitudes,

$$\begin{bmatrix}\phi^{l}_{-}\\ \phi^{r}_{+}\end{bmatrix}=\begin{bmatrix}S_{11} & S_{12}\\ S_{21} & S_{22}\end{bmatrix}\begin{bmatrix}\phi^{l}_{+}\\ \phi^{r}_{-}\end{bmatrix}\ . \tag{46}$$

from Eq. (44) we obtain the unitarity constraint on S,

$$SS^{+}=1\ . \tag{47}$$

The explicit connections between the particlelike elements of M in direction space and the corresponding elements of S are

$$M=\begin{bmatrix}S_{21}^{-1} & -S_{21}^{-1}S_{22}\\ S_{11}S_{21}^{-1} & S_{12}-S_{11}S_{21}^{-1}S_{22}\end{bmatrix}\ , \tag{48}$$

which may be written more conveniently, using the unitarity of S,

$$M=\begin{bmatrix}S_{21} & 0\\ 0 & S_{12}^{+}\end{bmatrix}^{-1}\begin{bmatrix}1 & -S_{22}\\ -S_{22}^{+} & 1\end{bmatrix}\ . \tag{49}$$

Similar relations hold between the hole components of $\tilde{M}$ [Eq. (40)] and the corresponding hole components of $\hat{S}_{\alpha\beta}=S_{\alpha\beta}(\hat{1}+\hat{\tau}_3)/2+\tilde{S}_{\alpha\beta}(\hat{1}-\hat{\tau}_3)/2$; it is then straightforward to show that $\tilde{S}_{\alpha\beta}(\mathbf{p}_{\parallel})=S_{\beta\alpha}(-\mathbf{p}_{\parallel})^{\text{tr}}$.

In addition to particle conservation, the interface Hamiltonian may possess additional symmetries including, (1) spin-current conservation, (2) time-reversal symmetry, (3) reflection symmetries, and (4) rotational symmetry. The transfer matrix M, or the S matrix, will obey the following additional constraints.

(1) Spin-current conservation,

$$\begin{aligned}&M^{+}\gamma_3\boldsymbol{\sigma}M=\gamma_3\boldsymbol{\sigma}\ ,\\ &S^{+}\boldsymbol{\sigma}S=\boldsymbol{\sigma}\ .\end{aligned} \tag{50}$$

(2) Time-reversal symmetry,

$$\begin{aligned}&M(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=\gamma_1\sigma_2M^*(\hat{\mathbf{n}},-\mathbf{p},-\boldsymbol{\mu})\sigma_2\gamma_1\ ,\\ &S(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=\sigma_2S^{T}(\hat{\mathbf{n}},-\mathbf{p},-\boldsymbol{\mu})\sigma_2\ .\end{aligned} \tag{51}$$

(3) Reflection symmetry in a plane perpendicular to $\mathbf{p}_{\parallel}=(0,0,p_{\parallel})$,

$$\begin{aligned}&M(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=\sigma_3M(\hat{\mathbf{n}},\Pi_{xy}\mathbf{p},\Pi_{xy}\boldsymbol{\mu})\sigma_3\ ,\\ &S(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=\sigma_3S(\hat{\mathbf{n}},\Pi_{xy}\mathbf{p},\Pi_{xy}\boldsymbol{\mu})\sigma_3\ .\end{aligned} \tag{52}$$

Note that the reflection Π_{xy} in the (x,y) plane changes only the sign of the z component of a polar vector, while for an axial vector it is the x and y components which change sign.

(4) Rotational symmetry,

$$M(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=U^{\dagger}(R)M(R\hat{\mathbf{n}},R\mathbf{p},R\boldsymbol{\mu})U(R)\ ,$$
$$S(\hat{\mathbf{n}},\mathbf{p},\boldsymbol{\mu})=U^{\dagger}(R)S(R\hat{\mathbf{n}},R\mathbf{p},R\boldsymbol{\mu})U(R)\ . \quad (53)$$

The M and S matrices depend on the unit normal $\hat{\mathbf{n}}$ of the interface, the momentum of an incoming wave $\mathbf{p}$ with $\hat{\mathbf{n}}\cdot\mathbf{p}>0$, and in general the magnetization $\boldsymbol{\mu}$ of the interface. The operator $U(R)$ generates a rotation R in spin space.

Spin-current conservation is particularly restrictive; combining (50) with current conservation gives $M\boldsymbol{\sigma}=\boldsymbol{\sigma}M$ (or $S\boldsymbol{\sigma}=\boldsymbol{\sigma}S$), implying that the interface reflects and transmits either spin configuration equally. Note that time-reversal invariance of the interface alone does not guarantee spin-current conservation; in particular spin-orbit scattering, in general, leads to spin-current nonconservation.[12]

D. ELIMINATION OF DRONE AMPLITUDES

The boundary condition [Eq. (43)] involves the *drone* amplitudes C^S_{+-},C^S_{-+} which are the amplitudes for the rapidly oscillating parts of the Green's function. These amplitudes are useful in deriving the boundary condition, but they do not carry any relevant physical information in the quasiclassical limit; thus, following Zaitsev,[21] we eliminate these amplitudes since they have fulfilled their purpose. The price one pays for the elimination of the *drone* amplitudes is a set of nonlinear boundary conditions connecting the remaining quasiclassical amplitudes. The elimination procedure is not unique; different algebraic elimination schemes lead to apparently different boundary conditions.[21,22] However, these different boundary conditions must be physically equivalent, and can be transformed one into another.

