Charge Transport and Quantum Phase Transitions in Singlet Superconductor - Ferromagnet - Singlet Superconductor Junctions

Boris Kastening\textsuperscript{1,2}, Dirk K. Morr\textsuperscript{3,4}, Lambert Alff\textsuperscript{2}, and Karl Bennemann\textsuperscript{4}

\textsuperscript{1} Institut für Theoretische Physik, Technische Hochschule Aachen, Physikzentrum, 52056 Aachen, Germany
\textsuperscript{2} Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany
\textsuperscript{3} Department of Physics, University of Illinois at Chicago, Chicago, Illinois 60607, USA
\textsuperscript{4} Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

(Dated: September 25, 2018)

We study the Josephson current, \(I_J\), in a junction consisting of two \(s\)-wave superconductors that are separated by a ferromagnetic barrier possessing a magnetic and non-magnetic scattering potential, \(g\) and \(Z\), respectively. We discuss the general dependence of \(I_J\) on \(g\), \(Z\), and the phase difference \(\phi\) between the two superconductors. Moreover, we compute the critical current, \(I_c\), for given \(g\) and \(Z\), and show that it possesses two lines of non-analyticity in the \((g,Z)\)-plane. We identify those regions in the \((g,Z)\)-plane where the Josephson current changes sign with increasing temperature without a change in the relative phase between the two superconductors, i.e., without a transition between a 0 and \(\pi\) state of the junction. Finally, we show that by changing the relative phase \(\phi\), it is possible to tune the junction through a first-order quantum phase transition in which the spin polarization of the two superconductors' combined ground state changes from \(\langle S_z \rangle = 0\) to \(\langle S_z \rangle = 1/2\).

PACS numbers: 74.50.+r, 74.45.+c, 74.78.-w, 85.25.Cp

I. INTRODUCTION

Heterostructures consisting of magnetically active layers provide new possibilities for manipulating charge (and potentially spin) transport and are hence of great interest for the field of spin electronics\textsuperscript{1}. Josephson junctions consisting of conventional \(s\)-wave superconductors and a ferromagnetic barrier fall into this category, and their study has led to the discovery of a number of fundamentally new phenomena (for a recent review, see Ref.\textsuperscript{2} and references therein). Among these is the transition from a 0-state to a \(\pi\)-state in junctions with a metallic ferromagnetic barrier, which is accompanied by a sign change (and hence directional change) of the Josephson current. This transition signifies an intrinsic phase change of \(\pi\) between the superconductors forming the Josephson junction which arises from a temperature dependent decay length and oscillation length of the superconducting order parameter inside the ferromagnetic metal. Such a transition was predicted theoretically\textsuperscript{3}, and subsequently also observed experimentally\textsuperscript{4}. It was recently shown, by using a phenomenological \(S\)-matrix scattering formalism, that a sign change of the Josephson current with increasing temperature can also occur in insulating ferromagnetic barriers\textsuperscript{5,6}. Changing the direction of the Josephson current by increasing temperature or by varying the relative phase between the superconductors, leads to novel types of current switches that possess potential applications in quantum information technology\textsuperscript{7,8}. Since most ferromagnetic barriers do not only possess a magnetic scattering potential, but also a non-magnetic one, the question naturally arises to what extent the interplay between these two types of scattering potentials either alters the effects discussed above or leads to qualitatively new phenomena.

In this article, we study the Josephson current, \(I_J\), in a one-dimensional (1D) Josephson junction consisting of two \(s\)-wave superconductors and a thin (\(\delta\)-function type) ferromagnetic barrier (SFS junction). We start from a microscopic Hamiltonian in which the barrier possesses a magnetic and non-magnetic scattering potential, described by \(g\) and \(Z\), respectively, the former being directly proportional to the barrier’s magnetization. We discuss the general dependence of the charge Josephson current on \(g\), \(Z\), and the relative phase, \(\phi\), between the two superconductors. In particular, we demonstrate that in certain regions of the \((g,Z)\)-plane, \(I_J\) varies continuously with \(\phi\), while in other regions, and particularly around \(Z = g\), \(I_J\) exhibits discontinuities. We compute the critical current, \(I_c\), defined as the maximum Josephson current for a given \(g\) and \(Z\), and show that it possesses two lines of non-analytic behavior in the \((g,Z)\)-plane. These non-analyticities correspond to discontinuities in the first and second derivative of \(I_c\) (with respect to \(g\) or \(Z\)). We show that \(I_c\) exhibits qualitatively different dependencies on the scattering strength in different parts of the \((g,Z)\)-plane, which opens the interesting (and quite counterintuitive) possibility to increase the critical current through the junction by increasing the junction’s magnetization. Moreover, we identify those regions of the \((g,Z)\)-plane in which the Josephson current changes sign (and thus direction) with increasing temperature without a change in the relative phase between the two superconductors, i.e., without a transition between a 0 and \(\pi\) state of the junction. In addition, we find that while the total spin Josephson current, \(I_s\), flowing through the junction is zero, there are two contributions to \(I_s\), arising from the Andreev and continuum states, respectively, that are equal in magnitude but possess opposite signs. We show that if these two contributions can be
independently measured, this would open new venues for employing the combined spin and charge degrees of freedom in such a junction. Finally, we demonstrate that by changing the phase $\phi$ between the superconductors, it is possible to tune the junction through a first-order quantum phase transition in which the spin polarization of the superconductors’ ground state changes from $\langle S_z \rangle = 0$ to $\langle S_z \rangle = 1/2$.

The theoretical methods used in this study provide direct insight into the explicit dependence of the Josephson current and the Andreev states on the magnetization of the junction, and into the interplay between magnetic and non-magnetic scattering potentials.

## II. THEORETICAL METHODS

We take the 1D SFS junction to be aligned along the $z$-axis and to be described by the Hamiltonian

$$
\mathcal{H} = \int dz \left\{ \sum_\sigma \psi_\sigma^\dagger(z) \left[ -\frac{\hbar^2 \partial^2}{2m} - \mu + U(z) \right] \psi_\sigma(z) - \left[ \Delta(z) \psi_\sigma^\dagger(z) \psi_\sigma^\dagger(z) + H.c. \right] - \frac{g_\mu B M_0}{\hbar} \mathbf{M}(z) \cdot \sum_{\alpha,\beta} \psi_\alpha^\dagger(z) \sigma_{\alpha\beta} \psi_\beta(z) \right\},
$$

(1)

where $\psi_\sigma^\dagger(z)$ and $\psi_\sigma(z)$ are the fermionic operators that create or annihilate a particle with spin $\sigma$ at site $z$, respectively. $\Delta(z)$ is the s-wave superconducting gap, and $U(z) = U_0 \delta(z)$ describes the non-magnetic (i.e., potential) scattering strength of the junction at $z = 0$. Without loss of generality, we choose the magnetization of the junction, $\mathbf{M}(z)$, to be parallel to the $z$-axis, i.e., $\mathbf{M}(z) = M_0 (0, 0, 1) \delta(z)$. In order to simplify the notation, we set $g_\mu B M_0 / \hbar = 1$. Moreover, to facilitate the discussion of the spin structure of the Josephson current and the junction’s ground state, we choose the quantization direction to coincide with the direction of the magnetic moment, i.e., with the $z$-direction.

In the following, we use two complementary theoretical approaches in order to compute the Josephson current through the interface: one follows the Blonder-Tinkham-Klapwijk (BTK) approach (see Sec. II A), the other one starts from the quantum mechanical definition of the current operator and computes its expectation value (see Sec. II B).

### A. BTK Ansatz

At the interface between the two superconductors, two Andreev bound states with energies $E_{\alpha,\beta}$ are formed. As was discussed before, and as we will explicitly show in Sec. II B, the charge Josephson current flows solely through these two bound states, and is hence given by

$$
I_J = I_J^0 + I_J^\beta = -\frac{e}{\hbar} \sum_{j = \alpha, \beta} \frac{\partial E_j}{\partial \phi} \tanh \left( \frac{E_j}{2k_B T} \right),
$$

(2)

where $\phi$ is the phase difference between the superconducting order parameters on the left and right side of the junction. In order to compute $E_{\alpha,\beta}$, we start from Eq. (1) and derive the Bogoliubov-de Gennes (BdG)

$$
\Psi_{n,j}(z) = \begin{pmatrix} u_{n,j}(z) \\ v_{n,j}(z) \end{pmatrix},
$$

(4)

with $j = \alpha, \beta$, the BdG equation is given by

$$
\hat{H}_j \Psi_{n,j}(z) = E_{n,j} \Psi_{n,j}(z).
$$

(5)

Here $E_{n,j}$ is the energy of the state $\Psi_{n,j}$,

$$
\hat{H}_j = \begin{pmatrix} H_0 + H_M & -\Delta \\ -\Delta^* & -H_0 + H_M \end{pmatrix},
$$

(6)

where the upper (lower) sign corresponds to $j = \alpha (\beta)$ and

$$
H_0 \equiv -\frac{\hbar^2 \partial^2}{2m} - \mu + U_0 \delta(z),
$$

(7a)

$$
H_M \equiv M_0 \delta(z),
$$

(7b)

$$
\Delta \equiv \begin{cases} \Delta_0 & z < 0 \\ \Delta_0 e^{-i\phi} & z > 0 \end{cases},
$$

(7c)

with $\Delta_0$ chosen real. The case $n = 0$ corresponds to the Andreev bound states, and in what follows, we use $E_j$ as a shorthand notation for their energies, $E_{0,j}$.

