Enhanced spin-triplet pairing in magnetic junctions with s-wave superconductors

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A common path to superconducting spintronics, Majorana fermions, and topologically-protected quantum computing relies on spin-triplet superconductivity. While naturally occurring spin-triplet pairing is elusive and even common spin-triplet candidates, such as Sr₂RuO₄, support alternative explanations, proximity effects in heterostructures can overcome these limitations. It is expected that robust spin-triplet superconductivity in magnetic junctions should rely on highly spin-polarized magnets or complex magnetic multilayers. Instead, we predict that the interplay of interfacial spin-orbit coupling and the barrier strength in simple magnetic junctions, with only a small spin polarization and s-wave superconductors, can lead to nearly complete spin-triplet superconducting proximity effects. This peculiar behavior arises from an effective perfect transparency: interfacial spin-orbit coupling counteracts the native potential barrier for states of a given spin and wave vector. We show that the enhanced spin-triplet regime is characterized by a huge increase in conductance magnetoanisotropy, orders of magnitude larger than in the normal state.

Realizing equal-spin triplet superconductivity provides an important platform for implementing superconducting spintronics and topologically-protected Majorana bound states (MBS) [1–7]. While naturally occurring triplet pairing remains elusive, transforming materials through proximity effects [8] offers a promising path to tailor the desired superconducting pairing [9–13].

For superconducting spintronics equal-spin triplet supports pure spin currents and the coexistence of superconductivity and ferromagnetism through long-range superconducting proximity effects in ferromagnet/superconductor (F/S) junctions [12,14]. Such junctions typically rely on multiple ferromagnetic and superconducting regions [12,13,15,17], complex ferromagnets with spiral magnetization [18], or complete spin polarization in half-metallic ferromagnets [19–21].

With alternative paths towards spin-triplet pairing, where interfacial spin-orbit coupling (SOC) could relax the requirement of a complex magnetic structure, it is expected that both a strong spin polarization and strong SOC are needed [22,23]. However, we reveal that for nearly complete spin-triplet proximity-induced superconductivity even weakly spin-polarized ferromagnet and smaller SOC could be desirable. Our findings could complement the paths towards MBS where proximity-induced spin-triplet pairing is sought through strong SOC and half-metallic ferromagnets [11,26,28].

A microscopic understanding of a superconducting proximity effect is obtained from the process of Andreev reflection (AR) at interfaces with superconductors where an electron is reflected backwards and converted into a hole with opposite charge and spin. This implies the doubling of the normal state conductance [29] since two electrons are transferred across the interface into the S region where they form a spin-singlet Cooper pair. In contrast to this conventional AR, a spin-active interface with interfacial spin-flip scattering also yields AR with an equal spin of electrons and holes [30], responsible for a spin-triplet Cooper pair.

We consider F/S junction, depicted in Fig. 1, having a flat interface (I) at z = 0 with potential and Rashba spin-orbit scattering (SOC). M is the magnetization and the current flows normal to I. (b) Schematic band structure in each region. Spin are denoted by arrows: In the F region red (blue) for parallel (antiparallel) to M; with interfacial SOC, spins are parallel to the interface and ⊥ to the in-plane component of the momentum, k∥. Excitation picture in the S region, the dashed line shows the normal state dispersion.

We consider F/S junction, depicted in Fig. 1, having a flat interface (I) at z = 0 with potential and Rashba SOC scattering [31]. We generalize the Blonder-Tinkham-Klapwijk formalism [29,32,33] to solve Bogoliubov-de Gennes equation for quasiparticle states Ψ(r) with energy E [34].

\[
\begin{pmatrix}
\hat{H}_e & \Delta \Theta(z)I_{2 \times 2} \\
\Delta^* \Theta(z)I_{2 \times 2} & \hat{H}_h
\end{pmatrix}
\]

\[
\Psi(r) = E \Psi(r),
\]

where the single-particle Hamiltonian for electrons is
\[ \hat{H}_0 = -(\hbar^2/2)\nabla [1/m(z)] \nabla - \mu(z) - (\Delta_{xc}/2)\Theta(-z) \mathbf{m} \cdot \mathbf{\tilde{\sigma}} + [V_0 d + \alpha(k_F\mathbf{\tilde{\sigma}} - k_z\mathbf{\tilde{\sigma}_y})]d(z) \] for holes \( \hat{H}_h = -\mathbf{\tilde{\sigma}_y} \hat{H}_e \mathbf{\tilde{\sigma}_y} \). They contain the effective mass \( m(z) \), the chemical potential \( \mu(z) \), and the exchange spin splitting \( \Delta_{xc} \). Magnetization, \( \mathbf{M} \), has orientation \( \mathbf{m} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \). \( \mathbf{\tilde{\sigma}} \) are Pauli matrices, and \( k \) is wave vector. The interfacial scattering is modeled by delta-like potential barrier with effective height \( V_0 \) and width \( d \) and the Rashba SOC with strength \( \alpha \), due to structure inversion asymmetry [31]. The s-wave superconductor is described by the constant pair potential \( \Delta \).

