Supplementary Material: Charge transport properties of the Majorana zero mode induced noncollinear spin selective Andreev reflection*

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Text A: Theoretical Model

As shown in Figure S1, we consider a topological insulator (TI) covered by a superconductor. Superconductivity is induced in the TI via the proximity effect, and a vortex state is formed in the surface of the TI under a magnetic field. At the center of the vortex core(r = 0), the spin polarization of the MZM is parallel to the magnetic field.

Let us construct the Hamiltonian of the vortex state in a topological superconductor (TS). This TS is modeled by a helical surface state with Rashba spin--orbit coupling and proximity-induced superconductivity [S1]. The helical surface state is the surface state of a 3D topological insulator in the x--y plane. We can generalize the Hamiltonian in the x--y plane to a spherical surface of radius R.

The single-electron Hamiltonian of a helical surface state is [S1]:

$$H_{0e} = -\frac{\alpha}{R\hbar}\hat{L} \times \hat{\sigma} - \mu, \quad \text{(s1)}$$

where α is the spin-orbit coupling strength, $\hat{\sigma}$ is the Pauli matrices, $\hat{L}$ are the orbital angular momentum, and μ is the chemical potential. The single-hole Hamiltonian (H_{0h}) defined as -$\sigma_y H_{0e} \sigma_y^*$ and σ_y is a pauli matrix.

The Hamiltonian of the proximity-induced superconducting state can be described as:

$$H_\Delta = \Delta(c_\downarrow c_\uparrow - c_\uparrow c_\downarrow) + \Delta^*(c_\downarrow^+ c_\uparrow^+ - c_\uparrow^+ c_\downarrow^+), \quad \text{(s2)}$$

where Δ is the proximity induced superconducting order parameter ans $c_\sigma^{(+)}$ is the electron annihilation (creation) operator with $\sigma =\uparrow\downarrow$ denoting the spin.

Then, in the standard Nambu representation, the field operator can be defined as

$$\hat{\psi}(r) = [\hat{c}_\uparrow, \hat{c}_\downarrow, \hat{c}_\downarrow^+, -\hat{c}_\uparrow^+]^T. \quad \text{(s3)}$$

The Hamiltonian of the proximity-induced superconducting state in then

$$H_\Delta = \begin{bmatrix} 0 & \Delta I \\ \Delta^* I & 0 \end{bmatrix}, \quad \text{(s4)}$$

where I is the unit matrix.

The Hamiltonian of the vortex state can be written as:

$$H_v = \begin{bmatrix} H_{0e} & \Delta I \\ \Delta^* & H_{0h} \end{bmatrix}, \quad \text{(s5)}$$

where H_{0h} is the single-hole Hamiltonian of a helical surface state defined as -$\sigma_y H_{0e} \sigma_y^*$ and σ_y is a pauli matrix.

The vortex state can be described as $\Delta = \Delta(\theta)e^{i\phi}$. Here the factor $e^{i\phi}$ describes a vortex with a winding number of 1 and $\Delta(\theta) = \Delta_0 tanh(\frac{Rsin\theta}{\xi_0})$, where ξ_0 characterizes the size of the vortex core.

By diagonalzingH_v, we can define a new quantum number of K_z [S1], where$K_z|\Phi_m >= m|\Phi_m >$, where m and $|\Phi_m >$ are the eigenvalue and eigenfunction of K_z. Here $K_z = l_z + \sigma_z + \tau_z$ is the orbital quantum number in the z direction, σ_z is the spin quantum number in the z direction, τ_z is the spin-orbit-pseudospin quantum number referring to the particle-hole degree of freedom and $|\Phi_m>$ is the four-component wave function [S1].

$$|\Phi_m>=[e^{im\phi}u_1, e^{i(m+1)\phi}u_2, e^{i(m-1)\phi}v_1, e^{im\phi}v_2] \tag{s6}$$

The eigenvalue problem then becomes

$$H_v|\Phi_m>=E_m|\Phi_m>. \tag{s7}$$

The four-component eigenfunction basis [S1-S2] in $|\Phi_m>$ can be expressed in terms of the spherical harmonic functions: $e^{im\phi}u_1=\sum_l a_l Y_l^m$, $e^{i(m+1)\phi}u_2=\sum_l b_l Y_l^{m+1}$, $e^{i(m-1)\phi}v_1=\sum_l c_l Y_l^{m-1}$, $e^{im\phi}v_2=\sum_l d_l Y_l^m$, where $Y_l^m(\theta,\phi)=P_l^m(cos\theta)e^{im\phi}/\sqrt{2\phi}$ and $P_l^m(cos\theta)$ is the associated Legendre polynomial.