For the bound states’ wave-function on the left and right hand sides of the junction, $\Psi_{0,j,L}(z)$ and $\Psi_{0,j,R}(z)$,
respective, we make the ansatz
\[ \Psi_{0,j,s}(z) = e^{iV_0 j z} \sum_{\delta=\pm} \left( \frac{u_{0,j,s,\delta}}{v_{0,j,s,\delta}} \right) e^{i k_F z}, \]
with \( s = L, R, c_{L,R} = \pm 1, \) and \( k_F \) is the Fermi momentum. Note that the decay length of the Andreev state, \( \kappa^{-1} = \hbar v_F / \sqrt{\Delta^2 - E_j^2} \) with \( v_F = \hbar k_F / m \), itself depends on \( E_j \). The solutions of Eq. \( (5) \) are subject to the boundary conditions
\[ \Psi_{0,j,L}(0) = \Psi_{0,j,R}(0), \]
\[ \partial_z \Psi_{0,j,L}(R) = \partial_z \Psi_{0,j,R}(0) = \frac{2m}{\hbar^2} \left( U_0 \mp M_0 \right) \Psi_{0,j,L}(0), \]
where again the upper (lower) sign corresponds to \( j = \alpha(\beta) \). In the limit \( k_F \gg \kappa_j \), which holds for superconductors with coherence length \( \xi = v_F / \Delta_0 \gg 1 / k_F \), the solution of the BdG equation yields two Andreev states with energies
\[ \frac{E_j}{\Delta_0} = \frac{\sqrt{A + B} \mp \sqrt{A - B}}{\sqrt{2 [1 + (g + Z]^2] [1 + (g - Z)^2]}}, \]
where the upper (lower) sign corresponds to \( j = \alpha(\beta) \) and
\[ A = (1 + Z^2 - g^2) \left[ \cos^2 \left( \phi / 2 \right) + Z^2 - g^2 \right] + 2g^2, \]
\[ B = \sqrt{1 + (g + Z)^2} \left[ 1 + (g - Z)^2 \right], \]
with \( g = m M_0 / \hbar^2 k_F \) and \( Z = m U_0 / \hbar^2 k_F \). Without loss of generality we assume \( g, Z \geq 0 \) from here on. While \( E_\beta \) does not change sign as a function of \( \phi \) (for \( Z \neq 0 \)), \( E_\alpha \) changes sign if \( 0 < g^2 - Z^2 < 1 \) (hence for \( g \leq Z \) or \( g \geq \sqrt{1 + Z^2} \), no sign change of either bound state takes place). This sign change, which occurs at a phase difference \( \phi_c \) given by \( \cos^2 \left( \phi_c / 2 \right) = g^2 - Z^2 \), indicates a first-order phase transition in which the spin polarization of the superconductors’ ground state changes, as discussed in more detail in Sec. III C.

For the subsequent discussion, it is necessary to consider the spin structure of the Andreev states. To this end, we compute the local density of states (LDOS), \( N(\sigma, z) \), (i.e., the local spectral function) for the spin-up and spin-down components of the Andreev states, using the Bogoliubov transformation presented in Eq. \( (4) \), are readily obtained as
\[ N(\uparrow, z) = |u_{0,\alpha}(z)|^2 \delta(\omega - E_\alpha) + |v_{0,\beta}(z)|^2 \delta(\omega - E_\beta), \]
\[ N(\downarrow, z) = |u_{0,\beta}(z)|^2 \delta(\omega - E_\beta) + |v_{0,\alpha}(z)|^2 \delta(\omega - E_\alpha). \]
Hence, \( \omega > E_{\alpha(\beta)} > 0 \) the wave-function of the \( \alpha \) state, \( |\Psi_{0,\alpha}\rangle \), possesses a particle-like spin-down component, and a hole-like spin-up component, i.e., \( |\Psi_{0,\alpha}\rangle = |p, \downarrow\rangle + |h, \uparrow\rangle \).
Similarly for the \( \beta \) state, \( |\Psi_{0,\beta}\rangle = |p, \uparrow\rangle + |h, \downarrow\rangle \). When \( E_\alpha \) changes sign, the occupation numbers of the spin-up and spin-down components of the respective wave-function are interchanged. We thus find that the LDOS near the junction barrier contains four peaks inside the superconducting gap, in agreement with the results obtained in Refs. \[ [6, 10] \]. As an important check of our calculations, we consider the limit \( \phi = 0 \), where the Josephson junction is identical to a system, in which a single magnetic impurity is located inside a 1D s-wave superconductor. In this limit, Eq. \( (10) \) yields that only one of the Andreev states exists inside the superconducting gap with \( E_\alpha < \Delta_0 \), while the other Andreev state possesses the energy \( E_\beta = \Delta_0 \) and is thus part of the continuum (see Fig. \( 1(a) \)). These results are in agreement with those of \( \tilde{T} \)-matrix and Bogoliubov-de Gennes approaches used in the context of impurity scattering in s-wave superconductors (for a recent review, see Ref. \[ 16 \]). We note that in this limit, \( \phi = 0 \), our results (and those of Ref. \[ 16 \]) for \( E_{\alpha,\beta} \) do not agree with the findings in Refs. \[ 5, 6 \] [see also Ref. \[ 17 \]].

**B. Quantum Mechanical Current**

Using the operator definition of the quantum mechanical current, we may resolve the spin-up and spin-down particle currents \( I_I(z) \) and \( I_L(z) \), which in turn allows to compute the charge and spin currents via
\[ I_I(z) \equiv -e [I_I(z) + I_L(z)], \]
\[ I_S(z) \equiv \frac{\hbar}{2} [I_I(z) - I_L(z)]. \]

In order to obtain appropriately defined current operators \( I_I(z) \) and \( I_L(z) \), whose expectation values are the currents \( I_I(z) \) and \( I_L(z) \), we note that the density operator of spin-\( \sigma \) electrons is
\[ \rho_\sigma(z) = \rho_\sigma(z, z') \big|_{z'=z}, \]
where
\[ \rho_\sigma(z, z') \equiv \psi_\sigma(z) \psi_\sigma(z'). \]

The quantum mechanical particle current operator corresponding to \( \rho_\sigma(z) \) then follows from
\[ \hat{I}_\sigma(z) = \frac{i\hbar}{2m} \left( \partial_z - \partial_{z'} \right) \rho_\sigma(z, z') \big|_{z'=z} = \frac{i\hbar}{2m} \left\{ \left[ \partial_z \psi_\sigma^\dagger(z) \psi_\sigma(z) - \psi_\sigma^\dagger(z) \partial_z \psi_\sigma(z) \right] \right\}, \]
and its expectation value
\[ I_\sigma(z) = \frac{\hbar}{m} \text{Im} \left\langle \psi_\sigma^\dagger(z) \partial_z \psi_\sigma(z) \right\rangle \]
is the corresponding particle current. In what follows, we refer to $I_\sigma(z)$ as the “conventional” form of the particle current.

After diagonalizing the Hamiltonian with the Bogoliubov transformation of Eq. (3), the currents given in Eq. (13) possess in general contributions from both the Andreev bound states and the continuum states. The calculation of the latter is prohibitively cumbersome when using the form of $I_\sigma$ given in Eq. (17). It turns out, however, that one can use an alternative formulation to evaluate $I_\sigma$ by defining a “symmetrized” form of the current operator. Specifically, using the anticommutator
\[ \{\psi_\sigma(z),\psi_\sigma(z')\} = \delta_{z,z'} \delta(z - z'), \]
we can write
\[ \hat{\rho}_\sigma(z,z') \equiv \frac{1}{2} \left[ \psi_\sigma(z)\psi_\sigma(z') - \psi_\sigma(z')\psi_\sigma(z) \right]. \]

