Quasiclassical description of transport through superconducting contacts

J. C. Cuevas
Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

M. Fogelström
Institute of Theoretical Physics, Chalmers University of Technology and Göteborgs University, S-41296 Göteborg, Sweden
Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We present a theoretical study of transport properties through superconducting contacts based on a new formulation of boundary conditions that mimics interfaces for the quasiclassical theory of superconductivity. These boundary conditions are based on a description of an interface in terms of a simple Hamiltonian. We show how this Hamiltonian description is incorporated into quasiclassical theory via a T-matrix equation by integrating out irrelevant energy scales right at the onset. The resulting boundary conditions reproduce results obtained by conventional quasiclassical boundary conditions, or by boundary conditions based on the scattering approach. This formalism is well suited for the analysis of magnetically active interfaces as well as for calculating time-dependent properties such as the current-voltage characteristics or as current fluctuations in junctions with arbitrary transmission and bias voltage. This approach is illustrated with the calculation of Josephson currents through a variety of superconducting junctions ranging from conventional to d-wave superconductors, and to the analysis of supercurrent through a ferromagnetic nanoparticle. The calculation of the current-voltage characteristics and of noise is applied to the case of a contact between two d-wave superconductors. In particular, we discuss the use of shot noise for the measurement of charge transferred in a multiple Andreev reflection in d-wave superconductors.

I. INTRODUCTION

At the end of the 1960’s several authors demonstrated that the complete standard theory of superconductivity, both in equilibrium and out of equilibrium, can be formulated in terms of a quasiclassical transport equation. This theory, known as quasiclassical theory of superconductivity, combines Landau’s semiclassical transport equations for quasiparticles with the concept of pairing and particle-hole coherence that are the basis of the BCS theory. The quasiclassical theory provides a full description of superconducting phenomena ranging from inhomogeneous superconductors to superconducting phenomena far from equilibrium. In its traditional form, the quasiclassical theory of superconductivity is restricted to the description of weak perturbations of a superconductor: the external perturbations (magnetic field, variations in the chemical potential, etc) should be weak $(V \ll E_F)$, where $E_F$ is the Fermi energy, of long wavelength $(q \gg k_F^{-1})$, where $k_F^{-1}$ is the Fermi wavelength, and of low frequency $(\hbar \omega \ll E_F)$. Although this limit covers many situations of interest in superconductivity, some important cases fall outside the range of validity of the usual scheme of the quasiclassical theory: strong impurities, walls, interfaces, etc. In the case of the analysis of the transport properties of superconducting contacts, the quasiclassical theory is complemented by appropriate boundary conditions, the so-called Zaitsev boundary conditions or by its generalization to magnetically active interfaces by Millis, Rainer and Sauls. Although these boundary conditions provide a formal solution of the problem of a strong perturbation due to interfaces, their highly non-linear form introduces many problems, e.g. these boundary conditions have spurious solutions which require special care, in particular in numerical implementations. At this point, we should mention that the recent progress in the solution of these boundary conditions make them much more tractable.

In the field of electronic transport through superconducting junctions there are many basic situations in which a complete understanding is still lacking. This is partially due to the difficulty of applying the quasiclassical theory because of the lack of simple and manageable boundary conditions. Most of these situations are related to either the current-voltage (I-V) characteristics of contacts between two superconductors with arbitrary transmission, or to situations in which there are magnetically active interfaces giving rise to spin-dependent transport. For instance, in the context of high temperature superconductors (HTS), which by now are believed to be d-wave superconductors, we can mention N-I-S tunnel junctions, grain boundary junctions, widely used for the realization of Josephson junctions, and YBCO S-N-S edge junctions. In the two latter systems the description of the I-V characteristics requires an analysis of multiple Andreev reflections (MAR), while all systems above require a careful self-consistent study of the superconducting state in the presence of pair-breaking, caused by bulk or surface impurities and by the surface itself, in order to account for results obtained in
experiments. Other examples, which take place in the context of conventional superconductors, are the S-N-S point contacts, where the normal region $N$ has a length comparable to the superconducting coherent length $\xi$. These systems demand from the theory a detailed analysis of the interplay between the proximity effect superconductivity in the normal metal and the occurrence of MAR. This analysis is currently in progress making use of the approach described in this work.

With respect to the transport through spin active interfaces there have been an extensive experimental effort to explore tunneling through magnetic insulator barriers by probing the proximity effect in S/F/structures and by constructing S/F-multilayers (see also references therein). Andreev reflection using ferromagnet/superconductor point contacts have also been used to probe the spin polarization of the ferromagnet. Finally, supercurrents have been reported in S/F/S-junctions by Veretennikov et al and by Gandit et al. To model an S/F/S-junction one can follow one of two routes. The first route is to assume an extension of a ferromagnetic metal, now characterized by a length and an exchange field, separating the two superconductors. Following this route, both critical current oscillations and the effect of the exchange field on the Andreev bound states have been studied. The limitation here is that the approach is restricted to small exchange fields in the ferromagnet, i.e. fields that are comparable to the superconducting gap. The second route, which we subscribe to, is to treat the effect of the ferromagnet as a boundary problem connecting the two superconducting half-spaces. Using Bogoliubov-deGennes equations and a WKB-approach for the ferromagnetic barrier, i.e. the scattering approach, Josephson current-phase relations and quasiparticle tunneling have been studied for both conventional s-wave and unconventional d-wave superconductors.

Parallel to the quasiclassical treatment of interfaces, a different formalism referred to as the Hamiltonian approach has emerged as a new interesting tool for the analysis of transport through superconducting contacts. This approach is based on modeling the contact by a simple Hamiltonian in combination with non-equilibrium Green’s function techniques. The origin of this approach can be traced back to the work of Bardeen who introduced the tunnel Hamiltonian approximation in order to describe a tunnel junction. Most of the calculations of current through superconducting contacts in the early 60’s were based on this tunnel Hamiltonian, and were restricted to the lowest order transport processes such as the calculation of the Josephson current in a S-I-S junction. Multi-particle tunneling was first discussed by Schrieff and Wilkins in their multiparticle tunneling theory as a possible explanation for the observed sub-gap structure in superconducting tunnel junctions. The contributions of these higher order processes were found to be divergent, which has led to the quite extended belief that the Hamiltonian approach is pathological except for describing the lowest order tunneling processes. However, in a series of works, Caroli and coworkers in the 70’s, and, more recently, Martín-Rodero and collaborators have shown that one can get rid of all the old pathologies of this approach by using a local representation and by summing the series of tunneling processes up to infinite order. In particular, within this technique a microscopic theory of Multiple Andreev reflections has been developed. This theory describes quantitatively the characteristic of superconducting atomic-size contacts.

In this paper we show how the Hamiltonian approach may be brought into the quasiclassical theory by integrating out large energies right at the onset. The resulting boundary condition reproduces results obtained by the conventional quasiclassical Zaitsev boundary condition or by boundary conditions based on the scattering approach. The boundary condition is also well suited for calculating time-dependent properties such as the current-voltage characteristics or the current fluctuations of S-I-S junctions. The paper is organized in the following manner: In section II we give the energy integration of the Hamiltonian approach and state the resulting boundary condition. In section III we show how the current through a contact may be calculated from the boundary t-matrix. In this section we also calculate the Josephson current resolved in energy and on trajectory for different types of superconductors and for different types of coupling between the two superconductors. In section IV, we discuss the boundary condition at a finite bias applied between the superconductors. This is then applied to the case of two coupled d-wave superconductors. Finally, in section V, current-fluctuations are discussed and the current-current correlator is derived within our method. This is then applied to compute the trajectory resolved current-fluctuations of two coupled d-wave superconductors.