Since the in-plane wave vector \( k_\parallel \) is conserved, the scattering states for incident spin \( \sigma \) electron are given by \( \Psi_\sigma (r) = e^{ik_\parallel r} \psi_\sigma (z) \) in a four-component basis [30], where the “bar” symbol denotes the spin-flip contribution

\[
\psi_\sigma (z) = \begin{cases} 
\chi_\sigma e^{ik_z z} + \alpha_\sigma \chi_{\sigma} e^{-ik_z z} + \beta_\sigma \chi_{\sigma} e^{-ik_z z} + \bar{\alpha}_\sigma \chi_{\sigma} e^{ik_z z} + \bar{\beta}_\sigma \chi_{\sigma} e^{ik_z z} + \chi_{\sigma} e^{-ik_z z} \quad & \text{for } z < 0, \\
\chi_\sigma e^{ik_z z} + \bar{\chi}_\sigma e^{-ik_z z} + \bar{\alpha}_\sigma \chi_{\sigma} e^{ik_z z} + \bar{\beta}_\sigma \chi_{\sigma} e^{ik_z z} + \chi_{\sigma} e^{-ik_z z} + \bar{\chi}_\sigma e^{ik_z z} \quad & \text{for } z > 0.
\end{cases}
\]

In the F region, the eigenspinors for electrons and holes are \( \chi_\sigma^e = (\sigma, 0)^T \) and \( \chi_\sigma^h = (0, \sigma)^T \) with

\[
\chi_\sigma = (1/\sqrt{2}) (\sigma \sqrt{1+ \sigma \cos \theta} e^{-i\phi}, \sqrt{1-\sigma \cos \theta})^T, \tag{3}
\]

where \( \sigma = 1(-1) \) refer to spin parallel (antiparallel) to \( \mathbf{M} \) and the z-components of the wave vector are \( k_\sigma^e(h) = \sqrt{k_F^2 + (2m_F/\hbar^2)[(-E + \sigma \Delta_{xc}/2) - k_\parallel^2]} \), with a spin-averaged Fermi wave vector, \( k_F [35] \). In the S region, coherence factors, \( u, v, \) satisfy \( u^2 = 1 - v^2 = (1 + \sqrt{E^2 - \Delta^2}/E)/2 \), while the z-components of the wave vector are \( q_\sigma^{e(h)} = \sqrt{q_F^2 + (2m_S/\hbar^2)\sqrt{E^2 - \Delta^2 - k_F^2}} \), with \( q_F \) the Fermi wave vector. Similar to Snell’s law [35], for a large \( k_\parallel \) these z-components can become imaginary representing evanescent states which carry no net current.

From the charge current conservation, we can express zero-temperature conductance at applied bias, \( V \),

\[
G(V) = \sum_\sigma \int \frac{dk_\parallel}{2\pi k_F^2} \left[ 1 + R_\sigma^e(-eV) - R_\sigma^e(eV) \right], \tag{4}
\]

normalized by the Sharvin conductance \( G_{Sh} = e^2k_F^2A/(2\pi\hbar) [31] \), where \( A \) is the interfacial area. Only the probability amplitudes from the F region are needed, for Andreev \( R_\sigma^e = \text{Re}[\langle k_\sigma^e(k_\sigma^h)\rangle \bar{a}_\sigma^e] + \langle k_\sigma^h(k_\sigma^e)\rangle \bar{a}_\sigma^h \rangle \) and specular reflection \( R_\sigma^s = \text{Re}[\langle \bar{b}_\sigma^e \rangle + \langle k_\sigma^h \rangle \bar{b}_\sigma^h \rangle \langle \bar{b}_\sigma^e \rangle \].