By directly diagonalizing the H_v, we can obtain the wave function and the energy spectrum. In our numerical calculations, we set $R=50\xi_0$, α=30 meV·nm, ξ_0=35 nm, Δ_0=1 meV, and μ =90 meV, which are comparable to the experiment data in Bi_2Se_3[S3]. Taking a cutoff in the orbital angular momentum l to be approximately 200, we find that for m = zero, E_0 = zero (numerically $\pm 4\times 10^{-6}$ meV). Here u_1=v_2 ≠0, and u_2=$v_1=0$; this means that a spin up electron and a spin up hole occupy the MZM. For the m=1 state, E_{-1}=-0.06 meV, v_1 ≠0, u_2=0, u_1=0 and v_2=0; only a hole with a down spin can occupy this state. Meanwhile, for m=-1, E_1=0.06$ meV, $u_2\neq 0$, u_1, v_1 and v_2=0, only a spin down electron can occupy this state. These are the first excited states of the vortex. When $|m|$>1, v_1, u_2, u_1,and v_2 are equal to zero at the core of the vortex.

Next, let us consider the total Hamiltonian of a system with a vortex state coupling to a spin polarization STM tip. The Hamiltonian of the electron on the STM tip can be described as[S4]:

$$H_{L,e}=\sum_\sigma \hat{d}_{L,\sigma}^{+}(\varepsilon_\sigma-\mu_L+\sigma M)\hat{d}_{L,\sigma} \tag{s8}$$

where $\hat{d}_{L,\sigma}^{+}$ denotes the electron annihilation (creation) operator of the STM tip with σ spin, μ_L indicates the chemical potential of the STM tip (set to zero), ε_σ is the kinetic energy of the STM tip with σ spin, $\widehat{M}$ is the spin related potential and $\hat{\sigma}$ are Pauli matrices.

The Hamiltonian of the STM tip is

$$H_L=\begin{bmatrix} H_{L,e} & 0 \\ 0 & H_{L,h}\end{bmatrix}, \tag{s9}$$

where ($H_{L,h}$) defined as -$\sigma_y H_{L,e}\sigma_y^*$ is the Hamiltonian of the electron(hole) on the STM tip.

The coupling between the vortex states and the STM tip can be described using the following Hamiltonian [S4]:

$$H_{L-v} = \sum_{n,\sigma}\{2t_{n\sigma}(cos\frac{\theta}{2}\hat{d}^{+}_{L,\sigma} - \sigma \cdot sin\frac{\theta}{2}\hat{d}^{+}_{L,\overline{\sigma}})\hat{c}_{n,\sigma} + H.c.\}, \quad \text{(s10)}$$

where t_c is the coupling strength between the vortex and the STM tip.

The total Hamiltonian of the system is:

$$H_{tot} = \begin{bmatrix} H_L & H_{L-v} \\ H_{v-L} & H_v \end{bmatrix}. \quad \text{(s11)}$$

The retarded Green's function of the system can be obtained via Dyson's equation:

$$G^{tot} = \frac{1}{(G^{0,R})^{-1} - \Sigma^r}. \quad \text{(s12)}$$

Here, the single-particle retarded Green's function $G^{0,R}$ can be constructed with the wave functions $\widehat{\Psi}_m$ and the eigenvalue E_m of the vortex state:

$$G^{0,R} = \sum_m \frac{|\widehat{\Psi}_m >< \widehat{\Psi}_m|}{E - E_m + i\delta}, \quad \text{(s13)}$$

Where $|\widehat{\Psi}_m >= [e^{im\phi}u_1, e^{i(m+1)\phi}u_2, e^{im\phi}v_2, e^{i(m-1)\phi}v_1]$ and $\delta\ is$ a positive infinitesimal.

We assume that the spin polarization of the FM tip $\widehat{M}$ has an angle θ with respect to the z direction(the direction of the MZM spin polarization).