We next define a “symmetrized” density via
\[ \hat{\rho}_\sigma^\text{sym}(z,z') = \frac{1}{2} \left[ \psi_\sigma(z)\psi_\sigma(z') + \psi_\sigma(z')\psi_\sigma(z) \right], \]
where the second term on the r.h.s. of Eq. (20) arises from the first term via a particle-hole transformation (this fact becomes important when discussing the form of the LDOS corresponding to $\hat{\rho}_\sigma^\text{sym}(z,z)$, see below). Since the $\delta$-function in Eq. (19) does not contribute to the particle current operator, it immediately follows that the densities defined in Eqs. (19) and (20) when inserted into Eq. (10) yield the same spin-$\sigma$ particle current operator. We can therefore write $I_\sigma$ as a “symmetrized” form as
\[ I_\sigma(z) = \frac{i\hbar}{2m} \left[ (\partial_z - \partial_{z'}) \hat{\rho}_\sigma^\text{sym}(z,z') \right]|_{z' = z} \]
\[ = \frac{i\hbar}{4m} \left\{ \psi_\sigma(z) [(\partial_z \psi_\sigma(z)] + \psi_\sigma(z) [(\partial_z \psi_\sigma^\dagger(z)] - \text{h.c.} \right\}. \]

One then obtains
\[ I_\sigma(z) = \frac{\hbar}{2m} \text{Im} \left\{ \psi_\sigma(z) \partial_z \psi_\sigma(z) + \psi_\sigma(z) \partial_z \psi_\sigma^\dagger(z) \right\} \] (22)
as the corresponding “symmetrized” form of the spin-$\sigma$ particle current. While the current thus defined is identical to the conventional form given in Eq. (17), it turns out that the calculation of the contributions from continuum states using the right hand side of Eq. (22) is considerably simplified. In what follows, we therefore discuss the contributions of continuum and Andreev states to the charge and spin current using the symmetrized form of the particle current, Eq. (22). Since the contributions to the particle current arising from individual (Andreev or continuum) states are different in the conventional and the symmetrized form, we distinguish between them by denoting with (without) a tilde the current flowing through a specific state within the symmetrized (conventional) definition. We then obtain
\[ I_{\uparrow(n)}(z) = \sum_n \tilde{I}_{\uparrow(n),n}(z), \] (23)
where
\[ \tilde{I}_{\uparrow,n}(z) \equiv \tilde{I}_{\uparrow}^\mu(n,z) \tan \frac{\beta E_{n,\alpha}}{2} + \tilde{I}_{\uparrow}^\nu(n,z) \tan \frac{\beta E_{n,\beta}}{2}, \] (24a)
\[ \tilde{I}_{\downarrow,n}(z) \equiv \tilde{I}_{\downarrow}^\mu(n,z) \tan \frac{\beta E_{n,\beta}}{2} + \tilde{I}_{\downarrow}^\nu(n,z) \tan \frac{\beta E_{n,\alpha}}{2}, \] (24b)
with amplitude functions
\[ I_{f,j}^\sigma(z) \equiv \frac{\hbar}{2m} \text{Im} \left[ f_{n,j}(z) \partial_z f_{n,j}^\ast(z) \right], \] (25)
where $f = u, v$ and $j = \alpha, \beta$, and the sum in Eq. (25) runs over all states of the system (including Andreev and continuum states).

We begin by computing the contribution to the total current arising from the continuum states. Using the general ansatz for the form of these states described in Appendix A, we find that the continuum states with momentum $\pm(k_F \pm q)$ are degenerate and that their energy $E_q$ is given by (in the limit $E_q \ll \mu$)
\[ E_q^2 = |\Delta_0|^2 + \left( \frac{\hbar^2 k_F q}{m} \right)^2. \] (26)
Diagonalizing the corresponding subspace, one obtains three important relations
\[ \sum_{n(E_q)} [\tilde{I}_{\uparrow,n}(z) + \tilde{I}_{\downarrow,n}(z)] \propto \sin 2q|z|, \] (27a)
\[ \sum_{n(E_q)} [\tilde{I}_{\uparrow,n}(z) - \tilde{I}_{\downarrow,n}(z)] = 0, \] (27b)
\[ \sum_{n(E_q)} \tilde{I}_{\uparrow}^\mu(n,z = 0) = \sum_{n(E_q)} \tilde{I}_{\downarrow}^\nu(n,z = 0), \] (27c)
where the sums run over an orthonormal basis of continuum states with energy $E_q$. The first relation, Eq. (27a), implies that given the definition of the charge Josephson current, $I_J$, in Eq. (13a), the contribution to $I_J$ from continuum states at the interface is identically zero within the symmetrized version of the current. As we show below, this result also holds when the conventional definition of the current operator is used. General arguments have been put forward that this result arises since the density of continuum states in the presence of a barrier is unchanged. However, away from the interface the continuum states carry a non-zero charge current since charge conservation requires that the (decaying) current through the Andreev states be compensated by a current carried through the continuum states. The second
relation, Eq. (27b), implies that the contribution of the continuum states to the spin Josephson current, as defined in Eq. (13b), is zero at any position z along the junction. Finally, the third relation, Eq. (27c), when combined with Eq. (24), yields that at the barrier, there are no contributions from the continuum states to either the spin-up or spin-down particle current.

Since the continuum states carry no charge current at the barrier (i.e., at \( z = 0 \)) the total charge Josephson current is solely carried by the Andreev states and thus given by

\[
I_j \equiv I_j(0) = -e\left[\tilde{I}_\downarrow(0) + \tilde{I}_\uparrow(0)\right], \tag{28}
\]

where \( \tilde{I}_\downarrow \) and \( \tilde{I}_\uparrow \) are the currents through the Andreev states in the symmetric formulation of the current. These are given by the \( n = 0 \) term in Eq. (28) for which one thus has

\[
\tilde{I}_\uparrow(0) = I_{\uparrow,0}(z) \tan \frac{\beta E_\sigma}{2} + I_{\uparrow,\beta}(z) \tan \frac{\beta E_\delta}{2}, \tag{29a}
\]

\[
\tilde{I}_\downarrow(0) = I_{\downarrow,0}(z) \tan \frac{\beta E_\sigma}{2} + I_{\downarrow,\alpha}(z) \tan \frac{\beta E_\delta}{2}. \tag{29b}
\]

It is straightforward to show that the bound state ansatz of Eq. (8) leads to

\[
I_{\uparrow,0}(z) = I_{\uparrow,0}(z) e^{-2\kappa|z|}, \tag{30a}
\]

\[
I_{\downarrow,\beta}(z) = I_{\downarrow,\beta}(z) e^{-2\kappa|z|}, \tag{30b}
\]

yielding \( \tilde{I}_\downarrow(0) = \tilde{I}_\uparrow(0) \). Together with Eq. (27b), this result implies that within the symmetrized form of the particle current, Eq. (22), neither the continuum states nor the Andreev bound states carry a spin current. Hence, we obtain that the total spin current \( I_S(0) \) defined in Eq. (13b) vanishes at any point along the junction, in agreement with the arguments in Ref. 22. This result holds even when the system undergoes a first order quantum phase transition in which the spin polarization of the junction’s ground state changes (see Sec. III C).

While the symmetrized form of the Josephson current used above allowed for a simpler evaluation of the contributions arising from the continuum states, any physical interpretation of the Josephson current has to be based on its conventional definition, given by Eq. (10), and the form of the spin density in Eq. (15). In what follows, we therefore discuss the form of the charge and spin currents within the conventional definition, and compare them with the symmetrized results presented above. A connection between the expressions for \( I_{\uparrow,n} \) and \( I_{\downarrow,n} \) (which represent the currents flowing through state \( n \) in the symmetrized and conventional definition, respectively) can be made by using the following identities

\[
\sum_n \left[ I_{\uparrow,n,\alpha}(z) - I_{\uparrow,n,\beta}(z) \right] = 0, \tag{31a}
\]

\[
\sum_n \left[ I_{\downarrow,n,\beta}(z) - I_{\downarrow,n,\alpha}(z) \right] = 0, \tag{31b}
\]

where, as in Eq. (23), the sum runs over all states of the junction. These identities are derived by applying \( \partial_z - \partial_{z'} \) to the anticommutator in Eq. (15), and subsequently setting \( \sigma' = \sigma \) and \( z' = z \), and using the form of \( \psi_\uparrow(z) \) and \( \psi_\downarrow(z) \) given in Eq. (31). One then finds that by subtracting the left hand side of Eq. (31a) [Eq. (31b)] from the right hand side of Eq. (23) for \( \sigma = \uparrow [\sigma = \downarrow] \), one obtains the corresponding expressions for \( I_{\uparrow,n} \) and \( I_{\downarrow,n} \). In particular, within the conventional definition, the Josephson current through the Andreev bound states is given by

\[
I_{\uparrow,\sigma}(z) = -I_{\uparrow,0,\sigma}(z) \left( 1 - \tanh \frac{\beta E_\sigma}{2} \right) \tag{32a}
\]

\[
+ I_{\uparrow,\sigma}(z) \left( 1 + \tanh \frac{\beta E_\delta}{2} \right), \tag{32b}
\]

\[
I_{\downarrow,\sigma}(z) = -I_{\downarrow,0,\sigma}(z) \left( 1 - \tanh \frac{\beta E_\sigma}{2} \right) \tag{33a}
\]

\[
+ I_{\downarrow,\sigma}(z) \left( 1 + \tanh \frac{\beta E_\delta}{2} \right). \tag{33b}
\]

Given the result for \( I_j \) in Eq. (28), it immediately follows that

\[
I_j = -e \left[ I_{\uparrow,\sigma}(0) + I_{\downarrow,\sigma}(0) \right], \tag{34}
\]

implying that also within the conventional definition of the particle current, the total charge Josephson current at \( z = 0 \) is solely carried by the Andreev states with no contribution arising from the continuum states. This result justifies the use of Eq. (2) in the BTK approach of Sec. II A for the calculation of the total charge Josephson current. Moreover, since the charge Josephson currents computed within the BdG approach of Sec. II A should be the same as that of the quantum mechanical method of Sec. II B, one requires [by combining Eqs. (2), (28), (29), and (31)] that the following important identity be satisfied

\[
\frac{\partial E_j}{\partial \phi} = 2\hbar I_{\uparrow,\sigma}(0), \tag{35}
\]

with \( j = \alpha, \beta \). We have carried out an extensive numerical survey in the parameter space of our system and found this relation to always hold.