We use formula (49) for the scattering M matrix in terms of the S matrix to obtain the following two relations from the general boundary condition [Eq. (43)]:

$$\hat{C}^r_{++}-\hat{C}^r_{+-}\hat{S}^+_{22}-\hat{S}_{22}\hat{C}^r_{-+}+\hat{S}_{22}\hat{C}^r_{--}\hat{S}^+_{22}=\hat{S}_{21}\hat{C}^l_{++}\hat{S}^+_{21}\ , \quad (54)$$

$$\hat{C}^r_{--}-\hat{S}^+_{22}\hat{C}^r_{+-}-\hat{C}^r_{-+}\hat{S}_{22}+\hat{S}^+_{22}\hat{C}^r_{++}\hat{S}_{22}=\hat{S}^+_{12}\hat{C}^l_{--}\hat{S}_{12}\ . \quad (55)$$

Since multiplication by the S matrices does not affect the Keldysh indices or the energy and time dependence of the $\hat{C}$ or $\hat{S}$ matrices, we drop the multiplication symbol $\otimes$, except where it is essential. Two additional relations follow from Eq. (43), which we replace by the analogous relations to Eqs. (54) and (55), with the right- and left-hand sides interchanged,

$$\hat{C}^l_{++}-\hat{C}^l_{+-}\hat{S}_{11}-\hat{S}^+_{11}\hat{C}^l_{-+}+\hat{S}^+_{11}\hat{C}^l_{--}\hat{S}_{11}=\hat{S}^+_{21}\hat{C}^r_{++}\hat{S}_{21}\ , \quad (56)$$

$$\hat{C}^l_{--}-\hat{S}_{11}\hat{C}^l_{+-}-\hat{C}^l_{-+}\hat{S}^+_{11}+\hat{S}_{11}\hat{C}^l_{++}\hat{S}^+_{11}=\hat{S}_{12}\hat{C}^r_{--}\hat{S}^+_{12}\ . \quad (57)$$

The boundary condition for a transparent interface ($S_{11}=S_{22}=0$) is easily obtained from the above equations,

$$\hat{C}^r_{++}=\hat{S}_{21}\hat{C}^l_{++}\hat{S}^+_{21}\ , \quad (58)$$

$$\hat{C}^r_{--}=\hat{S}^+_{12}\hat{C}^l_{--}\hat{S}_{12}\ . \quad (59)$$

For spin-inactive interfaces, the S matrices commute with the C matrices, and we obtain the standard condition of continuity for fully transparent interfaces,

$$\hat{C}^r_{++}=\hat{C}^l_{++}\ , \quad (60)$$

$$\hat{C}^r_{--}=\hat{C}^l_{--}\ . \quad (61)$$

In the general case of spin-active, partially transmitting interfaces the multiplication rules in Eqs. (29) and (30) must be used to discover the QC boundary condition. The basic relations which are used to eliminate the drone amplitudes in the general case are,

$$(\hat{C}^l_{++}-i)\otimes\hat{C}^l_{+-}=(\hat{C}^l_{--}+i)\otimes\hat{C}^l_{-+}=\hat{C}^l_{+-}\otimes\hat{C}^l_{--}=\hat{C}^l_{-+}\otimes\hat{C}^l_{++}=0\ ,$$
$$\hat{C}^r_{+-}\otimes(\hat{C}^r_{--}+i)=\hat{C}^r_{-+}\otimes(\hat{C}^r_{++}-i)=\hat{C}^r_{--}\otimes\hat{C}^r_{-+}=\hat{C}^r_{++}\otimes\hat{C}^r_{+-}=0\ . \quad (62)$$

Multiplying Eq. (54) by $\hat{C}^r_{++}$ on the left and by $(\hat{C}^r_{++}-i)$ on the right gives

$$\hat{C}^r_{++}\otimes\hat{S}_{22}\hat{C}^r_{--}\hat{S}^+_{22}\otimes(\hat{C}^r_{++}-i)=\hat{C}^r_{++}\otimes\hat{S}_{21}\hat{C}^l_{++}\hat{S}^+_{21}\otimes(\hat{C}^r_{++}-i)\ . \quad (63)$$

