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## Conversion of spin to charge current in topological insulator: role of the interface

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Three dimensional spin current density injected onto the surface of a topological insulator (TI) produces a two dimensional charge current density on the surface of the TI, which is the so-called inverse Edelstein effect (IEE). The ratio of the surface charge current density on the TI to the spin current density injected across the interface defined as the IEE length was shown to be exactly equal to the mean free path in the TI determined to be independent of the electron transmission rate across the interface [Phys. Rev. B 94, 184423 (2016)]. However, we find that the transmission rate across the interface gives a non-zero contribution to the transport relaxation rate in the TI as well as to the effective IEE relaxation rate (over and above any surface hybridization effects), and the IEE length is always less than the original mean free path in the TI are modified by the interface transmission time. The correction becomes significant when the transmission time across the interface becomes comparable to or less than the original momentum scattering time in the TI. This correction is similar to experimental results in Rashba electron systems in which the IEE relaxation time was found shorter in case of direct interface with metal in which the interface transmission rate will be much higher, compared to interfaces incorporating insulating oxides. Our results indicate the continued importance of the interface to obtain a better spin-to-charge current conversion and a limitation to the conversion efficiency due to the quality of the interface.

Manipulation of spin current by charge transport and vice versa are the central goals of spintronics, where spin-orbit coupling (SOC) plays an important role in connecting the charge with spin degree of freedom<sup>1,2</sup>. Topological insulators (TIs) have gained considerable attention as a strong SOC material having an insulating bulk and metallic surface states with a Dirac cone dispersion<sup>3</sup>. The spin and momentum of the two dimensional (2D) surface states of a three dimensional (3D) TI are helically locked in the Fermi contour. Because of spin-momentum locking, a 3D spin current density injected onto the surface of a TI will produce a 2D charge current density on the surface, which is known as the inverse Edelstein effect (IEE)<sup>4</sup>. Recently, the IEE was shown experimentally by spin pumping<sup>5,6</sup>, in which a spin current is produced by ferromagnetic resonance and is injected through a nonmagnetic metal layer onto the surface of the TI, and a surface charge current is obtained as shown in Fig. 1. The spin-charge conversion efficiency is measured by the IEE length defined as the ratio of the 2D charge current density on the surface of the TI to the 3D spin current density injected through the interface. In a theoretical paper by Zhang and Fert<sup>7</sup>, it was calculated that the IEE length is exactly equal to the mean free path in the TI independent of the transmission rate across the interface. However, we find that the IEE length will be modified due to the interface transmission rate, and define a modified IEE relaxation rate that will be determined by the momentum scattering rate and the interface transmission rate. We show that the transport relaxation rate in the TI also is modified by the interface transmission rate.

In this article, we calculate the transport in a TI/metal bilayer using the spinor Boltzmann equation following, Zhang and Fert<sup>7</sup>, and solve the spinor distribution function for the TI surface states. However, in this work we: (i) consider the general Boltzmann equation incorporating an inhomogeneous diffusion term to show a modification of the transport relaxation time due to the finite interface transmission time; (ii) obtain the solution to the distribution function in the steadystate homogeneous case showing a modification of the IEE relaxation time because of the finite interface transmission time as well; (iii) derive the expression for the transmission time across the interface considering both the case in which the interface is smooth so that the in-plane momentum is conserved during tunneling, and the case where the interface is rough so that the tunneling is momentum randomizing; (iv) show different dependencies of the spin current density across the interface on the in-plane and the out-of-plane components of the spin electrochemical potential in the metal even under the same physical assumptions as Zhang and Fert<sup>7</sup>. Furthermore, in the appendix, we provide an alternate approach based on quantum kinetic equation using Keldysh Green's function that reproduces the results of the semi-classical Boltzmann equation. Our main result is a modification of the IEE relaxation time in the presence of strong tunneling across the interface, which is consistent with the experimental findings of IEE relaxation time on Rashba 2D electron gas (2DEG) with strong  $SOC^{8-10}$ , where the IEE relaxation time is found to be shorter for an interface to a metal as compared to an oxide. This result shows the crucial importance of the interface in obtaining a better spin-to-charge current conversion.