We next consider the form of the spin current in the conventional definition of the currents. While the result of a vanishing total spin current, that we obtained within the symmetrized form, also has to hold within the conventional framework, we find that the contributions from the Andreev and continuum states differ. In particular, using the results of Eq. (32), we find that the contribution of the Andreev states to the spin current, \( I_{\downarrow,\sigma} \), is given by

\[
I_{\downarrow,\sigma}(z) = \hbar \left[ I_{\downarrow,0,\sigma}(z) - I_{\downarrow,\sigma}(z) \right], \tag{36}
\]

which in general does not vanish. However, since the total spin current still needs to be zero, it immedi-
ately follows that within the conventional definition of the particle current, a spin current of equal magnitude, but opposite sign to \( I_{AS}^{\uparrow} \) flows through the continuum states. Note, however, that while a spin Josephson current flows through the continuum states, the charge current through these states is zero, as discussed above. The contribution to the spin current provided by the continuum states thus compensates the spin current through the Andreev states and leads to a zero total spin current [we return to a discussion of these two (opposite) contributions to the spin current in Sec. [III B]. In contrast, in the symmetrized version, the spin current through each of the continuum states and the Andreev states is exactly zero.

In order to understand the different origin of the zero spin current in these two frameworks, and to gain insight into its physically correct interpretation, we consider the local density of states of the Andreev states, \( N_{sym}(\sigma, z) \), corresponding to the density \( \rho_{\sigma}^{sym}(z) = \langle \rho_{\sigma}^{sym}(z, z') \rangle \), which is given by

\[
N_{sym}(\uparrow, z) = \frac{1}{2} \left| u_{0,\alpha}(z) \right|^2 \left[ \delta(\omega + E_\alpha) + \delta(\omega + E_\beta) \right] + \frac{1}{2} \left| v_{0,\beta}(z) \right|^2 \left[ \delta(\omega - E_\beta) + \delta(\omega - E_\beta) \right],
\]

(36a)

\[
N_{sym}(\downarrow, z) = \frac{1}{2} \left| u_{0,\alpha}(z) \right|^2 \left[ \delta(\omega - E_\beta) + \delta(\omega + E_\beta) \right] + \frac{1}{2} \left| v_{0,\beta}(z) \right|^2 \left[ \delta(\omega + E_\alpha) + \delta(\omega + E_\alpha) \right].
\]

(36b)

Here, the second term on the right hand side of each equation is obtained from the first one via a particle-hole transformation, in agreement with the definition of \( \rho_{\sigma}^{sym}(z, z') \) in Eq. (20). As a result, the system now possesses two sets of two degenerate bound states, i.e., a total of four Andreev bound states, each with a spectral weight of 1/2. Within each set, the degenerate bound states differ by their spin quantum number: one bound state possesses a particle (hole) branch which is spin-\( \uparrow \) (spin-\( \downarrow \)), and vice versa for the second bound state. Using the relations in Eqs. (30) and (34), and the definition of the Josephson current in Eqs. (2) and (15a), one immediately finds that such a LDOS leads to the expressions for \( I_{AS}^{\uparrow,\downarrow}(z) \) given in Eq. (20). Since the spin quantum numbers are opposite between the degenerate bound states, it naturally follows that the spin current through the Andreev states is zero. Note, however, that the LDOS given in Eq. (30) is unphysical: it does not reflect the symmetry-breaking of the ferromagnetic barrier since for every spin-\( \uparrow \) branch, there exists a degenerate spin-\( \downarrow \) branch. Moreover, in the limit \( \phi = 0 \) (where the barrier represents a single magnetic impurity in a 1D s-wave superconductor), the symmetrized LDOS of Eq. (30) is in disagreement with that obtained from \( \hat{T} \)-matrix and Bogoliubov-de Gennes approaches. In contrast, the LDOS of Eq. (12) which is based on the conventional definition of the density operator reflects the symmetry-breaking of the ferromagnetic barrier. It is therefore physical and in full agreement with the results of Ref. [16] for \( \phi = 0 \). It then follows that the physically correct interpretation regarding the origin of a zero total spin current is that both the Andreev states and the continuum states carry a spin current of equal magnitude, but opposite sign. We propose that this conclusion can be tested by using a spin-resolved STM experiment which can distinguish between the LDOS presented in Eq. (12) on one hand, and that given in Eqs. (30) on the other hand.

### III. RESULTS

#### A. Charge Transport

The general dependence of the Andreev state energies and the Josephson current on the scattering strength of the barrier is presented in Fig. 1 where we plot \( \pm E_{\alpha,\beta} \) [Fig. (1a)] and the resulting Josephson current at \( T = 0 \) [Fig. (1b)] as a function of \( \phi \) for several values of \( Z \) and \( g \) (the columns in Figs. (1a) and (1b) from left to right correspond to \( g = 0, \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \), respectively, while the rows from bottom to top correspond to \( Z = 0, \frac{1}{2}, 1 \), respectively.) For a purely non-magnetic barrier [i.e., \( g = 0 \), left column of Fig. (1a)], we find in agreement with earlier results\(^{5,12,13,14,20}\) that the Andreev states are degenerate with energies

\[
\frac{E_{\alpha,\beta}}{\Delta_0} = \sqrt{\frac{\cos^2(\phi/2) + Z^2}{1 + Z^2}}.
\]

(37)

This degeneracy is lifted by a non-zero magnetic scattering potential of the junction (i.e., \( g \neq 0 \) as shown in the three right columns of Fig. (1a)). A qualitatively similar result was also found in Refs. [6,10,17,19]. Specifically, for a purely magnetic scattering potential of the junction (i.e., \( Z = 0 \), bottom row of Fig. (1a)), the energies of the Andreev states are given by

\[
\frac{E_{\alpha,\beta}}{\Delta_0} = \frac{1}{1 + g^2} \left[ \cos(\phi/2) \mp g \sqrt{g^2 + \sin^2(\phi/2)} \right].
\]

(38)

In agreement with the analytical results presented in Eqs. (37) and (38) we find that with increasing \( g \gg Z \) [plots in the lower right corner of Fig. (1a)] and \( Z \gg g \) [plots in the upper left corner of Fig. (1a)] the energies of both bound states move toward the gap edge. An interesting situation occurs for \( g = Z \) [plots along the diagonal of Fig. (1a)], since in this case, the effective scattering strength for the spin-\( \downarrow \) and spin-\( \uparrow \) electrons is \( V_{eff}^\downarrow = g + Z = 2Z \) and \( V_{eff}^\uparrow = g - Z = 0 \), respectively. In the unitary scattering limit \( g = Z \gg 1 \), we then find that the energies of the Andreev states are given by

\[
\frac{E_{\alpha}}{\Delta_0} = \frac{\cos^2(\phi/2)}{2Z} + O(Z^{-3}),
\]

(39a)
FIG. 1: (Color online). (a) Energies $\pm E_{\alpha,\beta}$ of the Andreev states. The columns from left to right correspond to $g = 0, \frac{1}{3}, \frac{2}{3}, 1$, respectively, while the rows from bottom to top correspond to $Z = 0, \frac{1}{3}, \frac{2}{3}, 1$, respectively. The energies of the $\alpha$ and $\beta$ states are indicated by red (grey in print) and black lines, respectively, while the spin-$\uparrow$ and spin-$\downarrow$ components are indicated by dashed-dotted and solid lines. For $g = 0$ (left column) the $\alpha$ and $\beta$ states are degenerate. (b) The resulting $I_J$ at $T = 0$ for several $g$ and $Z$ as a function of $\phi$. 
\[ \frac{E_\beta}{\Delta_0} = 1 - \frac{\sin^4(\phi/2)}{8Z^2} + O(Z^{-4}). \]  

(39b)

Hence, in the limit \( g = Z \rightarrow \infty \), the \( \alpha \)-state becomes a zero energy (midgap) state, while the \( \beta \)-state moves into the continuum. This analytical result is confirmed by the numerical results shown in the plots along the diagonal of Fig. 1(a).