II. DESCRIPTION OF THE APPROACH

The system of study is two semi-infinite superconducting electrodes coupled over some type of interface barrier. Our approach is to artificially separate the problem in to two parts in order to pose a boundary condition for the interface. The first part consists of calculating the Green’s function of either conductor, extending to $\pm \infty$ respectively, in presence of a hard surface at $x = 0$. To this part of the problem, the quasiclassical theory is our theory of choice. It has been shown that strong perturbations, such as rigid walls may be included into quasiclassical theory by means of effective boundary conditions posed for the quasiclassical Green’s function. To couple the two electrodes, from now denoted left (L) and right (R), we assume a phenomenological Hamiltonian as
\[
\hat{H}_T = \sum_{\sigma} \hat{c}^\dagger_{L,\sigma} v_{LR} \hat{c}_{R\sigma} + \hat{c}^\dagger_{R,\sigma} v_{RL} \hat{c}_{L\sigma}.
\]

(1)

The potentials \(v_{LR}\) and \(v_{RL}\), with \(v^\dagger_{RL} = v_{LR} = v\), act as hopping elements connecting the two electrodes \(L\) and \(R\). The perturbation given by \(\hat{H}_T\) is short ranged \((\sim \lambda_F \ll \xi_o)\) and may be strong \((v \sim E_F)\). The local character of \(\hat{H}_T\) allows us to view it as a single strong impurity in case of a point contact or as a line of strong impurities in case of an extended contact between the two electrodes. Following the work of Thuneberg and co-workers, the single impurity or, in case of the line of impurities following the work of Buchholtz and Rainer, this strong perturbation may also be incorporated into quasiclassical theory via a T-matrix equation. Anticipating the result for the T-matrix, the effect of the contact between the two electrodes on the physical quasiclassical Keldysh-Nambu matrix Green’s function, or propagator, \(\tilde{g}_i\), in electrode \(i = (L, R)\) enters as a source term in the transport equation for \(\tilde{g}_i(\mathbf{p})\) along a trajectory \(\mathbf{p}\).

\[
i \mathbf{v} \cdot \nabla_\mathbf{a} \tilde{g}_i(\mathbf{p}) + [\mathbf{v}, \tilde{g}_i(\mathbf{p})]_\mathbf{a} = \frac{\hbar^2}{2m} [\hat{\Sigma}_i(\mathbf{p}), \tilde{g}_i(\mathbf{p})]_\mathbf{a} \delta(\mathbf{R} - \mathbf{R}_c).
\]

(2)

Here \(\mathbf{R}_c\) is the position of the contact and \(\mathbf{v}\) is the Fermi velocity at point \(\mathbf{p}\) on the Fermi surface. The Green’s function \(\tilde{g}_{\infty,i}\) is an intermediate Green’s function obtained by solving the hard wall boundary condition of the separate electrodes, i.e. without taking the contact into account but using the self energies \(\hat{\Sigma}_i\) and evaluated using the physical propagator, \(\tilde{g}_i\), satisfying Eq. (3).

Our objective is to find the quasiclassical T-matrix, \(\tilde{T}\), giving the source term in the transport equation (2) above. The starting point is a conventional many-body perturbation theory for the Hamiltonian \(\hat{H}_T\). To proceed we artificially enlarge our Hilbert space with a ”reservoir quantum number” \((L, R)\) and the functions entering are the matrices

\[
\tilde{G} = \begin{pmatrix} \tilde{G}_{LL} & \tilde{G}_{LR} \\ \tilde{G}_{RL} & \tilde{G}_{RR} \end{pmatrix}, \quad \tilde{T} = \begin{pmatrix} \tilde{T}_{LL} & \tilde{T}_{LR} \\ \tilde{T}_{RL} & \tilde{T}_{RR} \end{pmatrix},
\]

\[
\tilde{G}_{\infty} = \begin{pmatrix} \tilde{G}_{\infty,L} & 0 \\ 0 & \tilde{G}_{\infty,R} \end{pmatrix}, \quad \tilde{v} = \begin{pmatrix} 0 & \tilde{v}_{LR} \\ \tilde{v}_{RL} & 0 \end{pmatrix}.
\]

The matrix elements are the usual Keldysh-Nambu matrices of non-equilibrium superconductivity. Especially, the Green’s functions \(\tilde{G}_{\infty,L}\) and \(\tilde{G}_{\infty,R}\) are the Green’s functions for the uncoupled left and right electrode. The coupling elements, \(\tilde{v}_{LR,RL}\), between \(L\) and \(R\) are proportional to the unit matrix in the Keldysh space and in Nambu space adopt the form

\[
\tilde{v}_{LR} = \tilde{v}_{RL}^\dagger = \begin{pmatrix} v & 0 \\ 0 & -v^\dagger \end{pmatrix}.
\]

With this, we write the T-matrix equation

\[
\tilde{T} = \tilde{v} + \tilde{v} \circ \tilde{G}_{\infty} \circ \tilde{T} = \tilde{v} + \tilde{v} \circ \tilde{G} \circ \tilde{v},
\]

(3)

which together with the Dyson equation

\[
\tilde{G} = \tilde{G}_{\infty} + \tilde{G}_{\infty} \circ \tilde{T} \circ \tilde{G}_{\infty} = \tilde{G}_{\infty} + \tilde{G}_{\infty} \circ \tilde{v} \circ \tilde{G}
\]

(4)

constitutes a closed set of equations that are to be brought into quasiclassical form. We have given two different ways of summing the series which correspond either to ”dressing” the perturbation (equations (3) and (4)) or to ”dressing” the Green’s function (equations (5) and (6)). The two sets of equations are equivalent and two useful relations

\[
\tilde{v} \circ \tilde{G} = \tilde{T} \circ \tilde{G}_{\infty} \quad \text{and} \quad \tilde{G}_{\infty} \circ \tilde{T} = \tilde{G} \circ \tilde{v}
\]

(7)

follow directly. Here, and above, the \(\circ\)-product is shorthand for integration or summation over common arguments. Starting from equation (4), using equation (6) and the second of the two relations (7), it is straightforward to get the following closed set of equations, closed separately for one and each of the components, \(\tilde{T}_{ij}\), of the T-matrix.

\[
\begin{align*}
\tilde{T}_{LL} &= \tilde{v}_{LR} \circ \tilde{G}_{\infty,R} \circ \tilde{v}_{RL} \\
\tilde{T}_{RR} &= \tilde{v}_{RL} \circ \tilde{G}_{\infty,L} \circ \tilde{v}_{LR} \\
\tilde{T}_{LR} &= \tilde{v}_{LR} + \tilde{v}_{LR} \circ \tilde{G}_{\infty,L} \circ \tilde{v}_{RL} \circ \tilde{G}_{\infty,R} \circ \tilde{T}_{LL} \\
\tilde{T}_{RL} &= \tilde{v}_{RL} + \tilde{v}_{RL} \circ \tilde{G}_{\infty,L} \circ \tilde{v}_{LR} \circ \tilde{G}_{\infty,R} \circ \tilde{T}_{RR}.
\end{align*}
\]

(8)

The equations above depend only on the Green’s functions \(\tilde{G}_{\infty,L}\) and \(\tilde{G}_{\infty,R}\) of the two uncoupled systems. Since the full Green’s function \(\tilde{G}_{ij}\) has been eliminated from the T-matrix equations there are no Green’s functions with spatial arguments in both systems. Together with the short range of \(\tilde{v}_{LR,RL}\) this means that we can directly perform the quasiclassical \(\xi\)-integration on the T-matrix equations and substitute the quasiclassical Green’s functions, \(\tilde{g}_{\infty,i}\), for the full ones, \(\tilde{G}_{\infty,i}\), above.

At the quasiclassical level, the Green’s functions \(\tilde{g}_{\infty,i}(\mathbf{p}_i, t, t')\) at the interface in equations (9) depend on the position on the Fermi surface, \(\mathbf{p}_i\), and of two times \((t, t')\). The coupling elements will be assumed to be time independent but may couple different points \(\mathbf{p}_i\) and \(\mathbf{p}_j\) on the Fermi surfaces of the two conductors. The exact form of the \((\mathbf{p}_i, \mathbf{p}_j)-dependence\) of \(\tilde{v}_{LR}\) is a degree of freedom in the model that allows us to consider different types of transport through the interface. We can now write down the equations for the quasiclassical \(t\)-matrix components.
where we suppressed the explicit dependence of the functions on $\tilde{p}$, and on time variables. The earlier $\times$-product in Eq. (5) is replaced by the $\otimes$-product in the quasiclassical expression. The $\otimes$-product stands for an integration over a common time variable together with a normal matrix multiplication in the combined Keldysh-Nambu and spin space. A left-over from the $\xi$-integration is the intermediate averaging over position on the Fermi surface as indicated by $\langle \cdots \rangle = \int d\tilde{p} \cdots d\hat{p}$. The quasiclassical $\tilde{t}$-matrix entering in to equation (9) is the forward scattering limit

$$
\tilde{t}_{ij} = t_{ij}(\hat{p}, \tilde{p}; t, t')
$$

of Eq. (4) and in general it depends on two times $(t, t')$. Following Ref. 2, let us summarize the procedure for calculating the quasiclassical propagators in the presence of an interface:

1. To find $\hat{g}_{\infty}$, we solve the conventional quasiclassical equations, the Eilenberger equation or the Usadel equation, for the uncoupled electrodes in equilibrium using hard-wall boundary conditions.

2. Use $\hat{g}_{\infty}$ to solve the quasiclassical T-matrix equations (2).

3. Solve the inhomogeneous quasiclassical equation (2) for the physical propagator $\hat{g}$.

4. Use $\hat{g}$ to calculate the “smooth” self-energies $\tilde{\epsilon}_i$ and $\Delta_i$, which enter the quasiclassical equations for $\hat{g}_{\infty}$ and for $\hat{g}$.