We focus on the zero-bias conductance, \( G(0) \), where there is no quasiparticle transmission and, from the probability conservation [30] [34], can be expressed using AR such that in Eq. (4) the integration kernel is \( 2|R_\sigma^e(0)| \). The total conductance can be decomposed into four processes: conventional and spin-flip AR for spin-up (spin-down) \( \uparrow(\downarrow) \) incident electron, corresponding, respectively, to the spin-singlet and spin-triplet superconducting correlations at the interface. It is convenient to introduce spin polarization

\[
P = \Delta_{xc}/2\mu_F, \quad \text{and dimensionless parameters for barrier strength } Z = V_0d/\sqrt{m_F\mu_S/\hbar^2} \] and Rashba SOC \( \lambda = 2\alpha\sqrt{m_F\mu_S/\hbar^2} \). As we present trends for a large parameter space, unless otherwise specified, we will consider the case for \( m_F = m_S = m \) and \( k_F = q_F \).

In Figs. (a) and (b) we show the conductance ratio between the spin-flip and conventional AR, \( G_{AR}/G_{AR} \), our proxy for singlet and triplet interfacial pairing, as

\[ \text{FIG. 2. The conductance ratio between the spin-flip and conventional Andreev reflection as a function of barrier potential } Z \text{ and Rashba SOC strength } \lambda \text{ for spin polarization (a) } P = 0.2, \text{ (b) } P = 0.7 \text{ (b) with in-plane } \mathbf{M} \text{. The insets: out-of-plane } \mathbf{M}. \text{ (c) The total conductance as a function } Z \text{ and } \lambda \text{ for in-plane and out-of-plane (inset) } \mathbf{M} \text{ with } P = 0.7 \text{ and (d) its contributions from different processes, solid (dashed) arrows: incoming electrons (reflected holes), violet arrows: spin parallel (up) and antiparallel (down) to } \mathbf{M}. \]
function of the barrier strength and SOC. Remarkably, $G_{AR}/G_{AR} \gg 1$, even for a small spin polarization, $P = 0.2$, a nearly complete triplet pairing is possible, $> 90\%$ (96\%) for in-plane (out-of-plane) $M$. A striking enhancement of the triplet contribution is feasible for a wide range of barrier strengths, accompanied with a suitable SOC. As shown in Fig. 2 the triangle region of this dominance increases considerably for a larger $P = 0.7$ and it is approximately delimited with lines T1 and T2,

$$\text{T1: } \lambda = 2Z/\sqrt{1-P}, \quad \text{T2: } \lambda = 2Z,$$  

excluding the half-metals, $P = 1$. Our findings suggest that even simple s-wave junctions with only one magnetic region of a small $P$ and interfacial SOC can support robust spin-triplet currents. These trends are also preserved for an out-of-plane $M$ [Figs. 2(a), (b) inset].

To explore this peculiar behavior and the origin of the triangle region with enhanced triplet pairing, in Fig. 2(c) we consider the total $G$ for $P = 0.7$ showing G1 and G2 which denote local maxima in $G$. This high-$G$ region, delimited by G1,2, shows a similarity, but not complete overlap with the enhanced triplet region. Such a relatively high-subgap overlap with the enhanced triplet region. Such a relatively high-subgap $G$ is in contrast to the common expectation that for a strong barrier ($Z > 1$) normal metal/S (N/S) junction would resemble a tunnel contact with a small interfacial transparency $T = 1/(1 + Z^2) \ll 1$.

For highly-polarized F region, $P = 0.7$, conventional AR is strongly suppressed. $G$ for such F/S junction should be even lower than for the N/S counterpart with the same large $Z$. A striking discrepancy with these expectations comes from the neglect of the SOC and unconventional AR. Even for a strongly-polarized F region, high $G$ is compatible with large $Z$ and strong SOC. In the opposite regime of no SOC ($\lambda \rightarrow 0$), the triplet component will vanish [Fig. 2(b)], but there is still a region with only small SOC, $\lambda \sim 0.5$, and a large triplet pairing.

In Fig. 2(d) we resolve $G$ for four AR processes, responsible for proximity effects, to examine the evolution of relative contribution of singlet and triplet pairing with interfacial parameters. While local maxima of $G$ along G1 arise from singlet contributions $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ and a tiny minority spin-triplet pairing $|\uparrow\downarrow\rangle$, G2 occurs from majority spin-triplet pairing $|\uparrow\uparrow\rangle$. This opens a path to tailor junctions parameters which would selectively remove the singlet contribution and ensure that transport properties are dominated by (majority) spin-triplet pairing.