The self-energy $\Sigma^r = H_{v-L}\lambda^r H_{L-v}$ with $\lambda^r = \sum_m \frac{|\phi^1_m >< \phi^1_m|}{E - E_m + i\delta}$ is the single-particle retarded Green's function of the STM tip. E_m is the eigenvalue of H_L and $|\phi^1_m >$ is the eigenfunction of H_L, $\delta\ is$ a positive infinitesimal.

Then, the general form of λ^r is:

$$\lambda^r = \begin{bmatrix} \lambda_{e\uparrow\uparrow} & \lambda_{e\uparrow\downarrow} & 0 & 0 \\ \lambda_{e\downarrow\uparrow} & \lambda_{e\downarrow\downarrow} & 0 & 0 \\ 0 & 0 & \lambda_{h\uparrow\uparrow} & \lambda_{h\uparrow\downarrow} \\ 0 & 0 & \lambda_{h\downarrow\uparrow} & \lambda_{h\downarrow\downarrow} \end{bmatrix}, \quad \text{(s14)}$$

where $\lambda_{e\uparrow\uparrow,\mathrm{nn}} = t^2_{en,\uparrow}cos^2\frac{\theta}{2}\lambda_1 + t^2_{en,\uparrow}sin^2\frac{\theta}{2}\lambda_2$, $\lambda_{e\uparrow\downarrow,\mathrm{nn}} = t_{en\uparrow}t_{en\downarrow}cos\frac{\theta}{2}sin\frac{\theta}{2}(\lambda_1 - \lambda_2)$, $\lambda_{e\downarrow\uparrow,\mathrm{nn}} = t_{en\uparrow}t_{en\downarrow}cos\frac{\theta}{2}sin\frac{\theta}{2}(\lambda_1 - \lambda_2)$, $\lambda_{e\downarrow\downarrow,\mathrm{nn}} = t^2_{en,\downarrow}cos^2\frac{\theta}{2}\lambda_1 + t^2_{en,\downarrow}sin^2\frac{\theta}{2}\lambda_2$, $\lambda_{h\uparrow\uparrow,\mathrm{nn}} = t^2_{hn,\uparrow}cos^2\frac{\theta}{2}\lambda_3 +$

$t_{hn,\uparrow}^2 sin^2\frac{\theta}{2}\lambda_4$, $\lambda_{h\uparrow\downarrow,\mathrm{nn}} = t_{hn,\uparrow}t_{hn,\downarrow}cos\frac{\theta}{2}sin\frac{\theta}{2}(\lambda_3 - \lambda_4)$, $\lambda_{h\downarrow\uparrow,nn} = t_{hn,\uparrow}t_{hn,\downarrow}cos\frac{\theta}{2}sin\frac{\theta}{2}(\lambda_3 - \lambda_4)$,

$\lambda_{h\downarrow\downarrow,\mathrm{nn}} = t_{hn,\downarrow}^2 cos^2\frac{\theta}{2}\lambda_3 + t_{hn,\downarrow}^2 sin^2\frac{\theta}{2}\lambda_4$, with $\lambda_1 = (E - (e_0 + M) + i\delta)^{-1}$, $\lambda_2 = (E - (e_0 - M) + i\delta)^{-1}$, $\lambda_3 = (E + (e_0 + M) + i\delta)^{-1}$, $\lambda_4 = (E + (e_0 - M) + i\delta)^{-1}$, n denote the state of vortex.Here, we use the parameter as: e=10Δ, $|M|$=7Δ,$t_{e0,\uparrow} = t_{h0,\uparrow} = t_{e1(2),\downarrow} = t_{h-1(-2),\downarrow} =$ 0.7Δ, $t_{e1(2),\uparrow} = t_{h-1(-2),\uparrow} = t_{e0,\downarrow} = t_{h0,\downarrow} = 0.2t_{e0,\uparrow}$.

