Electrical and Thermal Transport in Antiferromagnet–Superconductor Junctions

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We demonstrate that antiferromagnet–superconductor (AF–S) junctions show qualitatively different transport properties than normal metal–superconductor (N–S) and ferromagnet–superconductor (F–S) junctions. We attribute these transport features to a new scattering process that occurs at the interface between the AF and S layers. This process is associated with the interplay between the AF exchange interaction and the Rashba spin-orbit coupling in the S layer, leading to anisotropic SHE scattering that affects the transport properties in AF–S junctions.

Introduction. Heterostructures composed of superconductors and nonsuperconducting materials exhibit technologically relevant quantum phenomena. Examples include superconducting qubits, microwave resonators, single-photon detectors, and AC Josephson junction lasers. Superconducting heterostructures also form the basis for experimental methods such as point contact spectroscopy, scanning tunneling spectroscopy, and scanning tunneling microscopy, allowing for the determination of the superconducting gap and the investigation of the phase diagram in unconventional superconductors.

The simplest superconducting heterostructure is a normal metal (N)–superconductor (S) junction. The low bias transport at low temperature is dominated by Andreev reflection (AR) in conventional AR, where an incident electron is retroreflected as a hole of the opposite spin, and a Cooper pair is transmitted into the S layer. The Cooper pair carries a charge of 2e and zero heat, AR enhances electrical conductance and suppresses thermal conductance. In a Josephson junction (S–N–S) [28], AR can occur repeatedly, resulting in Andreev bound states that carry a supercurrent across the junction. Josephson junctions enable technologies such as electrical and thermal interferometers.

The spin dependence of AR at superconducting interfaces causes the transport properties to change drastically when ferromagnetic layers are introduced, leading to additional scattering processes different from those in traditional superconducting junctions. In Josephson junctions, these new scattering processes create low-energy bound states that lead to anomalous phase shifts and atomic-scale 0–π transitions. The existence of Josephson supercurrents in S–AF–S junctions has been experimentally reported, and other theoretical predictions have yet to be explored.

Model. We consider a collinear and two-sublattice AF metal on a cubic lattice attached to a conventional s-wave superconductor. The AF and S are both semi-infinite and occupy the regions z < 0 and z > 0, respectively. To investigate the electrical and thermal transport, we use the Blonder-Tinkham-Klapwijk (BTK) scattering formalism, where the conductances are determined by the reflection coefficients of the scattering matrix. We obtain the reflection coefficients by solving the Bogoliubov–de Gennes (BdG) equation.

The BdG Hamiltonian of an AF–S junction in the con-
where \( V \) is the interfacial barrier potential \( H \), the chemical potential is \( \mu = \frac{e\phi}{\hbar c} \), and \( \tau \) the effective mass of the charge carriers, \( k_0 \) is the wavevector at which \( \gamma_{k_0} = 0 \), and \( \hbar \) is the reduced Planck constant. The chemical potential is \( \mu = \mu_{AF} \Theta(-z) + \mu_S \Theta(z) \), where \( \Theta(\cdot) \) is the Heaviside step function.

The \( s-d \) exchange interaction between localized antiferromagnetic moments and itinerant spins reads \( H_{AF} = J \tau_+ \otimes \sigma_z \otimes (\mathbf{n} \cdot \mathbf{s}) \), where \( J = J_0 \Theta(-z) \) denotes the \( s-d \) interaction strength and \( \mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \) is the Ncl vector direction in spherical coordinates.

The interfacial potential is described by, \( H_I = V \tau_z \otimes \sigma_0 \otimes s_0 + \lambda_R \tau_+ \otimes \sigma_z \otimes [(\mathbf{s} \times \mathbf{q}) \cdot \hat{z}] \), where \( V = V_0 \delta(z) \) is the strength of spin-independent potential barrier and \( \lambda_R = \lambda_0 \delta(z) \) is the strength of Rashba SOC (RSOC) [71] due to the inversion symmetry breaking in the \( z \) direction. These two terms permit spin-conserving and spin-flipped reflection processes, respectively.