The whole scheme amounts to a set of linear differential equations for $\hat{g}_{\infty}$ and $\hat{g}$, coupled in a non-linear way by the T-matrix and the self-energy equations. Substantial simplifications can be achieved in the case of low transmissive tunnel barriers or point contacts. In these cases one can neglect the influence of the neighboring electrodes in the calculation of the self-energies and then the equations for $\hat{g}_{\infty}$ and $\tilde{\epsilon}_i$ and $\Delta_i$ decouple.

### III. JOSEPHSON CURRENTS

As a first application of the boundary condition we calculate supercurrent through a variety of contacts connecting two superconducting reservoirs. The current contribution from a given trajectory, $\hat{p}$, and at a given energy, $\varepsilon$, may be calculated directly by integrating the transport equation (2) along the direction given by $\nu_i(\hat{p})$. This is easily seen as on the considered trajectory away from the contact the physical propagator $\hat{g}_c(\hat{p})$ coincides with the intermediate propagator $\hat{g}_{\infty,i}(\hat{p})$ calculated by the impenetrable surface condition. In absolute vicinity of the contact only the source term in Eq. (4), $[\tilde{t}_{ii}(\hat{p}, \hat{p}), \hat{g}_{\infty,i}(\hat{p})] \delta(R - \hat{R}_c)$, contributes and results in a jump in the Green’s function. The magnitude of this jump is given by integrating Eq. (2) over the interval $[0_-, 0_+[$. Performing the integral results in the scattered propagator

$$
\hat{g}_{i+}(\hat{p}) = \hat{g}_{i-}(\hat{p}) - \frac{i}{v_F \cos \phi_i} \langle \tilde{t}_{ii}(\hat{p}, \hat{p}), \hat{g}_{i-}(\hat{p}) \rangle,
$$

where $\phi_i$ is the angle $\nu_i(\hat{p})$ makes with the contact normal. Note that $\hat{g}_{i-}(\hat{p}) \equiv \hat{g}_{\infty,i}(\hat{p})$ and $\hat{g}_{i-}(\hat{p})$, i.e. the propagator along the trajectory (\hat{p}) coupled to $\hat{p}$ by pure surface scattering we must solve for $\hat{g}_{i+}(\hat{p})$ along the path given by $\nu_i(\hat{p})$. The propagator at the contact, computed in (10), may now be inserted in the current formula

$$
J(T) = eN_F \int \frac{d\varepsilon}{4\pi i} \text{Tr} (\nu_i(\hat{p}) \hat{g}^K(\hat{p}; \varepsilon)) \tilde{p}_i = eN_F \int \frac{d\varepsilon}{4\pi i} \langle j^K_\varepsilon(\hat{p}) \rangle_{\hat{p}_i},
$$

with $N_F$ the density of states at the Fermi level in the normal state. Since the Josephson current is an equilibrium property, the Keldysh Green’s function components of $\hat{g}$ are in this case simply related to the Retarded ($R$) and Advanced (A) ones as $\hat{g}^K = (\hat{g}^R - \hat{g}^A) \tanh(\varepsilon/2T)$, and with $\langle \hat{g}^A(\hat{p}; \varepsilon) \rangle^\dagger = \hat{\tau}_3 \hat{g}^R(\hat{p}; \varepsilon) \hat{\tau}_3$, we get the energy and trajectory resolved current contribution across the contact, evaluated in the left superconductor, as

$$
\langle j^K_\varepsilon(\hat{p}) \rangle = \text{Im} \left[ \text{Tr} \left\{ i \hat{\tau}_3 \left[ i \hat{t}_{LL}^{R}, \hat{g}^R_{\infty,L} \right] \right\} \right] \tanh(\varepsilon/2T).
$$

The lonely first intermediate Green’s function, $\hat{g}_{\infty,i}(\hat{p})$, in Eq. (11) explicitly drop out of the current in the angle average since they obey the impenetrable surface boundary condition.

So far no reference have been made to the modeling of the contact and the $\tilde{t}$-matrix element $\tilde{t}_{LL}^{R}$. The contact model depends on the choice of the momentum dependence of the coupling elements, $v_{RL} = v_{LR} = v(\hat{p}, \hat{p})$. Two
extreme models for the \((\hat{p}, \hat{p}')\)-dependence will be considered: a totally disordered contact, \(v(\hat{p}, \hat{p}') = v\), i.e. the coupling across the contact retains no memory of the momentum direction, and a momentum conserving contact with \(v(\hat{p}, \hat{p}') = v\delta(\hat{p} - \hat{p}')\). The \(\hat{t}\)-matrix equations for the two types of contact, dropping superfluous indexing, read
\[
\hat{t} = \hat{v} \langle \hat{g}_R(\hat{p}) \rangle \hat{v}^\dagger + \hat{v} \langle \hat{g}_R(\hat{p}) \rangle \hat{v}^\dagger \langle \hat{g}_L(\hat{p}) \rangle \hat{v}
\]
for the disordered contact and
\[
\hat{t}(\hat{p}) = \hat{v} \hat{g}_R(\hat{p}) \hat{v}^\dagger + \hat{v} \hat{g}_R(\hat{p}) \hat{v}^\dagger \hat{g}_L(\hat{p}) \hat{v}(\hat{p})
\]
for the momentum conserving contact. For either model, the \(\hat{t}\)-matrix equation above is simple to invert after inserting the retarded Green’s functions \(\hat{g}_R(\hat{p})\) and \(\hat{g}_L(\hat{p})\)
\[
\hat{g}(\hat{p})_{R(L)} = \left( -\hat{f}_{R(L)} e^{\mp i\chi/2} f_{R(L)} e^{\pm i\chi/2} \right),
\]
with the phase difference \(\chi\) across the junction and the upper (lower) signs of the phase refer to the right (left) electrode. In equilibrium the T-matrix equation is simply an algebraic equation in energy space, which can be trivially inverted. The energy and trajectory resolved current is written
\[
j_{c}(\hat{p}) = \text{Im} \left[ \frac{iD}{2 - D - Dg_{RG}} \right] \Delta \left( \frac{\varepsilon - Dg_{RL} \alpha + Dg_{RL} \alpha}{\varepsilon - Dg_{RL} \alpha - Dg_{RL} \alpha} \right) \tanh \left( \frac{\varepsilon}{2T} \right).
\]
Here we have traded in the coupling strength, \(v\), for the transmission coefficient \(D\). The two are simply related as
\[
D = \frac{4v^2}{1 + |v|^2}.
\]
The scalar coupling element, \(v\), is from now on a dimensionless quantity. We have normalized the original coupling element in units of \((1/\pi N_F)\) to get rid of the different prefactors that appear in the angle averages in the T-matrix equation \([3]\).

**A. Josephson current between two s-wave superconductors**

Assuming that the two electrodes both are s-wave superconductors, we have the Green’s functions on either side of the contact
\[
\hat{g}(\hat{p})_{R(L)} = \frac{\pi}{\Omega} \left( \begin{array}{cc} \varepsilon & \Delta e^{\pm i\chi/2} \\ -\Delta e^{\mp i\chi/2} & -\varepsilon \end{array} \right),
\]
where \(\Omega = [\Delta^2 - \varepsilon^2]^{1/2}\). Since the s-wave superconductor is isotropic it does not matter which model for the coupling, \([13]\) or \([14]\), we choose. Additionally, in the absence of surface depairing effects it is sufficient to know the bulk Green’s functions \([13]\) to calculate the current contribution \([12]\). Using Eq. (16) we find the known result that the Josephson current is carried by junction states \([12]\) located at \(\varepsilon_j(\chi, T) = \pm \Delta(T)[1 - D \sin^2(\chi/2)]^{1/2}\). The total current is the sum of all contributions and reads
\[
j(T) = eN_F D \frac{\pi \Delta(T) \sin \chi \tanh \left( \frac{\varepsilon_j(\chi, T)}{2T} \right)}{[1 - D \sin^2(\chi/2)]^{1/2}}.
\]
In equation \([19]\) it should be noted that a second temperature dependence enters via the the temperature dependent gap, \(\Delta(T)\).