The analogous manipulations applied to Eqs. (55)–(57) yield

$$\hat{C}^r_{--}\otimes\hat{S}^+_{22}\hat{C}^r_{++}\hat{S}_{22}\otimes(\hat{C}^r_{--}+i)=\hat{C}^r_{--}\otimes\hat{S}^+_{12}\hat{C}^l_{--}\hat{S}_{12}\otimes(\hat{C}^r_{--}+i)\ , \quad (64)$$

$$(\hat{C}^l_{++}-i)\otimes\hat{S}^+_{11}\hat{C}^l_{--}\hat{S}_{11}\otimes\hat{C}^l_{++}=(\hat{C}^l_{++}-i)\otimes\hat{S}^+_{21}\hat{C}^r_{++}\hat{S}_{21}\otimes\hat{C}^l_{++}\ , \quad (65)$$

$$(\hat{C}^l_{--}+i)\otimes\hat{S}_{11}\hat{C}^l_{++}\hat{S}^+_{11}\otimes\hat{C}^l_{--}=(\hat{C}^l_{--}+i)\otimes\hat{S}_{12}\hat{C}^r_{--}\hat{S}^+_{12}\otimes\hat{C}^l_{--}\ . \quad (66)$$

The four nonlinear boundary conditions, Eqs. (63)–(66), contain some redundancy; we require only two independent conditions for a full description of the interface. A minimal set of boundary conditions is derived below for the special case of a weakly transmitting boundary ($|\hat{S}_{12}|^2\ll 1$). The boundary conditions in the weakly transmitting limit are obtained perturbatively from the Eqs. (63)–(66) and the solutions for a perfectly reflecting interface. For the perfectly reflecting interface ($S_{12}=S_{21}=0$) we obtain from (63) and (64),

$$\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{+}_{22}\otimes[\hat{C}^{r}_{++}-i+(\hat{S}^{+}_{22})^{-1}(\hat{C}^{r}_{--}+i)\hat{S}^{+}_{22}]=0 \ , \quad (67)$$

which leads to

$$\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}\otimes(\hat{S}^{+}_{22}\hat{C}^{r}_{++}+\hat{C}^{r}_{--}\hat{S}^{+}_{22})=0 \ . \quad (68)$$

The term in parentheses is invertable, so that

$$\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}=0 \ . \quad (69)$$

Analogous arguments applied to Eq. (64) yield,

$$\hat{C}^{r}_{--}\otimes\hat{S}^{+}_{22}\hat{C}^{r}_{++}=0 \ . \quad (70)$$

Next we use the identity,

$$(\hat{C}^{r}_{++}-\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-i)=(\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-\hat{S}_{22}\hat{C}^{r}_{--}\otimes\hat{S}^{-1}_{22}\hat{C}^{r}_{++})\otimes(\hat{C}^{r}_{++}+\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22})^{-1} \ , \quad (71)$$

which follows from the algebraic rules [Eq. (43)]. Inserting Eqs. (69) and (70), and using the unitarity condition, $\hat{S}^{+}_{22}=\hat{S}^{-1}_{22}$, we obtain boundary condition for the right-hand side of a perfectly reflecting interface,

$$\hat{C}^{r}_{++}-\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-i=0 \ , \quad (72)$$

or, equivalently, using Eqs. (23),

$$\hat{g}^{r}(\hat{\mathbf{p}},x^{s};\epsilon,t)=\hat{S}_{22}\hat{g}^{r}(\underline{\hat{\mathbf{p}}},x^{s};\epsilon,t)\hat{S}^{-1}_{22} \ , \quad (73)$$

for x^{s} on the surface. Note that condition (73) reduces for a magnetically inactive surface ($\hat{S}_{22}$ commutes with $\hat{g}^{r}$!) to the standard condition $\hat{g}^{r}(\hat{\mathbf{p}},x^{s};\epsilon,t)=\hat{g}^{r}(\underline{\hat{\mathbf{p}}},x^{s};\epsilon,t)$. Starting from Eqs. (65) and (66), arguments similar to those leading to (72) give us the boundary conditions for the left side of a perfectly reflecting interface,

$$\hat{C}^{l}_{++}-\hat{S}^{-1}_{11}\hat{C}^{l}_{--}\hat{S}_{11}-i=0 \ , \quad (74)$$

$$\hat{g}^{l}(\hat{\mathbf{p}},x^{s};\epsilon,t)=\hat{S}^{-1}_{11}\hat{g}^{l}(\underline{\hat{\mathbf{p}}},x^{s};\epsilon,t)\hat{S}_{11} \ . \quad (75)$$

For a weakly transmitting interface there are correction terms to the above boundary conditions which can be obtained by expanding the general boundary conditions [Eqs. (63)–(66)] through second order in the S-matrix elements $\hat{S}_{12}$ and $\hat{S}_{21}$, which describe the transmission properties of the interface. It is useful to note that the following quantities are of second order (or higher) in the off-diagonal matrix elements: $\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}$, $\hat{C}^{r}_{--}\otimes\hat{S}^{+}_{22}\hat{C}^{r}_{++}$, $\hat{C}^{r}_{++}-\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-i$, $\hat{S}^{-1}_{22}-\hat{S}^{+}_{22}$, and the equivalent terms for the left-hand side of the interface. A useful consequence is that

$$\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{+}_{22}\otimes\hat{C}^{r}_{++}=O(|\hat{S}_{12}|^{4}) \ . \quad (76)$$