We next discuss the form of the Josephson current, resulting from the form of the Andreev states shown in Fig. 1(a). In the unitary scattering limit \( Z \gg \max\{g, 1\} \) the Josephson current at \( T = 0 \) is given by (to leading order in \( Z \))

\[ I_J = \frac{e \Delta_0}{\hbar} \sin \phi \left( \frac{1}{2Z^2} \right), \]

(40)

while for \( g \gg \max\{Z, 1\} \) one obtains to leading order in \( g \)

\[ I_J = -\frac{e \Delta_0}{\hbar} \sin \phi \left( \frac{1}{2g^2} \right). \]

(41)

Hence, the Josephson currents for a predominantly non-magnetic [Eq. (10)] and predominantly magnetic [Eq. (11)] barrier differ by a phase shift of \( \pi \) in the unitary scattering limit. This result also follows from a comparison of the \( I_J \) plots in the upper left \( (Z \gg g) \) and lower right \( (g \gg Z) \) corners of Fig. 1(b).

Whether the Josephson current in the junction considered here is carried by Cooper pairs, or by single electrons, depends on the relative strength of \( g \) and \( Z \). We first recall that in a purely non-magnetic junction (i.e., \( g = 0 \)) it was argued that the dependence of the Josephson current on \( Z \) in the unitary scattering limit, \( I_J \sim Z^{-2} \) [see Eq. (10)], implies that the current is carried by Cooper pairs. In contrast, in Josephson junctions consisting of unconventional superconductors the scaling of the Josephson current, \( I_J \sim Z^{-1} \), implies that it is carried by single electrons. Here, we find that for a predominantly magnetic junction with \( g \gg \max\{Z, 1\} \), \( I_J \) also scales with the inverse square of the scattering strength (see Eq. (11)) and the current should thus also be carried by Cooper pairs. In contrast, for the case \( Z = g \rightarrow \infty \), we obtain \( I_J \sim Z^{-1} \) and the Josephson current should thus be carried by single electrons. Further support for this conclusion comes from considering the dependence of \( E_\alpha \) on the scattering strength in the limit \( \phi = 0 \). As mentioned above, in this case, the junction is identical to a static impurity in a (1D) s-wave superconductor. If the impurity is purely magnetic, the Andreev state \( \alpha \) (which is better known in this context as a Shiba state) is formed through scattering processes involving the creation and destruction of Cooper-pairs. This immediately follows from a diagrammatic derivation of the scattering \( \bar{T} \)-matrix which includes diagrams that contain the anomalous Greens functions, \( F \) and \( F^* \), representing the creation and destruction of Cooper-pairs, respectively. As a direct result of the included anomalous Greens functions, one obtains \( E_\alpha \sim g^{-2} \), as in Eq. (38) which immediately leads to \( I_J \sim g^{-2} \) for \( \phi \neq 0 \). In contrast, for an impurity with scattering strength \( V_\text{eff}^\perp = 2Z \) and \( V_\text{eff}^\parallel = 0 \), the \( \bar{T} \)-matrix is given by a series of diagrams that contain the normal Greens function only (diagrams containing \( F \) and \( F^* \) are forbidden), and hence \( E_\alpha \sim Z^{-1} \). Note that for the same reason, Josephson junctions consisting of unconventional superconductors possess Andreev states whose energies also scale as \( E_i \sim Z^{-1} \). This connection between the scaling of \( E_\alpha \) and \( I_J \) for \( \phi \neq 0 \) with the case of impurity scattering for \( \phi = 0 \) demonstrates that the presence or absence of scattering diagrams involving the anomalous Greens function determines the nature of the Josephson current.

While the Josephson current is a continuous function of \( \phi \) for certain combinations of \( Z \) and \( g \), \( I_J \) also exhibits discontinuities, in particular in the vicinity of \( Z \approx g \), as shown in Fig. 1(b). These discontinuities arise from a zero energy crossing of an Andreev state at a certain phase, \( \phi_{\text{LC}} \), where \( \partial E_{\alpha,\beta}/\partial \phi \neq 0 \), as shown in Fig. 1(a). Since at \( T = 0 \), only the negative energy branches of the bound states are populated and thus contribute to \( I_J \), \( \partial E_{\alpha,\beta}/\partial \phi \neq 0 \) leads to a discontinuity in the Josephson current at \( \phi_{\text{LC}} \). In Fig. 2(a), we present a contour plot that represents in which parts of the \((g, Z)\)-plane, \( I_J \) exhibits a continuous or discontinuous dependence on \( \phi \). In the white regions of Fig. 2(a), \( I_J \) is continuous, while in the grey and black regions, which are located in the vicinity of the \( Z = g \) line, it exhibits discontinuities as \( \phi \) is varied.

This change between continuous and discontinuous behavior of \( I_J \) in the \((g, Z)\)-plane leads to an interesting form of the critical current, \( I_c \). Here, we define \( I_c \) for a given \( g \) and \( Z \) as the maximum absolute value of \( I_J \) for any \( 0 \leq \phi < \pi \), i.e., \( I_c = \max_\phi |I_J(\phi)| \). At that value of \( \phi \), for which \( |I_J(\phi)| \) exhibits the maximum value, \( I_J \) either possesses either a continuous extremum or a discontinuity. In the light (dark) grey areas of Fig. 2(a), \( I_c \) is realized at a continuous extremum (discontinuity), while the discontinuity (continuous extremum) realizes a local maximum of \( |I_J| \) only. In the black regions of Fig. 2(a), no continuous extremum exists. In order to investigate the origin of the qualitatively different behavior of \( I_J \) in the white, grey and dark regions, we consider six pairs of values \((g, Z)\), denoted by the dots in Fig. 2(a), and present the resulting Josephson currents as a function of \( \phi \) in Fig. 2(b). We find that the different behavior in the grey and black regions arises from a shift in the values of \( \phi \) at which the discontinuity in \( I_J \) occurs. As one moves from point (1) to (6) in Fig. 2, two discontinuities first emerge at \( \phi = \pi \), and then move symmetrically toward \( \phi = 0 \) and \( \phi = 2\pi \), respectively.
FIG. 2: (a) Behavior of $I_J(\phi)$ in the $(g,Z)$-plane. White regions: $I_J$ is continuous. Light (dark) grey regions: Maximum of $|I_J(\phi)|$ is realized at a continuous extremum (discontinuity). Black area: Only extrema at discontinuities exist. The white regions are bounded by $Z^2 = g^2$ and by $Z^2 = g^2 - 1$. (b) $I_J(\phi)$ at $T = 0$ for the six parameter pairs $(g,Z)$ indicated by dots in (a).

One finds

$$I_c(g=0,Z) = \frac{e\Delta_0}{\hbar} \left( 1 - \frac{Z}{\sqrt{1 + Z^2}} \right), \quad (42)$$

$$I_c(g,Z=0) = \begin{cases} \frac{e\Delta_0}{\hbar} \sqrt{1 - g^2} & 0 \leq g \leq g_m, \\ \frac{e\Delta_0}{\hbar} \left( \frac{g}{\sqrt{1 + g^2}} - \frac{g^2}{1 + g^2} \right) & g \geq g_m, \end{cases} \quad (43)$$

where $g_m \approx 0.915186$ is the largest real solution of the equation $4g^6 - 4g^2 + 1 = 0$.

Even though the critical current is a continuous function of $g$ and $Z$, it possesses two lines of non-analyticity in the $(g,Z)$-plane that asymptotically approach $Z = g$ for $Z,g \to \infty$. These lines are represented in Fig. 3(a) as solid black lines. Line (1), corresponding to the boundary between the light grey and the black region in Fig. 2(a), represents a discontinuity in the second derivative of $I_c$.

In contrast, line (2), which corresponds to the boundary between the light grey and dark grey region in Fig. 2(a), represents a discontinuity in the first derivative of $I_c$. Line (2) also represents a sign change in that value of $I_J$.
which determines \( I_c \). In other words, to the left (right) of line (2), \( I_c \) is realized by a positive (negative) value of \( I_J \). These non-analyticities become particularly apparent when one plots the critical current as a function of \( g \) (for constant \( Z \)) and \( Z \) (for constant \( g \)), as shown in Figs. 3(b) and (c), respectively (in Fig. 3(b), we indicated the non-analyticities for the curve with \( Z = 1/2 \) by arrows).