Finally, we model the S layer using a mean-field BCS Hamiltonian, \( H_S = \Delta(T) \tau_+ \otimes (\sigma_0 \otimes i s_y) + h.c. \), where \( \Delta(T) = \Delta_0 \tanh \left( \frac{1.74 \sqrt{(T_c/T) - 1}}{2} \right) \Theta(z) \) is an interpolation formula for the temperature-dependent gap of an \( s \)-wave superconductor with a critical temperature \( T_c \) [72, 73].

To determine the reflection coefficients, we solve the BdG eigenvalue problem, \( H \psi = E \psi \), where \( \psi \) is the BdG eigenvector and \( E \) is its eigenvalue, for more details see the Supplemental Material [74]. In our setup, the \( x \) and \( y \) directions are translationally invariant. Hence, the eigenvector takes the form \( \psi = e^{i q_{\parallel} \cdot r} e^{i q_{\perp} \cdot z} \), where \( q_{\parallel} = (q_x, q_y, 0) \) is the conserved component of the wavevector parallel to the interface and \( q_{\perp} \) is the wavevector component normal to the interface. The spinor \( \chi \) is expressed in the following basis [74]:

\[
\chi = (A e^{i \phi}, A e^{-i \phi}, B e^{i \phi}, B e^{-i \phi}, A h e^{i \phi}, A h e^{-i \phi}, B h e^{i \phi}, B h e^{-i \phi})
\]

Here, \( A (B), \uparrow (\downarrow) \), and \( e (h) \) refer to the sublattice, spin, and charge degrees of freedom, respectively. Upon substitution of the eigenvector into Eq. (6) for \( z < 0 \), we find the wavevectors \( q_{\pm} = q_{c(h)} \) in the AF layer,

\[
q_{\pm} = \sqrt{k_0^2 - q_0^2} \pm \frac{2m}{\hbar^2} \sqrt{(E + \mu_{AF})^2 - J^2}, \quad q_{c(h)} = \sqrt{k_0^2 - q_0^2} \pm \frac{2m}{\hbar^2} \sqrt{(E - \mu_{AF})^2 - J^2}.
\]

In Fig. 1, we plot the dispersion relations of the AF layer given in Eq. (8) and identify the possible scattering processes. In contrast to an N(F)–S junction, an AF–S junction permits both specular AR and retro normal reflection (NR) [56–58].
where $A$ is the interfacial cross section, and we introduce
\begin{equation}
\chi^\pm_{n,m} = \int_0^\infty dE d^2q_{\parallel} \frac{(E - eU)^n (1 - R_e \pm R_h)}{4(k_B T)^m \cosh^2 \frac{E - eV}{2k_B T}},
\end{equation}
where $n, m = \{0, 1, 2\}$. The total reflection probabilities for electrons ($e$) and holes ($h$) are
\begin{equation}
R_{e(h)} = \sum_s \left( R^{+}_{e(h),s} + R^{-}_{e(h),s} \right).
\end{equation}
Here, $R^{\pm}_{i,s}$ is the reflection probability for particles with wavevector $q^{\pm}_i$, where $i = e, h$ and $s = \uparrow, \downarrow$ [74]. AR results in a net charge transfer of $2e$, but zero heat transfer [76–78] across the interface; thus, AR increases the electrical conductance and decreases the thermal conductance. In the following, we focus on the electrical ($G_C$) and thermal ($L_Q$) conductance of the junction.