**B. Josephson current between two d-wave superconductors**

To emphasize the modeling of the \((\hat{p}, \hat{p}')\)-dependence of the coupling across the junction and the importance of using the correct surface Green’s functions, we now study the current-phase relation of two d-wave superconductors. A realization of a d-wave order parameter is \(\Delta_{\hat{p}} = \Delta \cos 2(\phi_{\hat{p}} - \alpha)\). The magnitude and sign of \(\Delta_{\hat{p}}\) depends on the position on the Fermi circle and this is measured by the angle, \(\phi_{\hat{p}}\), the angle \(\hat{p}\) makes with the crystal \(\hat{a}\)-axis. The angle \(\alpha\) tracks the relative junction-to-crystal \(\hat{a}\)-axis orientation. If \(\alpha = \pm \pi/4\) and specular quasiparticle scattering at the interface is assumed the order parameter seen along a trajectory changes sign at the surface and an Andreev bound state forms at zero energy for every trajectory \(\hat{p}\). \([16]\). We will stick with the junction realization \(\alpha = \pm \pi/4\). To incorporate the effect of these surface states into the current-phase relation one must use the surface Green’s function \([12]\)
\[
\hat{g}(\hat{p})_{R(L)} = \frac{\pi}{\varepsilon} \left( \begin{array}{cc} \Omega_{\hat{p}} & is \Delta_{\hat{p}} e^{\mp i\chi/2} \\ is \Delta_{\hat{p}} e^{\mp i\chi/2} & -\Omega_{\hat{p}} \end{array} \right),
\]
where \(\Omega_{\hat{p}} = [\Delta_{\hat{p}}^2 - \varepsilon^2]^{1/2}\). The factor \(s_R\) discriminates between two types of junction \([12]\) \(s_R = -1 (\alpha_R = \alpha_L)\).
is referred to as a symmetric, and \( s_R = 1 \) \((\alpha_R = -\alpha_L)\) as a mirror junction. The convention for signs of the phase, \( \chi \), are as for the s-wave superconductor. It should be said before proceeding that we are neglecting the pair-breaking effect of the surface, and we assume constant order parameters up to the interface. This is for the sake of simple illustration and for the comparison of analytical results with other boundary conditions.

Turning to the \( t \)-matrix equations and starting with the diffusive model of the point contact, one immediately find that the Josephson current is zero. This follows from the vanishing average, \( \langle \Delta_\rho \rangle_\rho = 0 \). Due to this property the anomalous propagators vanish and therefore the Josephson current as well (see Eq. (15)). In the opposite limit, using the momentum-conserving model (14), the Josephson current is not zero. After inverting the \( t \)-matrix equation and evaluating the commutator in (12), we find the energy resolved current at \( \tilde{p}_k \)

\[
j_\varepsilon(\tilde{p}_k) = \pm \Im \left[ D \frac{\sin \chi}{e^{2} - e^{2} \sin \frac{\chi}{2}} \right] \tanh \left( \frac{\varepsilon}{2T} \right). \tag{21}\]

The sign of \( j_\varepsilon(\tilde{p}_k) \) is (+) for a mirror and (-) for a symmetric junction. As in the case of the \( s \)-wave junction we have junction states carrying the Josephson current. The position of these states depend on the type of junction in the following way

\[
\varepsilon_j(\chi; \tilde{p}_k) = \pm \sqrt{D} |\Delta_\rho| \times \begin{cases} \sin \frac{\chi}{2}, & \text{mirror} \\ \cos \frac{\chi}{2}, & \text{symmetric}. \end{cases} \tag{22}\]

These junction states were first found by Riedel and Bagwell (68) using a scattering approach and, independently, by Barash (11), using what is known as the Zaitsev boundary condition (12). Performing the integral over the energy we write the trajectory resolved current-phase relations

\[
j(\tilde{p}_k) = \pm 2\pi \sqrt{D} |\Delta_\rho| \times \begin{cases} \cos \frac{\chi}{2} \tanh \left( \frac{\sqrt{D} |\Delta_\rho| \sin \frac{\chi}{2}}{2T} \right) \\ \sin \frac{\chi}{2} \tanh \left( \frac{\sqrt{D} |\Delta_\rho| \cos \frac{\chi}{2}}{2T} \right) \end{cases} \tag{23}\]

for the two junction types, the upper being the mirror and the lower the symmetric one. The total current is the trajectory average of \( j(\tilde{p}_k) \) multiplied by \( eN_F \).

The main purpose of this section was to show that the quasiclassical version of the point contact coupling of two electrodes is simple to use and can recover results known in literature. In case of unconventional superconducting electrodes results depend in a crucial way on how the contact is modeled. This gives the Hamiltonian boundary condition an advantage in flexibility to the conventional Zaitsev boundary condition which coincides with the momentum conserving contact (13) introduced above.

C. Josephson current through a spin active interface

As another illustration of the flexibility of this method we extend the discussion to currents through spin active interfaces, i.e. interfaces which flip the spin of the incident electrons either by spin-dependent scattering within the interface, or by a difference in spin-orbit coupling on either side of the interface. The general boundary conditions that connect the quasiclassical propagators for superconducting metals across magnetically active interfaces were introduced by Mills, Rainer and Sauls. Recently one of the authors\( ^\text{,} \) derived the explicit solution of these boundary conditions for equilibrium Green functions. In order to compare with this solution, as in Ref. [7], we shall analyze in this section the Josephson current through a contact of two isotropic s-wave superconductors connected through a small magnetically active junction.

In order to accommodate the spin dependence we enlarge our space in such a way that every quantity is now a \( 2 \times 2 \) matrix in spin space. In particular, the coupling elements are spin dependent and adopt the following general form

\[
\hat{v}_{LR} = \hat{v}^q_{RL} = \begin{pmatrix} v & 0 \\ 0 & v^q \end{pmatrix} \quad \text{where} \quad v = \begin{pmatrix} v_{\uparrow, \uparrow} & v_{\uparrow, \downarrow} \\ v_{\downarrow, \uparrow} & v_{\downarrow, \downarrow} \end{pmatrix}. \tag{24}\]

Let us stick to the case of S/F/S junction analyzed in Ref. [7]. In this case \( F \) stands for a small ferromagnetic particle or grain. This ferromagnetic material is treated as a partially transparent barrier which transmits the two spin projections differently. For spin-active interfaces the different components of the S-matrix, \( S_{ij} \), are \( 2 \times 2 \) spin matrices. To proceed further a specific S-matrix was chosen in Ref. [7] to model the magnetic barrier

\[
\hat{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} r & t \\ t & -r \end{pmatrix} \exp(i\sigma_3), \tag{25}\]

where \( \sigma_3 \) notes the Pauli-matrices spanning spin space and parameters \((t, r)\) are the usual transmission and reflection coefficients. The S-matrix (25) is one of the simplest choices that allows a variable degree of spin mixing at the interface and the spin mixing is parameterized by the spin-mixing angle \( \Theta \). By this construction \( \hat{S} \) only violates spin conservation, i.e. it does not commute with the quasiparticle spin operator \( \sigma \). The angle \( \Theta \) will be considered as a phenomenological parameter independent of the trajectory direction (for more details see Tokuyasu et al Ref. [71]). Within the approach presented of this paper, one can easily model the previous S-matrix with a spin dependent coupling

\[
\hat{v}_{LR} = \hat{v}^q_{RL} = v \begin{pmatrix} \exp(i\sigma_3) & 0 \\ 0 & \exp(-i\sigma_3) \end{pmatrix}. \tag{26}\]
Again the quasiclassical surface Green functions are the inputs in this approach, i.e. the Green’s functions at the interface calculated with impenetrable wall boundary conditions. The spin-active boundary condition must be used at the contact also for the reflecting surface. In this simple case of a magnetic barrier the resulting spin-dependent propagators can be written in a $4 \times 4$ block-diagonal form

$$
\hat{g}_{\text{block}}(\hat{p}_b; \Theta) = \left( \begin{array}{cc}
\hat{g}(\hat{p}_b; \Theta) & 0 \\
0 & \hat{g}(\hat{p}_b; -\Theta)
\end{array} \right) = \left( \begin{array}{cccc}
g_{\uparrow\uparrow}(\Theta) & f_{\uparrow\downarrow}(\Theta) & 0 & 0 \\
f_{\downarrow\uparrow}(\Theta) & g_{\downarrow\downarrow}(\Theta) & 0 & -f_{\downarrow\uparrow}(\Theta) \\
0 & 0 & g_{\downarrow\uparrow}(\Theta) & -f_{\downarrow\uparrow}(\Theta) \\
0 & 0 & -f_{\downarrow\uparrow}(\Theta) & g_{\downarrow\downarrow}(\Theta)
\end{array} \right),
$$

where the electron and anomalous parts of $\hat{g}(\hat{p}_b; \Theta)$ in the upper left corner of $\hat{g}_{\text{block}}(\hat{p}_b; \Theta)$ can be written as

$$
g_{\uparrow\uparrow}(\Theta) = -\pi \frac{\varepsilon R \cos(\Theta/2) - \Omega \sin(\Theta/2)}{\varepsilon R \sin(\Theta/2) + \Omega \cos(\Theta/2)},$$

$$f_{\uparrow\downarrow}(\Theta) = \pi \frac{\Delta e^{-i(\Theta + \chi)/2}}{\varepsilon R \sin(\Theta/2) + \Omega \cos(\Theta/2)},$$

$$f_{\downarrow\uparrow}(\Theta) = -\pi \frac{\Delta e^{i(\Theta + \chi)/2}}{\varepsilon R \sin(\Theta/2) + \Omega \cos(\Theta/2)},$$

for trajectories with $(\hat{p}_b \cdot \hat{n} > 0)$. For trajectories with reversed momentum, i.e. $(\hat{p}_b \cdot \hat{n} < 0)$, the phase factor $\exp[\mp i(\Theta + \chi)/2]$ for functions $f_{\uparrow\downarrow}(\Theta)$ and $f_{\downarrow\uparrow}(\Theta)$ goes to $\exp[\pm i(\Theta \pm \chi)/2]$. Above, as in the earlier examples, the phase difference, $\chi$, between the two reservoirs is included and the upper (lower) signs refer to the right (left) reservoir. The components of the propagator in the lower right corner of $\hat{g}_{\text{block}}$ are simply related to those in the upper left corner by the replacement $\Theta \rightarrow -\Theta$.