The different dependence of \( I_J \) on the scattering strength in the limits \( g \gg Z \) or \( Z \gg g \) [see Eqs. (40) and (41)] on one hand and \( g = Z \gg 1 \), where

\[
I_J^\alpha = \frac{e\Delta_0 \sin \phi}{4Z}, \quad (44a)
\]

\[
I_J^\beta = \frac{e\Delta_0 \sin \phi (1 - \cos \phi)}{16Z^2}, \quad (44b)
\]
on the other hand leads to the interesting possibility to increase the critical current by increasing the magnetization, and hence the scattering strength of the barrier. Specifically, we find \( I_c = \frac{\Delta_0}{Z} g^{-2} \) for \( g \gg Z \) and \( I_c = \frac{\Delta_0}{Z^2} Z^{-2} \) for \( Z \gg g \), while for \( Z = g \gg 1 \), we have \( I_c = \frac{\Delta_0}{Z^2} Z^{-1} \). As a result, we find that for fixed \( Z \gg 1 \) and increasing \( g \), the critical current exhibits a maximum at \( Z = g \). This effect is demonstrated in Fig. 4 where we present \( I_c \) as a function of \( g \) for \( Z = 20 \). Hence, for a given non-magnetic scattering strength of a paramagnetic barrier, it is possible to increase the critical current by increasing the magnetization of the barrier and thus its magnetic scattering strength. This increase of the magnetization can, for example, be achieved by applying a local magnetic field via atomic force microscopy.²

We next consider the temperature dependence of the Josephson current. Here, we find that the splitting of the Andreev states for a non-zero magnetic scattering strength can lead to an unconventional temperature dependence of \( I_J \) in which it changes sign with increasing temperature without a change in the relative phase, \( \phi \), between the two superconductors. This temperature dependence is demonstrated in Fig. 5(a), where we assume a BCS temperature dependence of the superconducting gap. In order to understand this sign change, we consider the \( \phi \)-dependence of \( E_{\alpha,\beta} \), which is shown in Fig. 5(b). At \( T = 0 \), only the branches indicated by 1 and 2, belonging to Andreev states \( \beta \) and \( \alpha \), respectively, are occupied. Since the derivatives \( \partial E_{\alpha}/\partial \phi \) and \( \partial E_{\beta}/\partial \phi \) possess opposite signs, the Josephson currents through them, \( I_J^\beta < 0 \) and \( I_J^\alpha > 0 \), flow in opposite directions with \( |I_J^\alpha| > |I_J^\beta| \). Since with increasing temperature, the occupation of branches 2 and 3 changes more rapidly than those of branches 1 and 4, it follows that the magnitude of \( I_J^\beta \) decreases more quickly than that of \( I_J^\alpha \). As a result, the total current, \( I_J = I_J^\alpha + I_J^\beta \), eventually changes sign. A possible sign change of \( I_J \) with increasing temperature was previously also discussed in Refs. 5,6. However, due to the differences between our results for \( E_{\alpha,\beta} \) and those in Refs. 5,6 (see also Ref. 17), it is presently unclear, whether the origin of the sign change in Refs. 5,6 is the same as the one discussed here.

The qualitative nature of the temperature dependence can be altered via a change of the couplings \( g \) and \( Z \), as follows from Fig. 5(a). We find that in general, a sign change of \( I_J \) with increasing temperature occurs when (a) the particle-like components of both Andreev states possess the same spin-polarization and (b) \( \phi \) is chosen such that the energy difference between the Andreev states is sufficiently large. These two conditions can easily be
satisfied if at least one of the Andreev states exhibits a zero-energy crossing, and \( \phi \) is chosen to be close to that crossing in the region where \( \langle S_z \rangle = 1/2 \). A zero energy crossing, however, occurs only in the grey and black regions of the \((g, Z)\)-plane shown in Fig. 2(a). Thus, in order to observe a sign change of \( I_J \) with temperature, one should select a barrier whose scattering potentials are close to the \( Z = g \) line. Note that a similar temperature dependent sign change discussed above is qualitatively different from the one reported by Ryazanov et al.\(^4\). There, the sign change arises from a transition of the junction from a 0-phase state at high temperatures to a \( \pi \)-phase state at low temperatures due to a temperature dependent coherence length. In contrast, in our case the sign change arises from a change in the population of the Andreev states, with the relative phase between the superconductors remaining unchanged.

### B. Spin Transport through Andreev States

We argued in Sec. II B that the origin of the zero total spin current lies in the fact that the spin current through the Andreev states is compensated by a spin current through the continuum states that is equal in magnitude, but opposite in sign. The question thus naturally arises if it is possible to separately measure these two contributions to the total spin current. While one could envision several experimental set-ups in which this could be achieved, for example, by using two Josephson tunneling STM tips, one on each side of the junction, we cannot provide a definite answer to this question at the moment. However, the ability to measure these contributions separately would open new venues for using the combined spin and charge degrees of freedom in such a junction. In particular, it would be possible to make use either of a spin polarized (non-zero) charge Josephson current by considering the current through the Andreev states, or of a spin Josephson current without a charge Josephson current by considering the current through the continuum states. To exemplify these possibilities, we consider in what follows the spin polarization of the Josephson current through the Andreev states. We first define a spin polarization \( P \) of the Josephson current via

\[
P = \frac{I_{AS}(0) - I_{AS}(0)}{I_{AS}(0) + I_{AS}(0)} = -\frac{I_{AS}(0) - I_{AS}(0)}{I_{J}}. \tag{45}
\]

For \( P = -1(1) \), the Josephson current through the Andreev states is completely spin polarized and thus solely carried by spin-\( \downarrow \) (spin-\( \uparrow \)) electrons. In Fig. 6 we present \( P \) as a function of \( \phi \) for \( g = 1/3, Z = 2/3 \) and \( T = 0 \) (the corresponding charge Josephson current is shown in the second panel of the second row in Fig. 3). We find that \( P \) is non-zero for all \( \phi \), and its magnitude reaches a maximum at \( \phi = \pi/2 \) (note that while \( P \to -1 \) at \( \phi \to 0 \), one has at the same time \( I_J \to 0 \)). At \( T = 0 \), \( I_{AS}(I_{AS}) \) is carried solely by the occupied particle-like branch of the \( \beta \)-state (\( \alpha \)-state), as follows immediately from Eq. (32). This is consistent with the observation in Eq. (12) that the particle-like component of the \( \alpha \) and \( \beta \) states possess the spin quantum number \( S_z = -1/2 \) (spin-\( \downarrow \)) and \( S_z = +1/2 \) (spin-\( \uparrow \)), respectively. Since \( |I_{AS}^\alpha| > |I_{AS}^\beta| \) for all \( \phi \), one finds that the Josephson current through the Andreev states is partially spin-\( \downarrow \) polarized, as shown in Fig. 6. The degree of spin-polarization varies with \( \phi \) due to the changing relative contributions of \( I_{AS}^\alpha \) and \( I_{AS}^\beta \) to \( I_J \). Finally, for \( g = 0 \), the two Andreev states are degenerate, and hence \( P = 0 \).

### C. First Order Quantum Phase Transition

Another interesting effect arising from the combination of magnetic and non-magnetic scattering strength of the barrier is the possibility to tune the Josephson junction through a first-order quantum phase transition in which the ground state of the entire system (i.e., the combined ground state of both superconductors) changes its spin polarization from \( \langle S_z \rangle = 0 \) to \( \langle S_z \rangle = 1/2 \) (assuming without loss of generality that the magnetization of the barrier points along the \( z \)-axis). This type of first order transition, which is well known from static magnetic impurities in \( s \)-wave superconductors, where it was first discussed by Sakurai\(^2\), can occur either with increasing scattering strength, \( J \), of a magnetic impurity\(^2\), or due to quantum interference effects\(^2\), its fingerprint is a zero-energy crossing of the impurity induced fermionic states inside the superconducting gap. The phase transition arises from a level crossing in the superconductor’s free energy, \( F \), resulting in a discontinuity of \( \partial F/\partial J \) at the transition; hence the first order nature of the transition (for a more detailed discussion see Ref.\(^1\)). The Josephson junction considered here provides a new possibility...
to tune the system through such a first-order phase transition by varying the phase difference between the superconductors. In Appendix B we explicitly show that the change in the spin polarization of the junction coincides with the zero energy crossing of the $\alpha$ state, and is thus solely driven by the Andreev states. In contrast, the contribution of the continuum states to the spin polarization vanishes.