**Numerical parameters.** Before presenting our numerical results, it is necessary to introduce our numerical dimensionless parameters: the spin-independent barrier strength $Z = V_0 m/2h^2 q_s$, the Rashba spin strength $J = 2A m/2h^2 q_s$, the exchange strength $J_0/\mu$, and the dimensionless temperature $T/T_c$. Here $q^2 = k^2_0 + q^2_F$, where $q^2_F = 2m\mu/h^2$. For simplicity, we set $\mu_{AF} = \mu_{SB} = \mu$ and normalize the electrical and thermal conductance with respect to the corresponding Sharvin conductance [8]: $G_C = G_{C}/G_{C}^{Sh}$ and $L_Q = L_{Q}/L_{Q}^{Sh}$. The Sharvin electrical (thermal) conductance is the electrical (thermal) conductance evaluated in the limit $\Delta_0 = J_0 = Z = 0$, i.e., the response functions of a normal metal with perfect transmission: $G_{C}^{Sh} = \pi^2 q^2 A/4\pi^2 \hbar$ and $L_{Q}^{Sh} = A_0 T_c q^2_F/12h$.

In our calculations, we estimate the effective mass to be $\hbar^2/2m = 0.5 eV \text{nm}^2$ based on a tight-binding model with typical material parameters [48, 69, 70]. Furthermore, the superconducting gap $\Delta_0$ is several orders of magnitude smaller than the chemical potential $\mu$. For concreteness, we set $\mu = 2 eV$ and allow the exchange strength to lie in the interval $0 < J_0/\mu < 1$, where the system is conducting. As $J_0/\mu \to 1$, the AF material becomes an insulator, and the transport properties vanish. We consider the temperature range $0 < T/T_c < 1$ so that superconductivity does not break down.

**Calculation of reflection probabilities.**– Figure 2 shows the behavior of the reflection probabilities as functions of energy for different exchange strengths in both the transparent ($Z = 0$) and tunneling ($Z \gg 1$) regimes in the absence of RSOC.

For simplicity, we first consider a transparent interface ($Z = 0$) and the subgap regime ($E < \Delta_0$). In the normal metal limit ($J_0 = 0$), we find that retro AR is the dominant scattering process [25]. Retro NR and specular AR increase as the exchange interaction $J_0$ increases. This is because with the onset of $J_0$, the new scattering channels associated with the sublattice degrees of freedom become available. In the supergap regime ($E > \Delta_0$), electron-like and hole-like charge carriers can propagate in the S layer.

If the interface is not transparent ($Z \neq 0$), AR is suppressed while NR is enhanced, because fewer electrons are allowed to enter the S layer to form Cooper pairs. Increasing $J_0$ leads to an increase in retro NR and a decrease in specular NR, see Fig. 2.

**Electrical and thermal conductance.**– Now, we numerically compute the electrical and thermal conductance using Eqs. (10) and (11). In Fig. 3, we plot the zero-temperature electrical conductance and the thermal conductance as functions of the voltage bias and temperature, respectively, for different exchange and barrier strengths in the absence of SOC.

First, we focus on the electrical conductance shown in
In the absence of a barrier and exchange interaction, the system behaves like a transparent N–S junction. In this case, each electron incident from the N layer enters the S layer and forms a Cooper pair. This results in 100% retro AR; consequently, the electrical conductance is \( \tilde{G}_C = 2 \). As the exchange strength increases, retro NR eventually becomes the dominant scattering process. Thus, with increasing \( J_0 \), less charge is in total transported across the junction, and the electrical conductance decreases. The total NR is also increased as the barrier strength \( Z \) increases.

In the tunneling limit (\( Z = 10 \)), there is a sharp peak in the electrical conductance at \( eU/\Delta_0 = 1 \), which originates from the singularity in the density of states (DOS) in the S layer. Since higher temperatures result in more transmission of particles, the thermal conductance increases with increasing temperature, as shown in Fig. 3.

In the transparent limit (\( Z = 0 \)), the retro NR increases with the exchange strength. Since less particles are transmitted into the S layer, the thermal conductance decreases with an increasing exchange strength. As the barrier strength increases, even fewer particles are transmitted into the S layer. In the tunneling limit (\( Z = 10 \)), the thermal conductance is strongly suppressed.