The angle $\Theta$ induces a mixing of the two otherwise separated spin bands. It is easy to see that the resulting density of states at the interface has Andreev bound states inside the gap. These states are located at $\varepsilon_{\Theta \uparrow(\downarrow)} = \pm \Delta \cos(\Theta/2)$, with $+(-)$ for the spin-up (down) branch. The existence of the sub-gap states alters the Josephson current-phase relation radically. The contribution to the current from the energy $\varepsilon$, the trajectory $\hat{p}_b$, and spin band $\uparrow (\downarrow)$ may be calculated directly from expression (10). Keeping in mind that the phase that enters in Eq. (10) is the phase difference over the contact we write

$$j_{\varepsilon, \uparrow}(\hat{p}_b; \Theta, \chi) = \text{Im} \left[ \Delta \Delta^2 \left( \frac{\sin \chi}{[\Omega \cos(\Theta/2) + \varepsilon \sin(\Theta/2)]^2 - \Delta \Delta^2 \sin^2(\chi/2)} \right) \right] \tan h \left( \frac{\varepsilon}{2T} \right),$$

for the current carried by the spin-up band. The current carried by the spin-down band is given simply as $j_{\varepsilon, \downarrow}(\hat{p}_b; \Theta, \chi) = j_{\varepsilon, \uparrow}(\hat{p}_b; -\Theta, -\chi)$. At a finite superconducting phase difference, the original two interface Andreev bound states are split up into four current carrying states located inside the gap at positions

$$\varepsilon_J = \pm \Delta \left[ \cos^2(\Theta/2) - D \cos(\Theta) \sin^2(\chi/2) \pm \sqrt{T} \sin(\Theta) \sin(\chi/2) \sqrt{1 - D \sin^2(\chi/2)} \right]^{1/2}.$$

These states give the total contribution to the current and their positions change from the tunnel regime, $\varepsilon_J = \pm \Delta \cos(\Theta/2)$, to $\varepsilon_J = \pm \Delta \cos((\chi \pm \Theta)/2)$ at perfect transmission.
The spin-mixing angle $\Theta$ is varied from top to bottom from 0 to $\pi$ in steps of $\pi$. The dashed lines indicate the value of $\Theta$ for which the contacts become $\pi$ junctions. The supercurrent is normalized in units of the critical current density, $j_c$, for the corresponding transmission and zero spin-mixing angle.

In figure 2 we show the current-phase relation for a set of transparencies $D = 0.1, 0.4, 0.8$, and 1.0. In each panel the spin-mixing angle $\Theta$ is varied from 0 to $\pi$ in steps of $\pi$. As seen, for each value of $D$ there is a range $\Theta > \Theta_c$ where the junctions are $\pi$-junctions. For small $D$, the critical spin-mixing angle $\Theta_c$ is close to $\pi$ and with increasing $D$, $\Theta_c$ increases towards $\pi$. The magnitude of the critical current is for all but the perfect transmission junction very asymmetric for $0$ and $10$.

To conclude this section, let us stress that these results reproduce the result obtained in Ref. 1 showing again the versatility of the boundary conditions introduced in this work.

![Graph showing current-phase relation for S/F/S contact](image)

FIG. 1. Zero-temperature supercurrent-phase relation for the S/F/S contact considered in this section. The four different panels correspond to $D = 0.1, 0.4, 0.8$, and 1.0. The spin-mixing angle $\Theta$ is varied from top to bottom from 0 to $\pi$ in steps of $\pi$. The dashed lines indicate the value of $\Theta$ for which the contacts become $\pi$ junctions. The supercurrent is normalized in units of the critical current density, $j_c$, for the corresponding transmission and zero spin-mixing angle.

To conclude this section, let us stress that these results reproduce the result obtained in Ref. 1 showing again the versatility of the boundary conditions introduced in this work.

![Graph showing current-phase relation for S/F/S contact](image)

FIG. 2. Energy resolved spectral current for the S/F/S contact with $D = 0.4$ and $\Theta = 0.7\pi$ (see Fig. 1 right upper panel). This figure shows the total spectral current, sum of both spin contributions, as a function of energy according to Eq. (2), without the thermal factor. The different curves show the evolution of the four current-carrying Andreev bound states inside the gap with the superconducting phase difference. The curves are shifted vertically for clarity.

**IV. SOLVING THE T-MATRIX EQUATION AT AN APPLIED VOLTAGE**

In this section we shall describe how the T-matrix equation (3) can be solved in the case of a voltage-biased superconducting contact. As a constant bias $V$ is applied across a junction between two superconductors, the phase difference oscillates with time according to the Josephson relation: $\phi(t) = \phi_0 + \omega_0 t$, where $\omega_0 = 2eV/h$ is the Josephson frequency. This makes that every Green’s function and T-matrix component depend on two time arguments. We show in this section how the time convolutions in the T-matrix equation can be handled.

As we shall show in next section the current can be expressed, for instance, only in terms of the advanced and retarded components of $\hat{t}_{LR}$. Thus, we concentrate ourselves in these components whose equations can be written as (see Eq. 9)

$$
\hat{t}_{LR}(t,t') = \hat{v}_{LR} + \int dt_1 \int dt_2 \hat{v}_{LR} \times \hat{g}_{LR}^R(t_1,t_2) \hat{g}_{LR}^A(t_2,t_2) \hat{t}_{LR}^R(t_2,t').
$$

(31)

Here, we have written explicitly the time convolutions for the sake of clarity and we have omitted the $\hat{p}_R$ integrations, since they do not affect the time convolutions. In this expression every quantity is a 4 $\times$ 4 matrix in Nambu and spin space, and from now to the end of this section we get rid of the superindexes $R, A$, since the equations for these two components are formally identical. We also drop the $\infty$ subindex, since all propagators in (31) are propagators of the separated electrodes. The electrode Green’s functions entering Eq. (31) take the form: $\hat{g}_j(t,t') = \hat{U}_j^{-1}(t)\hat{g}_j(t-t')\hat{U}_j(t')$, where $j = R, L$ and $\hat{U}_j(t) = \exp[i\phi_j(t)\hat{\tau}_3/2]$, $\phi_j(t)$ being the phase of the $j$th superconductor. In this expression, $\hat{g}_j(t) = \int \hat{g}_j(e)e^{\exp(-i\epsilon t)}de/2\pi$.

We use the transformation generated by $\hat{U}_j(t)$ to transfer the time dependence from the Green’s functions to the hopping elements

$$
\hat{t}_{LR}(t,t') = \hat{v}_{LR}(t)\delta(t-t') + \int dt_1 \int dt_2 \hat{v}_{LR}(t) \hat{g}_{LR}(t_1,t_1) \hat{g}_{LR}(t_1,t_2) \hat{t}_{LR}(t_2,t'),
$$

(32)

where $\hat{v}_{LR}(t) = \hat{U}_L(t)\hat{v}_{LR}\hat{U}_R^+(t) = \hat{v}_{RL}(t) = v \exp[i\phi(t)\hat{\tau}_3/2]$. One can easily show that all physical properties of the system are invariant under this gauge.
transformation. Thus, we shall usually consider the T-matrix equation in this gauge, i.e. in which the hopping elements are time-dependent and the electrode Green’s functions only depend on the time difference.