Similarly, one finds,

$$\hat{C}^{r}_{--}\otimes\hat{S}^{+}_{22}\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}=O(|\hat{S}_{12}|^{4}) \ . \quad (77)$$

Another useful relation is

$$\hat{S}^{+}_{22}=\hat{S}^{-1}_{22}-\hat{S}^{-1}_{22}\hat{S}_{21}\hat{S}^{+}_{21} \ . \quad (78)$$

Using these rules we can write Eq. (63), up to corrections of order $|\hat{S}_{12}|^{4}$, in the form

$$-i\hat{C}^{r}_{++}\otimes\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}=\hat{C}^{r}_{++}\otimes\hat{S}_{21}\hat{C}^{l}_{++}\hat{S}^{+}_{21}\otimes(\hat{C}^{r}_{++}-i) \ . \quad (79)$$

Similarly, we obtain from Eq. (64)

$$i\hat{S}_{22}\hat{C}^{r}_{--}\otimes\hat{S}^{-1}_{22}\hat{C}^{r}_{++}=(\hat{C}^{r}_{++}-i)\otimes\hat{S}_{21}(\hat{C}^{l}_{++}-i)\hat{S}^{+}_{21}\otimes\hat{C}^{r}_{++}+i(\hat{C}^{r}_{++}-i)\otimes\hat{S}_{21}\hat{S}^{+}_{21}\hat{C}^{r}_{++} \ . \quad (80)$$

The second term on the right-hand side is the correction term of order $|S_{12}|^{2}$ coming from the replacement of $\hat{S}^{+}_{22}$ by $\hat{S}^{-1}_{22}-\hat{S}^{-1}_{22}\hat{S}_{21}\hat{S}^{+}_{21}$ on the left-hand side of Eq. (64). We can cancel two terms on the right-hand side of Eq. (80) to obtain

$$i\hat{S}_{22}\hat{C}^{r}_{--}\otimes\hat{S}^{-1}_{22}\hat{C}^{r}_{++}=(\hat{C}^{r}_{++}-i)\otimes\hat{S}_{21}\hat{C}^{l}_{++}\hat{S}^{+}_{21}\otimes\hat{C}^{r}_{++} \ . \quad (81)$$

By adding Eqs. (79) and (81) and using the identity [Eq. (71)], as well as the relation

$$(\hat{C}^{r}_{++}+\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22})^{-1}=-(2\hat{C}^{r}_{++}-i)+O(|\hat{S}_{12}|^{2}) \ , \quad (82)$$

we obtain

$$i(\hat{C}^{r}_{++}-\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-i)=\hat{C}^{r}_{++}\otimes\hat{S}_{21}\hat{C}^{l}_{++}\hat{S}^{+}_{21}\otimes(-i\hat{C}^{r}_{++}-1)+(\hat{C}^{r}_{++}-i)\otimes\hat{S}_{21}\hat{C}^{l}_{++}\hat{S}^{+}_{21}\otimes(i\hat{C}^{r}_{++}) \ . \quad (83)$$

The terms of third order in the $\hat{C}$ amplitudes cancel on the right-hand side of Eq. (83), and we obtain

$$(\hat{C}^{r}_{++}-\hat{S}_{22}\hat{C}^{r}_{--}\hat{S}^{-1}_{22}-i)=-i[\hat{S}_{21}\hat{C}^{l}_{++}\hat{S}^{+}_{21},\hat{C}^{r}_{++}]_{\otimes} \ . \quad (84)$$

The algebraic steps leading from Eqs. (63) and (64) to Eq. (84) can be repeated starting from Eqs. (65) and (66) to obtain

$$(\hat{C}^{\,l}_{++}-\hat{S}^{-1}_{11}\hat{C}^{\,l}_{--}\hat{S}_{11}-i)=+i[\hat{S}^{+}_{21}\hat{C}^{\,r}_{++}\hat{S}_{21},\hat{C}^{\,l}_{++}]_{\otimes}\ . \tag{85}$$

We finally write Eqs. (84) and (85) in terms of the QC propagators evaluated at the interface,

$$\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon,t)-\hat{S}_{22}\hat{g}^{\,r}(\underline{\hat{\mathbf{p}}}^{\,r},x^{r};\epsilon,t)\hat{S}^{-1}_{22}=-\frac{i}{2\pi}[\hat{S}_{21}(\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon,t)+i\pi)\hat{S}^{+}_{21},\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon,t)]_{\otimes}\ , \tag{86}$$

$$\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon,t)-\hat{S}^{-1}_{11}\hat{g}^{\,l}(\underline{\hat{\mathbf{p}}}^{\,l},x^{l};\epsilon,t)\hat{S}_{11}=-\frac{i}{2\pi}[\hat{g}^{\,l}(\hat{p}^{\,l},x^{l};\epsilon,t),\hat{S}^{+}_{21}(\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon,t)+i\pi)\hat{S}_{21}]_{\otimes}\ . \tag{87}$$