As an example of such a phase transition we consider the case $Z = 1/3$ and $g = 2/3$, for which the energies of the Andreev states and the resulting Josephson current are shown in the third panel in the third row of Figs. 1(a) and (b), respectively [we indicate in the panel in Fig. 1(a) the spin quantum number of all the components of the Andreev states]. With increasing $\phi$, the $\alpha$ state crosses zero energy at $\phi^\alpha = 2\arccos \sqrt{g^2 - Z^2} \approx 0.608\pi$, such that for $\phi > \phi^\alpha$, the spin-$\uparrow$ component of the $\alpha$ state is particle-like, while its spin-$\downarrow$ component is hole-like. This transition results in a change of the ground state spin polarization from $\langle S_z \rangle = 0$ to $\langle S_z \rangle = 1/2$. Moreover, the $\alpha$ state crosses zero-energy again at $\phi^{\alpha'} = 2\pi - 2\arccos \sqrt{g^2 - Z^2} \approx 1.392\pi$, such that for $\phi > \phi^{\alpha'}$, its spin-$\uparrow$ component is hole-like, while its spin-$\downarrow$ component is particle-like. As a result, the spin ground state changes from $\langle S_z \rangle = 1/2$ back to $\langle S_z \rangle = 0$. The range of $\phi$ for which $\langle S_z \rangle = 1/2$ is indicated in the panel of Fig. 1(b) by dotted lines. In general, one finds that $\langle S_z \rangle = 1/2$ for those $\phi$ which satisfy $\cos^2(\phi/2) < g^2 - Z^2$. Consequently, as $g$ is further increased (keeping $Z$ fixed), the range of $\phi$ for which $\langle S_z \rangle = 1/2$ increases. When $g$ exceeds the upper critical value $g_c^\alpha = \sqrt{1 + Z^2}$, one finds $\langle S_z \rangle = 1/2$ for all $\phi$. In contrast, when $g$ is smaller than the lower critical value $g_c^\alpha = Z$, one has $\langle S_z \rangle = 0$ for all $\phi$. As already mentioned above, the total spin current through the junction is zero even in a state with $\langle S_z \rangle = 1/2$.

**IV. CONCLUSIONS**

In summary, we have studied the Josephson current, $I_J$, in a 1D Josephson junction consisting of two $s$-wave superconductors and a thin ($\delta$-function type) ferromagnetic barrier. To this end, we used two complementary theoretical approaches: the BTK method, and an approach starting from the quantum mechanical definition of the current operator. We discussed the general dependence of the charge Josephson current on $g$, $Z$, and the relative phase, $\phi$, between the two superconductors. Specifically, we showed that in certain regions of the $(g,Z)$-plane, $I_J$ varies continuously with $\phi$, while in other regions, and particularly around $Z = g$, $I_J$ exhibits discontinuities. We computed the critical current, $I_c$, defined as the maximum Josephson current for a given $g$ and $Z$, and we showed that it possesses two lines of non-analytic behavior in the $(g,Z)$-plane. These non-analyticities correspond to discontinuities in the first and second derivative of $I_c$ (with respect to $g$ or $Z$). We demonstrated that $I_c$ exhibits qualitatively different dependencies on the scattering strength in different parts of the $(g,Z)$-plane, which opens the interesting possibilities to increase the critical current through the junction by increasing the junction’s magnetization. This effect possesses potential applications in the fields of quantum information technology. Moreover, we showed that for certain values of $g,Z$, the Josephson current changes sign (and thus direction) with increasing temperature without a change in the relative phase between the two superconductors, i.e., without a transition between a 0 and $\pi$ state of the junction. We showed that this sign change is entirely due to a temperature-dependent change in the occupation of the Andreev states. In agreement with earlier results, we demonstrated that the continuum states do not contribute to the charge current, and that therefore the charge Josephson current is carried entirely by the Andreev states. We also showed that while the total spin Josephson current through the junction is zero, the Andreev states and the continuum states separately carry a non-zero spin current of equal magnitude but opposite sign. The possibility of measuring these contributions separately would open new venues for employing the combined spin and charge degrees of freedom in such a junction for potential applications in spin electronics and quantum information technology. Finally, we demonstrate that by changing the phase $\phi$ between the superconductors, it is possible to tune the junction through a first-order quantum phase transition in which the spin polarization of the superconductors’ ground state changes between $\langle S_z \rangle = 0$ and $\langle S_z \rangle = 1/2$.

Experimentally, the effects discussed here could be studied in junctions with magnetically doped insulating barriers based on MgO, ZnO, or TiO$_2$. In these materials one can imagine to vary $g$ independently via the substitution of magnetic dopants such as Co, Mn, etc. and/or by changing their concentration, or by applying a small magnetic field, for example, via atomic force microscopy. Moreover, $Z$ can be altered by the choice of material and the junction width. It is possible to control the barrier width of complex oxides using layer-by-layer growth techniques monitored by reflection high energy electron diffraction (RHEED) on the unit-cell level, which is much smaller than the coherence length of a typical $s$-wave superconductor. Hence, we expect that the results derived above for a $\delta$-functional barrier should be observable in experimental systems with a non-zero barrier width, $d$, as long as $d$ is much smaller than the superconducting coherence length. Note that the novel Josephson behavior described in this paper will occur in addition to the effects that are expected from the proximity induced sign change in the superconducting order parameter as a function of the ferromagnetic barrier thickness.

Finally, scattering off the barrier leads to a suppression of the superconducting order parameter near the barrier, which was not accounted for in the approach presented above. However, in $s$-wave superconductors, the length scale over which the order parameter recovers its bulk
value near scattering centers (such as a junction) is set by $1/k_F$. This length scale is in general much shorter than both the superconducting coherence length $\xi_c$ and the decay length of the Andreev bound states, $\kappa^{-1}$, with $\xi_c \leq \kappa^{-1} \lesssim 10^{-12}$, and we thus expect that the inclusion of a spatially varying order parameter does not alter the qualitative nature of our results presented above.

V. ACKNOWLEDGEMENTS

D.K.M. acknowledges financial support by the Alexander von Humboldt Foundation, the National Science Foundation under Grant No. DMR-0513415 and the U.S. Department of Energy under Award No. DE-FG02-05ER46225. B.K. acknowledges financial support by DLR (German Aerospace Center). We would like to acknowledge helpful discussions with P. Fulde, M. Sigrist, M. Kulić, F. Nogueira, I. Eremin, Y.S. Barash, M. Fogelström, P. Brydon, and D. Manske. Moreover, we are grateful to J. Michelsen, V.S. Shumeiko, and G. Wendin for useful communications.

APPENDIX A: CONTRIBUTION OF THE CONTINUUM STATES TO $I_L$ AND $I_R$

For the scattering states’ wave-function of Eq. (4) we make the ansatz

$$
\Psi_{n,j}(z) = \sum_{\delta,\epsilon = \pm} \left( u_{n,j,s,\delta,\epsilon} \right) e^{i(\delta k_F + \epsilon q)z},
$$

(A1)

with $s = L, R$ referring to the left ($z < 0$) and right ($z > 0$) hand side of the junction, respectively, with $j = \alpha, \beta$, with $q > 0$, and where $k_F$ is the Fermi momentum. The corresponding solutions of Eq. (5) are subject to the boundary conditions (9). For a given $E_q > |\Delta|$, there are eight continuum states with a positive- and a negative-energy branch for each. For energies small compared to the Fermi energy, $q$ is given by (26).

Define

$$
\cosh \gamma = \frac{E_q}{\Delta_0}
$$

(A2)

To be specific, consider the negative-energy branches with energy $-E_q$. The BdG equations imply

$$
y_{j,s,\delta,\epsilon} = e^{\delta \gamma/2} u_{j,s,\delta,\epsilon} = e^{i\phi_{\delta,\epsilon}} e^{-\delta \gamma/2} v_{j,s,\delta,\epsilon},
$$

(A3)

with $j = \alpha, \beta$ and $s = L, R$ and where we have omitted the index $n$ labeling the different states of energy $-E_q$.

With $\phi_L = 0$ and $\phi_R = -\phi$ and defining

$$
e^{i\tau_\pm} = \frac{1 + i(Z \pm g)}{\sqrt{1 + (Z \pm g)^2}}
$$

(A4)

so that

$$
-\frac{\pi}{2} < \tau_\pm < \frac{\pi}{2}
$$

(A5)

and

$$
Z = \frac{1}{2} (\tan \tau_+ + \tan \tau_-),
$$

(A6a)

$$
g = \frac{1}{2} (\tan \tau_+ - \tan \tau_-),
$$

(A6b)

we may organize the boundary conditions (9) in matrix form by writing

$$
z_j \equiv M_j y_{j,L} = M_j^T y_{j,R},
$$

(A7)

with

$$
y_{j,s} = (y_{j,s,+}, y_{j,s,+}, y_{j,s,-}, y_{j,s,-}, y_{j,s,-})
$$

(A8)

and

$$
\begin{pmatrix}
e^{-\gamma/2} & e^{i\phi/2+\gamma/2} & e^{+\gamma/2} & e^{i\phi/2+\gamma/2} & e^{-\gamma/2} \\
e^{-i\phi/2-\gamma/2} & e^{-i\phi/2-\gamma/2} & e^{-i\phi/2-\gamma/2} & e^{i\phi/2+\gamma/2} & e^{-i\phi/2-\gamma/2}
\end{pmatrix},
$$

(A9)

where the upper (lower) sign corresponds to $\alpha (\beta)$. Thus the negative-energy scattering states for a given energy $-E_q$ may be represented by $y_j$. Reinstating labels $m$ and $n$ for the different states for a given energy, we demand that for continuum-normalized orthogonal states

$$
\begin{align*}
\sum_{s=L,R} \sum_{\delta,\epsilon = \pm} y_{m,j,s,\delta,\epsilon} y_{n,j,s,\delta,\epsilon} &= z_{m,j}^T Q_j z_{n,j}, \\
&= \delta_{mn} C_\tau(E_q),
\end{align*}
$$