In order to solve Eq. (32) it is more convenient to work in energy space where it becomes an algebraic equation. Thus, we Fourier transform the T-matrix with respect to the temporal arguments

\[ i_{LR}(t, t') = \frac{1}{2\pi} \int dt \int dt' e^{-ie(t-t')} i_{LR}(\epsilon, \epsilon'). \]  

(33)

It is easy to convince oneself that, due to the special time dependence of the coupling elements, the T-matrix admits a Fourier expansion of the form

\[ i_{LR}(t, t') = \sum_n e^{im\phi(t')/2} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} i_{LR}(\epsilon, \epsilon + neV). \]  

(34)

In other words, Fourier transforming Eq. (32) one can show that \( i_{LR}(\epsilon, \epsilon') \) satisfies the following relation

\[ i_{LR}(\epsilon, \epsilon') = \sum_n \hat{i}_{LR}(\epsilon, \epsilon + neV) \delta(\epsilon - \epsilon' + neV). \]  

(35)

The problem of the calculation of the current can be reduced to the evaluation of the Fourier components \( \hat{i}_{nm}(\epsilon) \equiv i_{LR}(\epsilon + neV, \epsilon + neV) \). As it can be seen Fourier transforming Eq. (32), these components fulfill the following (infinite) set of algebraic linear equations

\[ \hat{i}_{nm} = \hat{v}_{m,n,\pm 1} + \hat{\xi}_n \hat{i}_{nm} + \hat{\nu}_{n,n-2} \hat{i}_{n-2,m} + \hat{\nu}_{n,n+2} \hat{i}_{n+2,m}, \]  

(36)

where \( \hat{v}_{m-1,m} = (1 + \hat{\tau}_3)/2, \hat{v}_{m+1,m} = v(1 - \hat{\tau}_3)/2, \) and the matrix coefficients \( \hat{\xi}_n \) and \( \hat{\nu}_{n,m} \) can be expressed in terms of the Green’s functions of the uncoupled electrodes, as

\[ \hat{\xi}_n = \begin{pmatrix} v g_{R,n+1} & v g_{R,n} & v g_{R,n+1} & v f_{L,n} \\ v^\dagger g_{R,n-1} & v f_{L,n} & v^\dagger g_{R,n-1} & v g_{L,n} \end{pmatrix}, \]

\[ \hat{\nu}_{n,n+2} = -v f_{R,n+1} v\begin{pmatrix} f_{L,n+2} & g_{L,n+2} \\ 0 & 0 \end{pmatrix}, \]

\[ \hat{\nu}_{n,n-2} = -v^\dagger f_{R,n-1} v\begin{pmatrix} 0 & 0 \\ g_{L,n-2} & f_{L,n-2} \end{pmatrix}, \]  

(37)

In these equations the short-hand notation \( v_{i,n} = g_i(\epsilon + neV) \) for the \( 2 \times 2 \) spin-dependent propagators has been used. Notice that the set of linear equations (36) are analogous to those describing a tight-binding chain with nearest-neighbor hopping parameters \( \hat{V}_{n,n+2} \) and \( \hat{V}_{n,n-2} \). A solution can then be obtained by standard recursive techniques (see Ref. [17] for details).

Finally, the \( \hat{p}_p \)-dependence of the Green’s function in Eq. (33) depends on our choice of the contact model. Thus for instance, for the disordered case the Green’s functions appearing in Eq. (36) are the angle averaged ones, while for the case of a momentum conserving contact we must include the trajectory dependent Green’s functions (see Eqs. 13-14).

### A. Current at finite voltage

As commented in a previous section, the current contribution from a given trajectory may be calculated directly by integrating the transport equation (3) along the trajectory over the discontinuity given by the source term. Thus, the time-dependent current reads as

\[ j(t) = eN_F \langle j(\hat{p}_p, t) \rangle_{\hat{p}_p}, \]  

(38)

where the contribution of given trajectory with momentum \( \hat{p}_p \) can be written as

\[ j(\hat{p}_p, t) = \text{Tr} \left\{ \hat{\tau}_3 \left[ \hat{f}_{LL} \otimes \hat{g}_{\infty,L} \right]_{\hat{p}_p} \right\}. \]  

(39)

This expression can be greatly simplified as follows. First, the Keldysh components of the T-matrix can be eliminated in favor of the advanced and retarded components using the relation \( \hat{t}^R = \hat{t}^R \otimes \hat{g}_{\infty,L}^R \otimes \hat{t}^A \). On the other hand, the four elements of the enlarged space are not independent. For instance, it is easy to show the following relations: \( \hat{t}_{LR} = (1 + \hat{t}_{LL} \otimes \hat{g}_{\infty,L}) \otimes \hat{v}_{LR} \) and \( \hat{t}_{RL} = \hat{v}_{RL} \otimes (1 + \hat{g}_{\infty,L} \otimes \hat{t}_{LL}) \). Using these relations it is rather straightforward to show that the current can be written as

\[ j(\hat{p}_p, t) = \text{Tr} \left\{ \hat{\tau}_3 \left[ \hat{t}_{LR} \otimes \hat{g}_{\infty,L} \right]_{\hat{p}_p} \right\}. \]  

(40)

where we have dropped the symbol \( \infty \), since from now on in this section the only Green functions which will appear are the surface Green functions.

Taking into account the Fourier expansion of the T-matrix (see Eq. 34), the current adopts the form

\[ j(\hat{p}_p, t) = \sum_{m=-\infty}^{\infty} j_m(\hat{p}_p)e^{im\phi(t)}, \]  

(41)
where the different Fourier current components can be expressed in terms of the Fourier components of the harmonics \( \tilde{t}_{nm}(\epsilon) \equiv t(\epsilon + neV, \epsilon + meV) \) as follows

\[
\tilde{j}_m(\hat{p}_i) = \int \, \sum_n \, \text{Tr} \left[ \tilde{\gamma}_3 \left( \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} - \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} \right) + \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} - \tilde{g}^R_{RL,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{R,nm} \right]. \quad (42)
\]

This is the general expression of the \( \epsilon \) ac Josephson effect in a superconducting contact. This indicates that in the case of constant bias voltage there appear alternating components which oscillate not only with the Josephson frequency \( \omega_{\theta} \), as in the case of a tunnel junction, but also with all its harmonics. When the voltage tends to zero all the harmonics sum up to yield the supercurrent.

We can further simplify the expression of the current harmonics, \( \tilde{j}_m \). Using the equations of the T-matrix components it can be shown that the general relation \( \tilde{t}^{A,R}_{RL,nm}(\epsilon) = \tilde{t}^{R,A}_{LR,znm}(\epsilon) \) holds. Thus, we can simply express the current in terms of harmonics \( \tilde{t}^{R,A}_{LR,znm} \equiv \tilde{i}^{R,A}_{znm} \) as follows

\[
\tilde{j}_m(\hat{p}_i) = \int \, \sum_n \, \text{Tr} \left[ \tilde{\gamma}_3 \left( \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} - \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} \right) + \tilde{g}^R_{LR,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{L,nm} - \tilde{g}^R_{RL,0n} \tilde{g}^K_{RL,nm} \tilde{g}^A_{R,nm} \right] . \quad (43)
\]

In order to illustrate this current formula we now investigate the dc component for a spin singlet superconductor with no spin active interface in two limiting cases: tunnel regime and perfect transmission. For the description of a poorly transmissive barrier one can solve perturbatively the equation for \( \tilde{t}^{R,A}_{LR,nm} \). Up to first order in the coupling element: \( \tilde{t}^{R,A}_{LR,nm} \approx (v/2) (1 + \tilde{\gamma}_3) \delta_{m,n+1} + (v/2) (1 - \tilde{\gamma}_3) \delta_{m,n-1} \) and higher harmonics can be neglected. Substituting this perturbative solution into the expression of the dc current, \( 0 \), one finds the traditional result

\[
\tilde{j}_0(\hat{p}_i) = D \int_{-\infty}^{\infty} \, \rho_L(\epsilon - eV) \rho_R(\epsilon) \times \left[ f_{FD}(\epsilon - eV) - f_{FD}(\epsilon) \right], \quad (44)
\]

where \( f_{FD} \) is the Fermi distribution function and \( \rho_{L,R} \) are the local densities of states at the corresponding side of the interface: \( \rho_i(\epsilon) = \frac{1}{\pi} \text{Im} \{ g_i^0(\epsilon) \} \).

In the case of a perfect transmissive contact \( (D = 1) \), the absence of backscattering greatly simplify the calculation of the different harmonics of the T-matrix components (see Ref. [13]). In the case of a symmetric contact the dc current for perfect transmission can be written as

\[
\tilde{j}_0(\hat{p}_i) = D \int_{-\infty}^{\infty} \, \rho_L(\epsilon - eV) \rho_R(\epsilon) \times \left[ f_{FD}(\epsilon - eV) - f_{FD}(\epsilon) \right], \quad (46)
\]

where \( f_{FD} \) is an energy and voltage dependent transmission coefficient given by

\[
\tilde{j}_0(V) = \int_{-\infty}^{\infty} \, \rho_L(\epsilon - eV) \rho_R(\epsilon), \quad (46)
\]

where \( \rho_i(\epsilon) \) is the local density of states at the interface.

In Fig. 3 we show the current-voltage characteristics and differential conductance for different values of the probability of a multiple Andreev reflection is basically the product of the different Andreev reflections that take place at each side of the interface.