The S matrix can be obtained via the Fisher-Lee formula [S5]:

$$\mathrm{S} = \begin{bmatrix} r_{ee} & r_{eh} \\ r_{he} & r_{hh} \end{bmatrix} = -I + i\Gamma^{\frac{1}{2}} \times G^{tot} \times \Gamma^{\frac{1}{2}}, \qquad \text{(s15)}$$

where, Γ is the broadening function, which is defined as $\Gamma = i(\Sigma^r - \Sigma^{r+})$, $r_{ee(hh)}$ is a 2× 2 matrix describing the probability of a electron(hole) being reflected as a electron(hole), while $r_{eh(he)}$ is a 2× 2 matrix describing the probability of a electron(hole) being reflected as a hole(electron) in spin space. The current I_c can be defined as:

$$I_c = \frac{e}{h}\int_0^\infty [< a_e^+(E)a_e(E) > - < b_e^+(E)b_e(E) > - < a_h^+(E)a_h(E) > + < b_h^+(E)b_h(E) >]dE, \qquad \text{(s16)}$$

where $a_{e(h)}^{+(-)}(E)$ is the generate (annihilation) operator of an incoming electron(hole), $b_{e(h)}^{+(-)}(E)$is the generate (annihilation) operator of a outgoing electron(hole). The differential conductance can also be obtained [S6].

The shot noise includes additional information concerning the fluctuation and can be calculated as [S7]

$$Sp(t - t') = \frac{1}{2} < \Delta I_L(t)\Delta I_L(t') + \Delta I_L(t')\Delta I_L(t) > \qquad \text{(s17)}$$

Where $\Delta I_L(t) = I_L(t) - I_{L0}$ and I_{L0} is the average of $I_L(t)$

The shot noise under the zero temperature limit can be obtained as follows

When eV>0,

$$Sp1 = \frac{2e^3V}{h}[\left(r_{he}^{+}a_e^{+}(E)r_{he}a_e(E)\right)\left(r_{hh}^{+}a_h^{+}(E)r_{hh}a_h(E)\right) +$$

$$\left(r_{ee}^{+}a_e^{+}(E)r_{ee}a_e(E)\right)\left(r_{eh}^{+}a_h^{+}(E)r_{eh}a_h(E)\right) - \left(r_{ee}^{+}a_e^{+}(E)r_{he}a_e(E)\right)\left(r_{hh}^{+}a_h^{+}(E)r_{eh}a_h(E)\right) -$$

$$\left(r_{he}^{+}a_e^{+}(E)r_{ee}a_e(E)\right)\left(r_{eh}^{+}a_h^{+}(E)r_{hh}a_h(E)\right)] \qquad \text{(s18)}$$

When eV<0, $a_e^{(+)}$ should change to $a_h^{(+)}$ and $r_{e(h)e(h)}^{(+)}$ should change to $r_{h(e)h(e)}^{(+)}$. This is because the carrier of the charge current is the change from electron to hole. When eV=0, the shot noise power should be $\frac{(Sp1(eV>0)+Sp1(ev<0))}{2}$.In other words, the shot noise power is 0 at zero temperature.

The shot noise power [6] can be simplified as *Sp:*

$$Sp = \frac{8e^3V}{h} r_{eh}^{+} r_{eh} r_{ee}^{+} r_{ee}. \qquad \text{(s19)}$$

The Fano factor [6] is defined as

$$F = \frac{Sp}{2eI}. \qquad \text{(s20)}$$

Both the shot noise power and the Fano factor can be obtained from the S-matrix.

Text B: Charge transport properties of SSAR when STM tip contact with the vortex core