Figure 3 shows that in the transparent limit the increase of exchange strength reduces both the electrical and thermal conductance, while in the tunneling regime, increases both of them. This behavior occurs due to the interplay between the exchange interaction and the barrier in the supergap regime (\( E > \Delta_0 \)), where tunneling into the S layer is also allowed. In the tunneling limit, the exchange interaction enhances the transmission of both electron-like and hole-like particles into the S layer, consequently increasing the electrical and thermal conductance.

Next, to compare the AF–S junction with the F–S junction, we plot the electrical conductance as a function of the exchange strength in Fig. 4. In the F–S junction, the electrical conductance decreases linearly with the exchange strength, \( \tilde{G}_C \approx 2(1 - J_0/\mu) \) [32]. On the other hand, in the AF–S junction, the relationship between the electrical conductance and the exchange strength is more subtle. The electrical conductance decays rapidly at small \( J_0/\mu \), is almost constant for intermediate \( J_0/\mu \), and decays as \( J_0/\mu \to 1 \). We have checked that these features are robust by varying \( m, \mu \), and \( \Delta_0 \) within the experimentally relevant intervals. The inset of Fig. 4 shows that the electrical conductance decays rapidly with the exchange strength on an energy scale set by the superconducting gap. In the regime where \( J_0 \ll \Delta_0 \), the system behaves like an N–S junction, such that \( \tilde{G}_C = 2 \). In the \( J_0 \sim \Delta_0 \) regime, we find that the reflection probabilities become dependent on the angle of incidence [74]. For electrons close to normal incidence, we find that retro AR dominates transport. For electrons with an angle of incidence nearly parallel to the interface, we find that retro AR is suppressed and specular NR is enhanced. This sudden enhancement of specular NR leads to the sharp decay of the electrical conductance observed in Fig. 4.

Numerically, we find that \( \tilde{G}_C \sim (J_0/\Delta_0)^{-1.0} \) [74].

In the regime where \( \Delta_0 \ll J_0 \ll \mu \), the DOS in the AF layer is approximately constant, and consequently, so is the electrical conductance [74]. As \( J_0/\mu \to 1 \), the AF layer starts to behave as an insulator, suppressing all transport properties.

**Anisotropic magnetoresistance.** We have not yet considered the effect of finite interfacial RSOC, due to the breaking of the inversion symmetry at the interface. For finite RSOC, an additional scattering channel is opened in which spin-flip scattering is allowed. Recently, it has been found that in F–S junctions, RSOC leads to a large anisotropic magnetoresistance (AMR) [33], while there is no AMR in N–S junctions.

In the AF layer, the spin quantization axis is determined by the Nel vector. Consequently, a finite RSOC leads to anisotropy in the electrical and thermal conductance for an AF–S junction. Since we consider only an interfacial RSOC with an inversion breaking axis in the \( z \) direction, this AMR depends only on the Nel vector’s polar angle \( \theta \).

Figure 5 shows the electrical AMR(\( \theta \)) as a function of the Nel vector direction for a fixed RSOC strength and temperature. We find that the minima and maxima occur at \( \theta = \{0, \pi\} \) and \( \theta = \pi/2 \), respectively. The inset shows that the maximum AMR increase with \( \lambda \). The qualitative features of the electrical and thermal AMR are identical. Thus, similar to F–S junctions and in contrast to N–S junctions, AF–S junctions show a strong AMR. In an AF–N junction (\( \Delta_0 \to 0 \)), the electrical
ional (thermal) AMR is approximately 75% smaller (50% larger) than that in an AF–S junction. The simultaneous enhancement of the electrical AMR and diminution of the thermal AMR in an AF–S junction can be attributed to the finite AR in the presence of the S layer.

Concluding remarks.—We demonstrate that the electrical and thermal conductance of AF–S junctions are qualitatively different from those of N(F)–S junctions due to the emergence of two new scattering processes: specular AR and retro NR. Furthermore, we show that there is a large AMR in the presence of a finite interfacial RSOC.

Our results reveal that superconducting spintronics based on antiferromagnetic materials, open up a fascinating playground for novel physical phenomena. We hope that this theoretical study will inspire new experimental work on AF–S heterostructures.

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