In order to illustrate our approach in the case of a voltage biased contact, we consider here a junction between two d-wave superconductors. Let us analyze in particular the symmetric junction mentioned in section III B, whose description is based on the Green’s functions of Eq. (20). Again, we neglect pair breaking effect and assume constant order parameter up to the interface. The proper self-consistent treatment of these junctions will be the subject of a forthcoming publication. In this contact geometry the zero-energy bound states in each side of the interface strongly affect the transport through this system. Of course, the results for the current depend on the contact model used. Let us first consider the case of a disordered contact. In this case, the propagators which enter in the current formula are the angle averaged ones. This implies that the anomalous propagators vanish, which means that the current is only due to single-quasiparticle processes. Thus, the current formula reduces to

\[
\tilde{j}_0(V) = 4 \pi^2 |v|^2 \langle \rho_L(\epsilon - eV) \rangle \hat{p}_i \langle \rho_R(\epsilon) \rangle \hat{p}_i \langle \rho_{LR}(\epsilon) \rangle, \quad (47)
\]

where \( \langle \rho_i(\epsilon) \rangle \langle \hat{p}_i \rangle \langle \rho_{LR}(\epsilon) \rangle \) is the local density of states at the interface.
the normal transmission coefficient $D$ for this disordered model. The only abrupt feature exhibited by the current inside the gap occurs in the tunnel regime. The resonant tunneling through the zero-energy bound states leads to a zero-bias anomaly and the subsequent negative differential conductance. As it is well known, the position and the height of the peak in the conductance depends on intrinsic width of zero-energy states;\textsuperscript{19,73–75} It is known theoretically that the elastic scattering with bulk impurities\textsuperscript{21} or a diffusive surface layer\textsuperscript{22} provide an intrinsic broadening, which for the case of Born scatterers is $\propto \sqrt{\Gamma \Delta}$, where $\Gamma = 1/2\tau$ is the effective pair-breaking parameter locally at the surface. In Fig. 3 we have introduced a small phenomenological broadening of $10^{-2}\Delta$ to mimic this intrinsic effect.

With this simple calculation we can already point out the following. Many calculations of the I-V curves in junctions of unconventional superconductors are limited to the tunneling regime, and make use of the traditional tunnel formula (see Eq. (44)). However, if bound states or divergencies are present in the density of states, this perturbative expression does not even give the correct result for a low transparent contact, and one needs to include high order processes as in Eq. (46). Indeed, this is a well known problem in the context of s-wave superconductors (for a discussion of this problem see for instance Ref. \textsuperscript{47}). In order to illustrate this fact, in Fig. 4 we compare the result of Eq. (46) and the tunneling result for a small transparency $D = 0.01$. One can see in Fig. 4(a) that there is a clear difference between these two results. In particular, in the low voltage regime the complete expression renormalizes the unphysical divergencies obtained with the tunnel formula. As the broadening of the level is increased the difference between these two results diminishes progressively (see Fig. 4(b)). Indeed, recent experiments in $ab$-plane tunneling into YBCO\textsuperscript{11} suggest that the broadening of the zero bias anomaly can be as large as 25% of the gap $\Delta$ (see Ref. \textsuperscript{23}). In this case, there is no significant difference in the resulting current between both expressions.
The angular dependence of the normal transmission coefficients. Thus, the final result depends on the model for the interface. The different curves correspond to different values of normal transmission coefficient. In order to see these curves in the same scale the current is normalized by the normal state conductance $G_N$ which includes the transmission coefficient. Moreover, the current and the voltage are normalized in units of the momentum-dependent gap. The vertical lines indicate the positions $eV_n = \Delta_p/n$, $n = 2, ..., 10$, as a guide for the eye.

Let us now consider the case of a momentum conserving contact, which is the usual assumption in the Zaitsev boundary conditions. To gain some insight into the final result, in Fig. 5 we show the contribution of an individual trajectory $\hat{\mathbf{p}}$. The current and voltage are normalized in units of the gap seen by this trajectory. As can be observed, the current exhibits a pronounced subgap structure at voltages $eV = \Delta_p/n$, where $n$ is an integer number, together with the appearance of negative differential conductance (this can be seen better in the lower panel of this figure). These features are a simple consequence of the resonant tunneling across the zero-energy bound states. Indeed, this type of I-V has been previously obtained in the context of a junction between two conventional superconductors coupled by means of a resonant transmission (see Ref. [76,77]). Notice also the presence of a zero bias peak, specially clear for low transparencies, and which is a consequence of the small broadening introduced in the calculation. The total current is obtained by averaging over the different trajectories. Thus, the final result depends on the model for the angular dependence of the normal transmission coefficient. With any reasonable reasonable model most of the features of the trajectory resolved current disappear. In particular, the subharmonic gap structure is washed out, and it only remains a peak in the conductance at $eV \approx \Delta$ (see for instance Ref. [73]).

V. CURRENT FLUCTUATIONS

During the last years it has become progressively clearer that a deep understanding of the electronic transport in mesoscopic systems requires the analysis of quantities which goes beyond the straightforward measurement of the current-voltage characteristics. In this sense the noise or time-dependent current fluctuations has emerged as a very useful tool which provides new information on the time correlations of the current, information about channel distributions, statistics and charge of the carriers. In the case of superconducting contacts, most of the activity has been restricted to the case of s-wave superconductors. In the case of unconventional superconductors there are only a few theoretical works in the context of hybrid structures like normal metal/d-wave superconductors. We believe that in the future the measurement of current fluctuations will be an important tool for a deeper understanding of the symmetry of the order parameter and origin of the superconductivity in general in the case of HTS materials. For this reason in this section we describe the calculation of the noise spectrum within our approach, valid for any type of contact between unconventional superconductors.

Let us remember that the noise is characterized by its spectral density or power spectrum $S(\omega)$, which is simply the Fourier transform at frequency $\omega$ of the current-current correlation function

$$S(\omega) = \int dt' e^{i\omega(t'-t)} \langle \delta j(t) \delta j(t') \rangle$$

$$\equiv \int dt' e^{i\omega(t'-t)} \langle \hat{\mathcal{K}}(t, t') \rangle,$$

where $\delta j(t) = j(t) - <j(t)>$ are the fluctuations in the current.

In order to obtain the expression of the current-current correlator, first we need an expression for the current operator. Within our model this operator evaluated at the interface can written as follows

$$j(t) = i e \sum_{\sigma} \left\{ v_{LR,\sigma} \hat{c}^\dagger_{L,\sigma}(t) \hat{c}_{R,\sigma}(t) - v_{RL,\sigma} \hat{c}^\dagger_{R,\sigma}(t) \hat{c}_{L,\sigma}(t) \right\}.$$

This expression is a simple consequence of the continuity equation for the current.

In order to calculate the noise we need in principle to evaluate correlators of four field operators. However, we are working in the framework of a mean field theory, which means that we can decouple these correlators in terms of one-particle Green's functions using the Wick theorem. With this in mind, it is straightforward to show...
that the kernel $K(t, t')$ can be expressed in terms of the interface Keldysh Green’s functions as follows:

$$K(t, t') = e^2 \{ \text{Tr} \left[ \hat{v}_{R \ell} \hat{G}_{LL}^<(t, t') \hat{v}_{L \ell} \hat{G}_{RR}^>(t', t) \right] + \hat{v}_{L \ell} \hat{G}_{RR}^<(t, t') \hat{v}_{R \ell} \hat{G}_{LL}^>(t', t) - \hat{v}_{L \ell} \hat{G}_{RL}^<(t, t') \hat{v}_{R \ell} \hat{G}_{RL}^>(t', t) \right] + (t \to t') \} ,$$

(50)

where the functions $\hat{G}^<$ and $\hat{G}^>$ are related to the usual advanced, retarded and Keldysh functions in the following way:

$$\hat{G}^< = \left( \hat{G}^K - \hat{G}^R + \hat{G}^A \right) / 2,$$

$$\hat{G}^> = \left( \hat{G}^K + \hat{G}^R - \hat{G}^A \right) / 2.$$

(51)

In order to compactify the notation, we introduce the trace $\tilde{\text{Tr}}$ and the matrix $\tilde{\tau}_3$ which act in the “reservoir” space. Then, the noise kernel reads

$$K(t, t') = -e^2 \tilde{\text{Tr}} \left[ \hat{v} \hat{G}^<(t, t') \tilde{\tau}_3 \hat{v} \hat{G}^>(t', t) + \hat{v} \hat{G}^>(t', t') \tilde{\tau}_3 \hat{v} \hat{G}^<(t', t) \right].$$

(52)