For equilibrium properties it is convenient to use the Matsubara propagators which depend on the Matsubara frequencies $\epsilon_n=(2n+1)\pi T$. These propagators are related to the equilibrium retarded and advanced propagators in the standard way, and identical arguments to those above give the following boundary conditions for systems in equilibrium:

$$\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon_n)-\hat{S}_{22}\hat{g}^{\,r}(\underline{\hat{\mathbf{p}}}^{\,r},x^{r};\epsilon_n)\hat{S}^{-1}_{22}=-\frac{i}{2\pi}[\hat{S}_{21}(\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon_n)+i\pi)\hat{S}^{+}_{21},\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon_n)]\ , \tag{88}$$

$$\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon_n)-\hat{S}^{-1}_{11}\hat{g}^{\,l}(\underline{\hat{\mathbf{p}}}^{\,l},x^{l};\epsilon_n)\hat{S}_{11}=-\frac{i}{2\pi}[\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon_n),\hat{S}^{+}_{21}(\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon_n)+i\pi)\hat{S}_{21}]\ . \tag{89}$$

Note that the matrix product refers only to multiplication of Nambu matrices.

Our notation for the four momentum directions $\hat{\mathbf{p}}^{\,l}$, $\underline{\hat{\mathbf{p}}}^{\,l}$, $\hat{\mathbf{p}}^{\,r}$, and $\underline{\hat{\mathbf{p}}}^{\,r}$ is shown in Fig. 2. Equations (86)–(89) establish the boundary conditions at a weakly transmitting interface, and generalize those derived by Zaitsev who assumes the interface to be spin inactive. An important consequence of the above boundary conditions is that spin current

$$\mathbf{J}^{S}_{i}=N(E^{S}_{F})\int\frac{d\Omega^{S}}{4\pi}\mathbf{v}^{S}_{F}T\sum_{n}\tfrac{1}{4}\mathrm{Tr}[\hat{\tau}_3\sigma_i\hat{g}^{\,S}(\hat{\mathbf{p}}^{\,S},\mathbf{R};\epsilon_n)] \tag{90}$$

is not necessarily conserved by the interface. The boundary conditions derived by Zaitsev necessarily imply that spin-current is conserved, in addition to particle current.

E. JOSEPHSON CURRENT THROUGH A MAGNETIC INTERFACE

Weakly transmitting interfaces provide a "weak link" that is necessary for a supercurrent to flow across an interface separating two superconductors. Here we derive a formula for the Josephson current in terms of the transmission amplitudes $\hat{S}_{21}$ for a spin-active interface. The equilibrium (dc) particle current flowing in the superconductor with $\mathbf{R}\in S$ $(=l$ or $r)$ is

$$\mathbf{j}^{S}=N(E^{S}_{F})\int\frac{d\Omega^{S}}{4\pi}\mathbf{v}^{S}_{F}T\sum_{n}\tfrac{1}{4}\mathrm{Tr}[\hat{\tau}_3\hat{g}^{\,S}(\hat{\mathbf{p}}^{\,S},\mathbf{R};\epsilon_n)]\ , \tag{91}$$

where $N(E^{S}_{F})$ is the quasiparticle density of states at the Fermi energy. In the rest of the paper $\hat{g}^{\,S}$ is the Matsubara propagator.

Here we are interested only in translationally invariant interfaces so we assume $\mathbf{j}^{S}=j^{S}\hat{\mathbf{x}}$, in which case particle conservation requires $j=j^{l}=j^{r}$, independent of x. Thus, we have the freedom to calculate the particle current using the propagators $\hat{g}^{\,S}(\hat{\mathbf{p}}^{\,S},x^{S};\epsilon_n)$, evaluated at the interface. We then express the current calculated on side $S=l,r$ of the interface as

$$j^{S}=N(E^{S}_{F})v^{S}_{F}\int_{+}\frac{d\Omega^{S}}{4\pi}(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}}^{\,S})T\sum_{n}K^{S}\ ,$$
$$K^{S}=\tfrac{1}{4}\mathrm{Tr}\{\hat{\tau}_3[\hat{g}^{\,S}(\hat{\mathbf{p}}^{\,S},x^{S};\epsilon_n)-\hat{g}^{\,S}(\underline{\hat{\mathbf{p}}}^{\,S},x^{S};\epsilon_n)]\}\ , \tag{92}$$

where the integration is over that portion of Fermi surface with $\hat{\mathbf{x}}\cdot\hat{\mathbf{p}}^{\,S}>0$, and $x^{S}=0+(0-)$ for $S=r(l)$. We now make use of the boundary conditions for a weakly transmitting interface. From Eq. (88) we obtain,

$$K^{l}=K^{r}=\frac{i}{8\pi}\mathrm{Tr}\{\hat{\tau}_3[\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon_n),S^{+}_{21}\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon_n)\hat{S}_{21}]\}\ , \tag{93}$$