(A10)
with

\[ Q_j \equiv (M_j M_j^\dagger)^{-1} + (M_j M_j^\dagger)^{-1*} \quad (A11) \]

and where \( C_r(E_q) \) is real and may be chosen to depend on the energy \( E_q \). That is, finding an orthonormal basis of scattering states for a given energy boils down to diagonalizing the \( Q_j \) and using \( (A3) \) and \( (A7) \) to obtain all corresponding coefficients \( u_{n,j,s,\delta,\epsilon} \) and \( v_{n,j,s,\delta,\epsilon} \). Numerically, we find that

\[
\sum_{n(E_q)} (|u_{n,j,s,+,\pm}|^2 - |u_{n,j,s,-,\mp}|^2) = 0, \quad (A12a)
\]

\[ u_{n,j,s,+,+}^* + u_{n,j,s,+,+} - u_{n,j,s,+,+}^* - u_{n,j,s,+,+} = 0, \quad (A12b) \]

and the same for the \( v_{n,j,s,\delta,\epsilon} \). Moreover, we numerically obtain

\[
\sum_{n(E_q)} \left[ u_{n,j,s,+,+}^* - u_{n,j,s,+,+} - u_{n,j,s,+,+}^* + u_{n,j,s,+,+} \right] = d_j A_r(E_q) + i c_s A_i(E_q), \quad (A13)
\]

and the same for the \( v_{n,j,s,\delta,\epsilon} \), with \( d_{\alpha,\beta} = \pm 1 \), \( c_{L,R} = \pm 1 \), and where \( A_r(E_q) \) and \( A_i(E_q) \) are dimensionless and generally nonzero real coefficient functions.

It is straightforward then to show that

\[
\sum_{n(E_q)} \text{Im} \left( u_{n,\alpha}^* \partial_z u_{n,\alpha} \pm v_{n,\alpha}^* \partial_z v_{n,\alpha} \right) \\
\quad \pm u_{n,\beta}^* \partial_z u_{n,\beta} + v_{n,\beta}^* \partial_z v_{n,\beta} \\
= 8 k A_i(E_q) \sin 2 q |z|, \quad (A14)
\]

leading immediately to the results \( (27) \).

**APPENDIX B: SPIN GROUND STATE OF THE JUNCTION AND FIRST ORDER PHASE TRANSITION**

The total spin of the system receives contributions from both the Andreev bound states and the scattering states. Define the spin density by

\[
\hat{\rho}_S(z) = \left. \frac{\hbar}{2} \left[ \hat{\rho}_s(z, z') - \hat{\rho}_n(z, z') \right] \right|_{z' = z}, \quad (B1)
\]

with \( \hat{\rho}_n(z, z') \) from \( (15) \). It is then straightforward to show that

\[
\rho_S(z) \equiv \langle \hat{\rho}_S(z) \rangle \\
= \frac{\hbar}{2} \sum_{n} \left\{ [\rho_{n,u,\alpha}(z) + \rho_{n,v,\alpha}(z)] \tanh \frac{\beta E_{n,\alpha}}{2} \right. \\
- \left. [\rho_{n,v,\beta}(z) + \rho_{n,u,\beta}(z)] \tanh \frac{\beta E_{n,\beta}}{2} \right\}, \quad (B2)
\]

where

\[
\rho_{n,f,j}(z) \equiv \frac{1}{2} f_{n,j}^*(z) f_{n,j}(z), \quad (B3)
\]

with \( f = u, v \) and \( j = \alpha, \beta \).

Note that for any given energy, there exist pairs of continuum states that differ only in the spin quantum numbers of their hole-like and particle-like branches. This result, combined with the normalization of the continuum states then yields that their contribution to the spin of the junction vanishes. Using next the normalization of the bound states

\[
\int_{-\infty}^{+\infty} dz |u_{0,j}^*(z) u_{0,j}(z) + v_{0,j}^*(z) v_{0,j}(z)| = 1, \quad (B4)
\]

with \( j = \alpha, \beta \), we obtain that the spin of the system is solely determined by the Andreev bound states and given by

\[
\langle S_z \rangle = \int_{-\infty}^{+\infty} dz \rho_S^{\text{AS}}(z) \\
= - \frac{\hbar}{4} \left( \tanh \frac{\beta E_{\alpha}}{2} - \tanh \frac{\beta E_{\beta}}{2} \right). \quad (B5)
\]

Since our conventions are such that always \( E_{\beta} > 0 \), but the sign of \( E_{\alpha} \) can vary, we obtain for \( T = 0 \)

\[
\langle S_z \rangle = \begin{cases} 
0 & E_{\alpha} > 0, \\
\hbar/2 & E_{\alpha} < 0,
\end{cases} \quad (B6)
\]

signaling a quantum phase transition caused by the zero-energy crossing of one of the Andreev bound states.

---

1. S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnar, M.L. Roukes, A.Y. Chtchelkanova, and D.M. Treger , Science 294, 1488 (2001), and references therein; I. Zutic, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004)

2. For recent reviews see S. Kashiwaya and Y. Tanaka, Rep. Prog. Phys. 63, 1641 (2000); A.A. Golubov, M.Yu. Kupriyanov, and E. Il’ichev, Rev. Mod. Phys. 76, 411 (2004); and references therein.

3. L.N. Bulaevskii, V.V. Kuzii, and A.A. Sobyanin, Zh. Eksp. Teor. Fiz. Pisma Red. 25, 314 (1977) [JETP Lett. 25, 290 (1977)]; A.V. Andreev, A.I. Buzdin, and R.M. Osgood,
Phys. Rev. B 43, 10124 (1991); A.I. Buzdin, B. Vujicic, and M.Yu. Kupriyanov, Zh. Eksp. Teor. Fiz. 101, 231 (1992) [Sov. Phys. JETP 74, 124 (1992)].

V.V. Ryazanov, V.A. Oboznov, A.Yu. Rusanov, A.V. Veretennikov, A.A. Golubov, and J. Aarts, Phys. Rev. Lett. 86, 2427 (2001).

M. Fogelström, Phys. Rev. B 62, 11812 (2000); M. Andersson, J.C. Cuevas, and M. Fogelström, Physica C 367, 117 (2002).

Y.S. Barash and I.V. Bobkova, Phys. Rev. B 65, 144502 (2002).

L.B. Ioffe, V.B. Geshkenbein, M.V. Feigel’man, A.L. Fauchère, and G. Blatter, Nature 398, 679 (1999).

G.E. Blonder, M. Tinkham, and T.M. Klapwijk, Phys. Rev. B 25, 4515 (1982).

A.F. Andreev, Phys. JETP 19, 1228 (1964).

R. Zikic, L. Dobrosavljevic-Grujic, and Z. Radovic, Phys. Rev. B 59, 14644 (1999).

R.A. Riedel and P.F. Bagwell, Phys. Rev. B 57, 6084 (1998).

A.M. Zagoskin, Quantum Theory of Many-Body Systems (Springer, New York 1998).

A. Furusaki, Superlattices Microstruct. 25, 809 (1999).

H.-J. Kwon, K. Sengupta, and V.M. Yakovenko, Eur. Phys. J. B 37, 349 (2003).

P.G. de Gennes, Superconductivity of Metals and Alloys (Addison-Wesley, New York, 1989).

A.V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. 78, 373 (2006).

In Ref. [5] a splitting of the Andreev states is found to occur for $\phi \neq 0$ only. The reason for this discrepancy with the results discussed above and those in Refs. [6,10] lies in the particular form of the $S$-matrix chosen in Ref. [5].

See Sec. 4.5.3 in Ref. [12].

J. Michelsen, V.S. Shumeiko, and G. Wendin, Phys. Rev. B 77, 184506 (2008).

Note that our $Z$ is, by definition, half the $Z$ of Ref. [14].

Y. Lu, Acta Phys. Sin. 21, 75 (1965); H. Shiba, Prog. Theor. Phys. 40, 435 (1968).

B. Kastening, D.K. Morr, D. Manske, and K. Bennemann, Phys. Rev. Lett. 96, 047009 (2006).

A. Sakurai, Prog. Theor. Phys. 44, 1472 (1970).

D.K. Morr and N.A. Stavropoulos, Phys. Rev. B 67, 020502(R) (2003).

D.K. Morr and J. Yoon, Phys. Rev. B 73, 224511 (2006).

B.E. Kane, Nature (London) 393, 133 (1998).

P. Schlottmann, Phys. Rev. B 13, 1 (1976); M.I. Salkola, A.V. Balatsky, and J.R. Schrieffer, Phys. Rev. B 55, 12648 (1997); D.K. Morr and J. Yoon, Phys. Rev. B 73, 224511 (2006).