Now, in order to eliminate the Green’s functions in favor of the T-matrix elements, we use the relation

$$\hat{G}^< = \left( 1 + \hat{G}^R \circ \hat{v} \right) \circ \hat{G}^< \circ \left( 1 + \hat{v} \circ \hat{G}^A \right),$$

(53)

where $\hat{G}^<(\epsilon) = \left[ \hat{G}^A(\epsilon) - \hat{G}^R(\epsilon) \right] f_{FD}(\epsilon)$ and $\hat{G}^>(\epsilon) = \left[ \hat{G}^A(\epsilon) - \hat{G}^R(\epsilon) \right] (f_{FD}(\epsilon) - 1)$. Now, making use of Eqs. (3-7) it is easy to see that the following relation holds

$$\hat{v} \circ \hat{G}^< = \hat{T}^R \circ \hat{G}^< \circ \left( 1 + \hat{T}^A \circ \hat{G}^A \right).$$

(54)

This expression allows us to write the noise kernel as follows

$$K(t, t') = -e^2 \tilde{\text{Tr}} \left\{ \left[ \hat{T}^R \circ \hat{G}^< \circ \left( 1 + \hat{T}^A \circ \hat{G}^A \right) \right] (t, t') \tilde{\tau}_3 \left[ \hat{T}^R \circ \hat{G}^> \circ \left( 1 + \hat{T}^A \circ \hat{G}^A \right) \right] (t', t) + (t \to t') \right\} .$$

(55)

As explained in section II, once we have eliminated the full Green’s functions in the noise kernel, we can perform the quasiclassical $\xi$-integration and substitute the quasiclassical Green’s functions, $\hat{g}_\infty$, for the full ones, $\hat{G}_\infty$. Thus, the noise kernel can be expressed finally as

$$K(t, t') = -e^2 \tilde{\text{Tr}} \left\{ \left[ \hat{T}^R \circ \hat{g}_\infty^< \circ \left( 1 + \hat{T}^A \circ \hat{g}_\infty^A \right) \right] (t, t') \tilde{\tau}_3 \left[ \hat{T}^R \circ \hat{g}_\infty^> \circ \left( 1 + \hat{T}^A \circ \hat{g}_\infty^A \right) \right] (t', t) + (t \to t') \right\} .$$

(56)

Let us stick now to the case of a constant bias voltage applied across the interface. In this case, for both contact models considered in section III, we can resolve the current fluctuations in trajectories as follows

$$S(\omega, t) = e^2 N_F \langle S(\hat{p}_\ell; \omega, t) \rangle \hat{p}_\ell,$$

(57)

where the time-dependent contribution of given trajectory with momentum $\hat{p}_\ell$ can be written as

$$S(\hat{p}_\ell; \omega, t) = \sum_{m=-\infty}^{\infty} S_m(\hat{p}_\ell; \omega) e^{im\phi(t)} ,$$

(58)

where the different ac-components of the noise can be expressed in terms of the Fourier component of the T-matrix elements in the following way

$$S_m(\hat{p}_\ell; \omega) = -\int dt \sum_{\kappa} \tilde{\text{Tr}} \left\{ \left[ \hat{T}^R \hat{g}_\infty^< \left( 1 + \hat{T}^A \hat{g}_\infty^A \right) \right]_{0m}(\epsilon) \tilde{\tau}_3 \left[ \hat{T}^R \hat{g}_\infty^> \left( 1 + \hat{T}^A \hat{g}_\infty^A \right) \right]_{nm}(\epsilon + \omega) + (\epsilon \to \epsilon + \omega) \right\} .$$

(59)

Notice that in the case of a junction between two superconductors, the noise, as the current, oscillates on time with all the harmonics of the Josephson frequency. Notice also that we have reduced the calculation of this quantity to the determination of the different Fourier components of the T-matrix elements, which has been detailed in section IV.

In order to illustrate the calculation of the current fluctuations, we consider the contact between d-wave superconductors analyzed in the previous section. In particular, we present results for the zero-frequency noise at zero temperature, $S$, i.e. the zero-frequency shot noise. At this point, it is worth remarking that by zero-frequency noise we mean noise at a frequency lower than any relevant energy scale in our problem, gap for instance, and high enough to neglect $1/f$ noise. Again, the final re-
result depends on the type of contact model under investigation. Let us start discussing the shot noise for the disordered contact. In this case, due to the vanishing of the anomalous Green’s functions, the whole calculation reduces to the determination of the quasiparticle contribution, which in term of the transmission coefficient of Eq. (47) can be written as

\[ S = \int_0^e d\epsilon \tau(\epsilon, V)(1 - \tau(\epsilon, V)). \]  

(60)

This is simply the result that one obtains for a normal contact with an energy and voltage dependent transmission coefficients. In Fig. 8 we show the result of Eq. (60) for different normal transmissions. In the tunneling regime the shot noise is \( S(V) \approx 2eV(V) \) and the most remarkable feature is the zero bias anomaly (see inset of Fig. 7). In the case of perfect transmission there is a non-zero noise due to the fact that the transmission coefficient \( \tau(\epsilon, V) \) is less than one in the gap region. For voltages much greater than the maximum gap, then \( \tau(\epsilon \gg \Delta, D = 1.0) \rightarrow 1 \), what makes that the noise at \( D = 1.0 \) saturates in the high voltage regime.

![FIG. 6. Zero-frequency shot noise for the disordered contact considered in Fig. 8. The inset show the low bias limit of the curve in the tunneling regime (\( D = 0.01 \)).](image)

More interesting is the case of the momentum conserving interface. In Fig. 8 we show the contribution of a trajectory of momentum \( p \). As in the case of the current, the shot noise exhibits a rich subharmonic gap structure, which persists almost up to perfect transmission. The shape of the different curves can be understood in the same terms as the BCS case (see Ref. [81]), with the additional ingredient of the resonant tunneling through the zero energy states. Of course, as in the case of the current, most of these features disappear after performing the angular average.

![FIG. 7. The upper panel shows the trajectory resolved zero-frequency shot noise for the momentum conserving case considered in Fig. 8. The shot noise and voltage are normalized by the trajectory-dependent gap \( \Delta_p \). In the lower panel one can see the effective charge defined as \( Q^* = S/2eV \) as a function of voltage for a transmission \( D = 0.6 \). The vertical lines indicate the position of the voltages \( eV_n = \Delta_p/n \), \( n = 2, ..., 10 \).

In the case of conventional superconductors, the shot noise has been proposed as a tool for measuring the multiple charge quanta transferred by the multiple Andreev reflections. Obviously we can pose here the same question in the case of unconventional superconductors. Indeed, a noise experiment has been recently proposed by Auerbach and Altman to discriminate between two possible explanations of the pronounced subharmonic gap structure observed in YBCO edge junctions. Namely, usual multiple Andreev reflections in a d-wave superconductor and magnon pair creation in the context of the SO(5) theory. In this latter case the observed charge should be \( Q^* = 2ne \), where \( n = 1, 2, ..., \) at a voltage \( eV_n = \Delta_p/n \). This result has to be compared with \( Q^* = ne \) expected in the traditional view of MAR. In order to contribute to the solution of this puzzle, we show in Fig. 8 (lower panel) the effective charge, \( Q^* = S/2eV \), for a transmission \( D = 0.6 \). This result confirm the traditional interpretation that in the MAR process of order \( n \) a charge \( ne \) is transferred. Usually, in order to observe a clear quantization of the charge one should go to the tunneling regime, but in this case this is not necessary due to the resonant tunneling through the zero-energy states. Notice again that this is the contribution of a single tra-
jectory and after angle averaging this clear quantization of the charge with voltage disappears. The exhaustive analysis of the shot noise in d-wave contacts will be presented in a forthcoming publication.

VI. CONCLUSIONS

We have shown how a Hamiltonian approach and the quasiclassical theory of superconductivity can be combined to give a powerful tool to analyze electronic and transport properties of superconducting junctions. In particular, we have demonstrated that a simple Hamiltonian description of an interface can be used to model a great variety of contacts. This Hamiltonian description can be brought into quasiclassical theory via a T-matrix equation, resulting in a new formulation of boundary conditions. These boundary conditions do not contain any spurious solution and can be efficiently solved to compute any transport property. The broad applicability of this formulation covers cases ranging from conventional superconductors to unconventional ones, clean systems and diffusive ones. Moreover, it can be applied to spin active interfaces and it is well suited for the description of time-dependent phenomena like the I-V characteristics and the noise properties of junctions with arbitrary transmission and bias voltage. We have illustrated this approach with the calculation of Josephson current in a transmission and bias voltage. We have illustrated this approach with the calculation of Josephson current in a great variety of situations. The calculation of I-V characteristics and the noise has been exemplified with the analysis of a contact between two d-wave superconductors. In particular, we have briefly discussed the use of shot noise as a possible tool for measuring the charge of the Andreev reflections in unconventional superconductors.

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