and it is straightforward to show that the boundary condition for weak transmission conserves particle number. Thus, the main result for the supercurrent flowing across a weakly transmitting interface is given by (choosing $S=l$),

$$j^{l}=N(E^{l}_{F})v^{l}_{F}\int_{+}\frac{d\Omega^{l}}{4\pi}(\hat{x}\cdot\hat{\mathbf{p}}^{\,l})\cdot\frac{i}{8\pi}T\sum_{n}\mathrm{Tr}\{\hat{\tau}_3[\hat{g}^{\,l}(\hat{\mathbf{p}}^{\,l},x^{l};\epsilon_n),\hat{S}^{+}_{21}\hat{g}^{\,r}(\hat{\mathbf{p}}^{\,r},x^{r};\epsilon_n)\hat{S}_{21}]\}\ . \tag{94}$$

The propagators that define the current in Eq. (94) are to be calculated in the limit of a *perfectly reflecting* interface. In general the calculation of the QC propagators at one interface requires a numerical calculation along the lines of Buchholtz and Zwicknagl's[27] calculation of the triplet order parameter $\hat{\Delta}(\hat{\mathbf{p}},x)$ for a nonmagnetic interface; once the order parameter is known the QC propagator can be obtained quite easily by solving the QC transport equations. Self-consistent solutions for the order parameter $\hat{\Delta}(\hat{\mathbf{p}},x)$ and propagator do not currently exist for magnetically active interfaces, but these calculations can be carried out with the aid of the boundary condition given in Eqs. (73) and (75).

Some qualitative results for the supercurrent can be obtained by evaluating Eq. (94) with the *bulk* propagators, but we emphasize that except for *s*-wave superconductors in contact with a nonmagnetic, perfectly reflecting interface this is a procedure which may yield only qualitatively correct results, particularly in unconventional superconductors where presumed spin and orbital correlations associated with the Cooper pairs may be destroyed by the interface potential. Since the results to follow are at best qualitatively accurate, we assume for simplicity that the Fermi surfaces of both metals are spherical and have the same volume.

First consider a nonmagnetic interface, in which case $\hat{S}_{21}=s_{21}\hat{1}$. The supercurrent, when evaluated with the weak-coupling bulk propagators (note that we assume only unitarity states, in which $\hat{\Delta}\,\hat{\Delta}=-|\Delta|^2\hat{1}$),

$$\hat{g}^S(\hat{\mathbf{p}},x;\epsilon_n)=\pi\frac{i\epsilon_n\hat{\tau}_3-\hat{\Delta}^S(\hat{\mathbf{p}},x)}{(\epsilon_n^2+|\Delta^S|^2)^{1/2}}$$
$$\hat{\Delta}^S=\begin{bmatrix}0 & \Delta^S(\hat{\mathbf{p}},x)\\ -\Delta^S(\hat{\mathbf{p}},x)^\dagger & 0\end{bmatrix}, \tag{95}$$

becomes

$$j^l=N(E_F^l)v_F^l\frac{\pi}{2}\int_+\frac{d\Omega^l}{4\pi}(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}})|s_{21}|^2T\sum_n\frac{\mathrm{Im}\{\mathrm{tr}_{\mathrm{spin}}[\Delta^l(\hat{\mathbf{p}},0-)\Delta^{r\dagger}(\hat{\mathbf{p}},0+)]\}}{(\epsilon_n^2+|\Delta^l|^2)^{1/2}(\epsilon_n^2+|\Delta^r|^2)^{1/2}}\ . \tag{96}$$

For conventional *s*-wave superconductors, with $\Delta^S=|\Delta^S|e^{i\alpha^S}$, we recover the Josephson current-phase relation with the maximum supercurrent calculated by Ambegaokar and Baratoff,[28]

$$j^l=\frac{\pi}{4}\langle|s_{21}|^2\rangle N(E_F^l)v_F^l\left[T\sum_n\frac{|\Delta^r||\Delta^l|}{(\epsilon_n^2+|\Delta^r|^2)^{1/2}(\epsilon_n^2+|\Delta^l|^2)^{1/2}}\right]\sin(\alpha^l-\alpha^r)\ , \tag{97}$$

where the angular brackets denote the appropriate average of the transmission probability over the Fermi surface.