The origin of the dominant triplet contribution bounded by the T1 and T2 can be traced to the normal-state properties in the corresponding F/N junction by taking $\Delta = 0$. This is further shown in Supplemental Material (See Ref. 37). At the interface (barrier region), the dispersion relation is $E = \hbar^2 k^2 / 2m - \mu + V_0 + \alpha k^2/\xi$. The energy band is split due to SOC [see Fig. 1(b)] and shifted up by the barrier potential (assuming $V_0 > 0$, but $V_0 < 0$ gives the same results). A spinor of an incident electron with $k_\parallel$ can be decomposed into barrier eigispinors, $|\chi_\parallel⟩ = (χ_+ |χ_\uparrow⟩ + (χ_− |χ_\uparrow⟩ + (χ_− |χ_\downarrow⟩ + (χ_+ |χ_\downarrow⟩),$ $χ_± = (1/\sqrt{2})(± e^{iγ}, 1)^T$, with helicity $±1$, where $γ = \tan^{-1}(k_x/k_y)$. We recognize that these two helicities for outer/inner band have inequivalent effective barriers.

$$Z^+_\text{eff} = 2Z + \lambda k_\parallel/k_F, \quad Z^-\text{eff} = 2Z - \lambda k_\parallel/k_F.$$  

Since $Z, \lambda k_\parallel/k_F \geq 0$, for positive helicity the barrier is enhanced, $Z^+\text{eff} \geq Z$. However, for negative helicity, at $Z = \lambda k_\parallel/2k_F$, $Z^-\text{eff}$ becomes effectively completely transparent and can give a dramatically increased $G$.

The effect of this selective barrier transparency and the resulting open channels for a given $k_\parallel$ and $\sigma$, can be clearly seen in Fig. 3(a). The dominant contribution to $k_\parallel$-resolved conductance comes from the open channels located on the circle of radius $k_\parallel = (2Z/\lambda)k_F$. To maximize $G$ for the F/N junction, we can identify several contributing factors. (i) The number of open channels, $N(Z, \lambda)$, should be large. Located on the circle of radius $k_\parallel = (2Z/\lambda)k_F$, their number increases with the perimeter, $N(Z, \lambda) \propto k_\parallel$. (ii) The open channels should exclude evanescent waves for large $k_\parallel$, not contributing to $G$. This range of $k_\parallel$ follows from the Snell’s law, for incident $\downarrow$ (↑) electron: $k_\parallel \leq k_\downarrow (k_\parallel \leq k_\uparrow)$. In the extreme cases, $k_\parallel \equiv (2Z/\lambda)k_F = k_\downarrow$ and $k_\parallel \equiv (2Z/\lambda)k_F = k_\uparrow$, we recover exactly T1 and T2 from Eq. 5. (iii) With spin-momentum locking of interfacial helical states, an enhanced F/N transmission depends also on the spin matching with the incident spin, in addition to the usual wave vector matching.

From these considerations we can understand why, instead of having full circles of open channels, in Fig. 3 we see crescent-like shapes with completely open channels only for both spin and $k_\parallel$ matching. This picture can be verified from a simple, but accurate, analytical description of F/N transmission using selective junction transparency. The transmission decomposed into spin-
conserving and spin-flip part, \( T_\sigma = T_{\sigma\sigma} + T_{\sigma-\sigma} \), yields

\[
T_{\sigma\sigma} \propto [1 - \sigma \cos(\gamma + \phi)]^2, \quad T_{\sigma-\sigma} \propto \sin^2(\gamma + \phi),
\]

confirming \( \pi/2 \) and \( \pi \) symmetry from Fig. 3(a), respectively. Here previously given angles \( \phi \) and \( \gamma \) describe the in-plane orientation of \( \mathbf{M} \) and the barrier eigenspinor.

This analysis applies also to F/S junctions, revealing in Fig. 3(b) a similar angular dependence of \( k_\parallel \)-resolved \( G \) due to conventional and spin-flip AR. Some quantitative modifications from the F/N case, can be understood already without SOC due to a different condition for a perfect F/S transparency at normal incidence were all the wave vectors can be unequal \( k_1 \neq k_2 \), [40]. For F/S junctions the condition for open channels again requires \( k_\parallel \leq k_F \) which excludes the evanescent states in AR. The only subtlety is \( G_{\parallel\parallel} \) from spin-flip AR where we could expect that \( k_F < k_\parallel \leq k_t \) is also possible. However, such a large \( k_t \) would result in a strongly decaying wave vector in the S region [recall the expression for \( q^e(h) \) with its inverse smaller than the BCS coherence length and thus render ineffective any contribution for spin-majority pairing with \( k_\parallel \leq k_F \). This provides a guidance for a choice of junction parameters giving an enhanced spin-triplet paring between the lines T1 and T2 in Eq. (5), even for previously unexpected regimes with only a small \( P \).