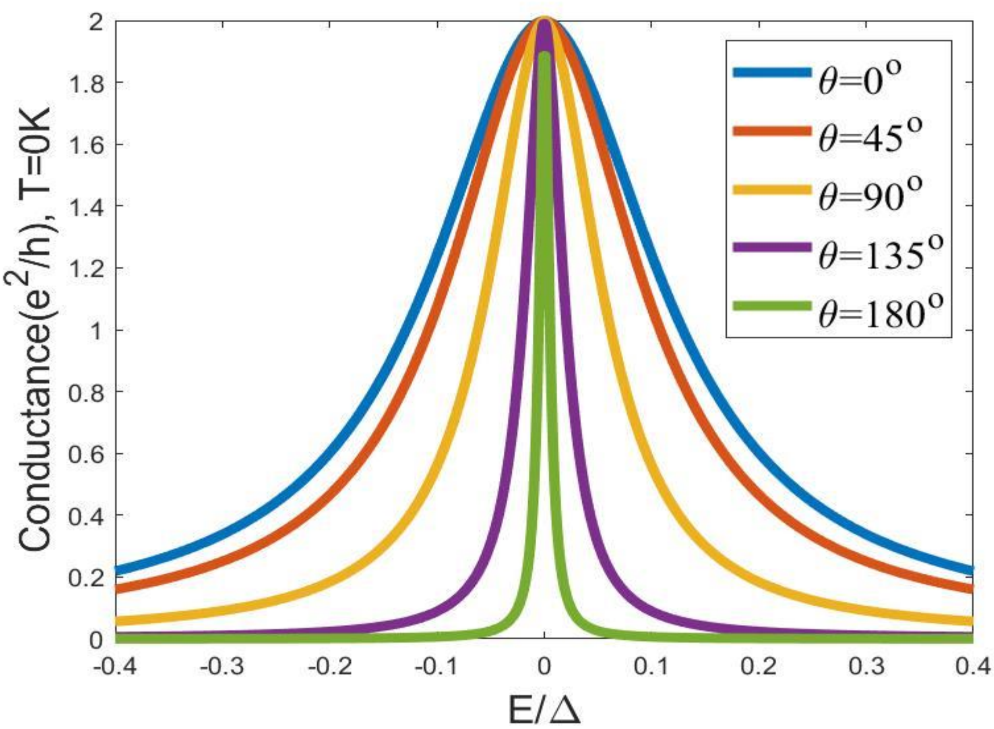

Fig. S1. The angular dependence of the conductance in the SSAR effect when STM tip contact with the vortex core. The conductance forms a peak with a maximum value of two and the width decreases with the increase of the angle, which is consistent with the previous studies [S8].

Text C: Influence of the first and second excited states on conductance

The different properties between the two conditions can be explained using the Green's function of system. From the wave function of the vortex states, we find that only the first term (u_1 for the spin-up electron, $e_\uparrow$ and the third term (v_2 for the spin-up hole, $h_\uparrow$) of the wave function($|\Psi_0>$) have non-zero values at the central of vortex when *m* = 0. When *m* = 1, only the fourth term (for the spin-down hole, $h_\downarrow$) of the wave function ($|\Psi_{-1}>$) has a non-zero value, while for *m* = -1, only the second term (for the spin-down electron, $e_\downarrow$) of the wave function ($|\Psi_1>$) has a non-zero value central of vortex. This means that the MZM is only local at the spin up channel of the hole and the electron, while the two first excited states are local at the spin-down channels of the electron and the hole, respectively. In the collinear case, the self-energy is a diagonal matrix and there is no coupling between the two spin channels. Only the coupling between the electron and the hole is local at the spin-up channel of the MZM.

However, in case of STM tip is contact with non-central area, the wave function of MZM have a little spin ↓ component. While the excited states have both of electron and hole component.

For example, the *m*=1 state，expect the spin-down hole, $h_\downarrow$, there are little component of spin up electron and spin up hole. Therefore, the excited states can contribute to the conductance in the non-central case. In this case, the excited states have two influence on the conductance, the first is more peaks at the energy of the excited states, second is decrease the conductance near the zero energy.

Here, we use the $t_{e(h),n,\uparrow(\downarrow)}$ to describe the coupling between the STM tip and vortex states. We set $t_{e0,\uparrow} = t_{h0,\uparrow} = t_{e1(2),\downarrow} = t_{h-1(-2),\downarrow} = 0.7\Delta$, $t_{e1(2),\uparrow} = t_{h-1(-2),\uparrow} = t_{e0,\downarrow} = t_{h0,\downarrow} = nt_{e0,\uparrow}$. We find that when *n*=0, the STM tip only coupling with the spin up channel of MZM and the spin down channel of the excited states. In this case, the coupling between electron and hole is only from the MZM. In case of *n* ≠0, the STM tip have coupling with the spin up channel of the excited states.

Then, the influence of excited states on the conductance will increase with increase of *n*.

Besides, with increase of the θ, the coupling between the spin up channel and spin down channel is strong. The spin down channel that is majority component of wave function may have more contribution of conductance. However, when $\theta = 180^o$, the energy broadening is too small to suppress the contribution of excited states.

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