The more interesting cases are those in which at least one side of the interface is an unconventional superconductor. If for example the left-hand side is a conventional *s*-wave superconductor and the right-hand side is a *d*-wave superconductor, then in the limit $T_C^{s\text{-wave}}\gg T_C^{d\text{-wave}}$ and $T\sim T_C^{d\text{-wave}}$, the supercurrent becomes,

$$j=\pi N(E_F^l)v_F^l\left[T\sum_n\frac{1}{|\epsilon_n|(\epsilon_n^2+|\Delta_o^l|^2)^{1/2}}\right]\times\int_+\frac{d\Omega}{4\pi}(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}})|s_{21}|^2\mathrm{Im}[\Delta_0^l\Delta_0^r(\hat{\mathbf{p}})^*]\ . \tag{98}$$

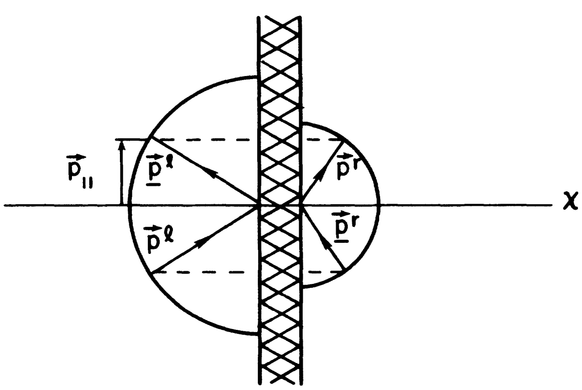

FIG. 2. *Interface scattering kinematics:* The four possible scattering states, for a given value of the conserved parallel momentum $\mathbf{p}_{\parallel}$, are labeled by their momenta, all on their respective Fermi surfaces.

In general, a supercurrent flows between an *s*- and *d*-wave superconductor provided the *d*-wave order parameter $\Delta_0^r(\hat{\mathbf{p}})=\sum_{m=-2}^{+2}C_mY_{lm}(\hat{\mathbf{p}})$, has a nonvanishing amplitude with $m=0$ relative to the $\hat{\mathbf{x}}$ direction. Note that this conclusion does not depend upon any momentum dependence of the transmission amplitude s_{21} and is obviously not restricted to the *d*-wave case, but is valid for any singlet order parameter.

Equation (96) may also be applied to the case of a supercurrent flowing across a nonmagnetic interface between two triplet superconductors. An interesting application is the Josephson current flowing between two vessels of superfluid ^{3}He-*A* separated by a weakly transmitting interface. In this case the order parameter on side $S(=1,r)$ is parametrized by a triad of orthonormal vectors $(\hat{\mathbf{n}}_s,\hat{\mathbf{m}}_s,\hat{l}_s=\hat{\mathbf{m}}_s\times\hat{\mathbf{n}}_s)$,

$$\Delta^S=\hat{l}_s(\hat{\mathbf{m}}_s+i\hat{\mathbf{n}}_s)\cdot\hat{\mathbf{p}}\ , \tag{99}$$

with $\hat{l}_s(x_s)=\pm\hat{\mathbf{x}}$.[29] There are two distinct cases; either (i) $\hat{l}_r=\hat{l}_l$ or (ii) $\hat{l}_r=-\hat{l}_l$, which yield very different results for the supercurrent. For case (i) we choose $\hat{\mathbf{m}}_l=\hat{\mathbf{y}}$, $\hat{\mathbf{n}}_l=\hat{\mathbf{z}}$ and then $\hat{\mathbf{m}}_r=\cos\alpha\hat{\mathbf{y}}+\sin\alpha\hat{\mathbf{z}}$ and $\hat{\mathbf{n}}_r=-\sin\alpha\hat{\mathbf{y}}+\cos\alpha\hat{\mathbf{z}}$.

The angle of rotation of the orbital axes plays the role of the relative phase between the superfluids, and we find a Josephson current proportional to

$$j \sim \int_+ \frac{d\Omega}{4\pi}(\hat{\mathbf{p}}\cdot\hat{\mathbf{x}})\,|\,s_{21}\,|^2 \mathrm{Im}[\boldsymbol{\Delta}_l(\hat{\mathbf{p}})\cdot\boldsymbol{\Delta}_r^*(\hat{\mathbf{p}})] \sim \sin\alpha \ . \quad (100)$$

In case (ii) with $\hat{l}_r = -\hat{l}_l$ the Josephson current is identically zero, the result originally obtained by Ambegaokar *et al.*[29] This vanishing of the supercurrent occurs because the right and left order parameters have opposite projections of the orbital angular momentum along the $\hat{\mathbf{x}}$ axis; i.e., $\boldsymbol{\Delta}_l \sim \hat{x}e^{i\phi}$ and $\boldsymbol{\Delta}_r \sim \hat{x}e^{-i\phi}$, where ϕ is the azimuthal angle in the y-z plane. The sensitivity of the Josephson current to the relative orientation of the two triplet order parameters across the interface is a generic feature of Josephson tunneling between triplet superconductors, and may be relevant to the lack of a Josephson current between two electrodes of UPt_3.[14]

For a triplet superconductor in contact with a singlet superconductor through a magnetically *inactive* interface we immediately obtain the result of Pals *et al.*,[10] namely that the Josephson current vanishes identically. Josephson tunneling between singlet and triplet superconductors is possible if the interface is spin active.[12] The transmission amplitude for a spin-active interface has the form,

$$\hat{S}_{21} = \begin{bmatrix} S_{21}(\hat{\mathbf{p}}) & 0 \\ 0 & S_{12}^{\mathrm{tr}}(-\underline{\hat{\mathbf{p}}}) \end{bmatrix} ,$$
$$S_{ij} = s_{ij} + \mathbf{m}_{ij}\cdot\boldsymbol{\sigma} \ . \quad (101)$$