In addition to directly measuring the spin structure of \( G \) or spin current, an experimental test of our predictions for enhanced spin-triplet pairing could be realized through probing magnetic anisotropy of conductance in F/S junctions, referred to as magnetic anisotropic Andreev reflection (MAAR) [34]. MAAR and it is better studied normal-state analog, tunneling anisotropic magnetoresistance (TAMR) [38, 39], can be expressed for out-of-plane rotation of \( \mathbf{M} \) [Fig. 1(a)] as [34]

\[
\text{TAMR}(\theta), \text{MAAR}(\theta) = [G(0) - G(\theta)]/G(\theta),
\]

where angle \( \theta \) is between \( \mathbf{M} \) and the interface normal. From the evolution of MAAR, shown in Figs. 4(a) and (b) for \( P = 0.2 \) and \( P = 0.7 \), we see that it closely follows the trends of the enhanced majority spin-triplet pairing from Figs. 2(a) and (b). It is this spin-triplet component that is responsible for a large increase of MAAR compared to TAMR, in the normal state, Figs. 4(a), (c), (d). Even for \( P = 0.2 \) the resulting increase can reach an order of magnitude and become much larger for \( P = 0.7 \) where it was recently measured in all-epitaxial Fe/MgO/V junctions [40] to exceed 1000! Rather than change MAAR to TAMR by increasing the temperature above the critical temperature (for vanadium \( \sim 4 \) K), experimentally it is more convenient to reach the normal state by increasing the bias, \( V > \Delta \) at a fixed temperature [40].

Such Fe/MgO/V junctions simplify the analysis of the observed magnetic anisotropy since they have two stable zero-field \( (B = 0) \) states with mutually orthogonal \( \mathbf{M}: \) in-plane and out-of-plane [40, 41]. This removes common complications in other F/S junction by decoupling the influence of the \( B \)-field required for rotating \( \mathbf{M} \) which could alter the magnitude of magnetic anisotropy and create spurious effects from vortices. Junction parameters \( Z = 0.83 \) (\( V_0 = 0.3 \) eV, \( d=17 \) nm), \( \lambda = 0.79 \), 1.44 (\( \alpha = 5.5 \) eVÅ), describing two measured Fe/MgO/V samples with MAAR of 10-20 \% (TAMR only \( \sim 0.01 \%) \) [40] are marked in Fig. 4(b). This small SOC, \( \lambda \sim 1 \), smaller than in Fe/GaAs/Au TAMR studies [38], is already sufficient for a dominant triplet pairing.

While we employ a simple approach which naturally suggests a number of generalizations, from inclusion of the self-consistent pair potential, finite \( B \)-fields, study of critical temperature, or more complex barrier description [42, 47], its transparency already reveals several important trends and can support peculiar experimental observation of a giant MAAR [40]. Our implications for enhanced triplet pairing and MAAR detection could also be relevant for two-dimensional materials, as supported by the work in Refs. [48, 49]. Another extension of this work could include the role of magnetic textures which themselves result in synthetic spin-orbit coupling and could be used to control Majorana bound states [50, 57].

Similar to the advances in realizing large magnetoresistive effect, not by employing complex ferromagnets with nearly complete spin polarization, but rather choosing a suitable nonmagnetic barrier [58, 59], our findings suggest what could constitute a suitable interface to realize enhanced spin-triplet proximity. In particular, to further enhance such triplet pairing with only a very small spin polarization of a ferromagnet, a challenge would be to

FIG. 4. Amplitude of out-of-plane magnetoanistotropic Andreev reflection (MAAR) as a function of interface parameters \( Z \) and \( \lambda \) for (a) \( P = 0.2 \) and (b) \( P = 0.7 \). (c) The corresponding tunneling anisotropic magnetoresistance (TAMR) when superconducting gap vanishes for \( P = 0.2 \). (d) A comparison between out-of-plane TAMR (yellow) and MAAR (blue), \( P = 0.2 \), \( Z = 5 \) and \( \lambda = 10.2 \).
design interfaces which could simultaneously provide a large spin-orbit coupling and large potential barrier.

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