The supercurrent, calculated assuming the bulk propagators in Eqs. (95) and (96), is given by Eq. (92) with

$$K^l = \pi \frac{\mathrm{Im}[\Delta_0^* \boldsymbol{\Delta}\cdot\mathbf{w}]}{(\epsilon_n^2 + |\,\Delta_0\,|^2)^{1/2}(\epsilon_n^2 + |\,\boldsymbol{\Delta}\,|^2)^{1/2}}$$
$$\mathbf{w} = (\mathbf{m}_{21}s_{12}^* - \mathbf{m}_{12}^* s_{21}) + i(\mathbf{m}_{21}\times\mathbf{m}_{12}^*) \ , \quad (102)$$

in agreement with the form of the Josephson current between a singlet and a triplet superconductor obtained in Ref. 12. The general feature of Eq. (102) to note is that the Josephson coupling depends on the relative phase between the spin-dependent transmission amplitudes $\mathbf{m}_{ij}$ and the spin-independent amplitudes s_{ij}, in addition to the phase difference between the singlet and triplet order parameters. In our model no spatial variations of the order parameter are necessary for a Josephson coupling, in contrast to a recent result of Fenton.[30] We would obtain Fenton's result if we assume full reflection symmetry at the interface of the superconductor-oxide-superconductor junction, and include the gradients of the order parameter near the interface. However, there is no reason to impose this symmetry, particularly for a nonsymmetric system such as a Josephson contact between an exotic (i.e., heavy-fermion) superconductor and a conventional superconductor.

The symmetry of the interface does constrain the interface scattering matrix. For the most symmetric spin-active interface, the interface potential is invariant under time reversal and reflections in a plane perpendicular to the interface; the corresponding transmission amplitudes satisfy,[31]

$$s_{ij}(\mathbf{p}_\parallel,\hat{\mathbf{n}}) = s_{ji}(-\mathbf{p}_\parallel,\hat{\mathbf{n}}) \ , \quad (103)$$

$$\mathbf{m}_{ij}(\mathbf{p}_\parallel,\hat{\mathbf{n}}) = \mathbf{m}_{ji}(-\mathbf{p}_\parallel,\hat{\mathbf{n}}) = c_{ij}(\hat{\mathbf{n}}\times\mathbf{p}_\parallel) \ . \quad (104)$$

The kernel K^l in Eq. (102) that determines the current becomes,

$$K^l \sim \mathrm{Re}(c_{21}s_{21}^*)\mathrm{Im}[\Delta_0^* \boldsymbol{\Delta}\cdot(\hat{\mathbf{n}}\times\mathbf{p}_\parallel)] \ , \quad (105)$$

indicating that current depends on (i) the relative phase of the singlet and triplet order parameter, (ii) the *orientation* of the triplet order parameter, and thus the underlying crystalline axes of the triplet superconductor, relative to the interface, and (iii) the relative phase of the spin-orbit transmission amplitude c_{21} and the spin-independent amplitude s_{21}. These latter two features are unique to unconventional superconductors in contact with a conventional s-wave superconductor. They imply that Josephson tunneling between triplet and singlet superconductors is sensitive to the internal structure of the interface and the type of contact made between the interface and the unconventional superconductor, but in general Josephson tunneling between a conventional superconductor, like Al and an unconventional superconductor, perhaps UPt_3, is not excluded. We emphasize again that these conclusions are based upon evaluating the current in Eq. (94) with the bulk propagators, which do not take into account the distortion of the order parameter by the interface. For unconventional superconductors the surface may lead to qualitative changes in the order parameter near the interface. Quantitative calculations of the structure and properties of unconventional superconductors near magnetically active interfaces, with the "tools" developed in the paper, are left to the future.[19]

III. SUMMARY

The main results of this paper are the boundary conditions [Eqs. (63)–(66)] relating the QC propagators for two metals in contact through a magnetically active interface, represented by an interface scattering matrix whose elements are related to the transmission and reflection coefficients of the interface. These boundary conditions supplement the QC transport equations for the bulk superconductors on either side of an interface and provide the necessary constraints to determine the structure of the perturbed superconducting region near an interface. Any quantitative calculation of the properties of inhomogeneous superconductors in contact with magnetic interfaces must start from an accurate calculation of the superconducting order parameter near the interface. The derivation of the boundary conditions for magnetically active interfaces given here follows closely the work of Zaitsev for a nonmagnetic interface; however, the same results can also be obtained by generalizing the T-matrix method developed by Kieselmann to magnetically active interfaces. Finally we want to re-emphasize that our boundary condition applies to perfectly smooth interfaces. Real boundaries always exhibit some degree of roughness, which is particularly important for interfaces with unconventional superconductors. The effects of roughness on superconductivity will be discussed in a forthcoming publication.

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