We start with the spinor Boltzmann equation for the surface states of the TI in a TI/metal bilayer, given by

$$\partial_{\mathbf{T}}\hat{g}_{\mathbf{p}} + \mathbf{v} \cdot \nabla_{\mathbf{R}}\hat{g}_{\mathbf{p}} = \sum_{\mathbf{k}} \Gamma_{\mathbf{k}\mathbf{p}}(\hat{f}_{\mathbf{k}} - \hat{g}_{\mathbf{p}}) + \sum_{\mathbf{p}'} \Delta_{\mathbf{p}\mathbf{p}'}(\hat{g}_{\mathbf{p}'} - \hat{g}_{\mathbf{p}}), \quad (1)$$

where  $\hat{f}_{\mathbf{k}}$  and  $\hat{g}_{\mathbf{p}}$  are the non-equilibrium spinor distribution functions for metal and the TI surface states, respectively. Here, **k** is the 3D momentum of the states in the metal and **p** is the 2D momentum of the TI surface states. The velocity operator for the surface states is  $\mathbf{v} = (1/\hbar)\partial H/\partial \mathbf{p} = v_{\mathrm{F}}(\boldsymbol{\sigma} \times \hat{\mathbf{z}})$ , where  $H = \hbar v_{\mathrm{F}} \boldsymbol{p} \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}})$  is the Hamiltonian of the surface states,  $v_{\mathrm{F}}$  is the Fermi velocity,  $\hat{\mathbf{z}}$  is the unit vector along the surface normal direction,  $\boldsymbol{\sigma}$  is the vector consisting of three Pauli spin matrices, p is the magnitude of  $\mathbf{p}$ , and  $\hat{\mathbf{p}} = \mathbf{p}/p$  is the unit vector along the momentum direction. The first term



FIG. 1. Spin-to-charge current conversion on the surface of a TI by spin-pumping experiment: a rotating magnetization  $\mathbf{M}(t)$  around the y-direction in the ferromagnetic metal (FM) produces a spin current density  $\mathbf{J}_s$  in the z-direction injected to the nonmagnetic metal (NM) with spins oriented along the y-direction. The injected spin current density  $\mathbf{J}_s$  onto the surface of the TI from the NM through the interface produces a charge current density  $\mathbf{J}_c$  in the x-direction on the surface of the TI due to the spin-momentum locking of the TI surface states on the Fermi contour as shown on the right.

in the left hand side of Eq. (1) represents the time derivative and the second term represents diffusion in the 2D surface of the TI, where T is the time and  $\mathbf{R}$  is the 2D position vector on the TI surface.

Because we find the interface tunneling rate is crucial in the transport, we will elaborate on the derivation of the interface tunneling rate and the assumptions made therein. The first term on the right hand side of Eq. (1) represents tunneling across the interface with the tunneling probability  $\Gamma_{\textbf{kp}}$  given from the Fermi's Golden Rule as  $\Gamma_{\textbf{kp}}$  =  $(2\pi/\hbar)|T_{\mathbf{kp}}|^2\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{p}})$ , where  $T_{\mathbf{kp}}$  is the tunneling matrix element between the metal and the TI surface states given by  $|T_{\mathbf{kp}}|^2 = |\langle \psi_{\mathbf{k}}(\mathbf{r})\chi_{\mathbf{k}}|V_{\mathrm{tun}}(\mathbf{r})|\psi_{\mathbf{p}}(\mathbf{r})\chi_{\mathbf{p}}\rangle|^2$ , where  $V_{\mathrm{tun}}(\mathbf{r})$  is the tunneling potential, and  $\mathbf{r}$  is the 3D position vector. The orbital part of the wave functions are  $\psi_{\mathbf{k},\mathbf{p}}(\mathbf{r})$ , and the spin part of the wave functions are  $\chi_{\mathbf{k},\mathbf{p}}$ . If the interface is considered to be rough enough to randomize momentum and the tunneling potential is assumed to be spin-independent and step-like in the surface normal direction, the interface potential can be modeled by  $V_{\text{tun}}(\mathbf{r}) = v_0 \Sigma_{i=1}^{N_s} \delta(\mathbf{r}_{\parallel} - \mathbf{R}_i^{\text{S}}) V_t(z)$ , where the roughness of the interface is modeled by  $N_s$  randomly distributed short-range delta potentials at positions  $\mathbf{R}_i^{s}$  at the interface,  $\mathbf{r}_{\parallel}$  is the component of  $\mathbf{r}$  parallel to the interface, and  $V_{\rm t}(z)$  is a step-like function along the z-direction. The orbital part of the wave functions are assumed to be of the form  $\psi_{\mathbf{k},\mathbf{p}}(\mathbf{r}) = \phi_{\mathbf{k},\mathbf{p}}(\mathbf{r}_{\parallel})\xi_{\mathbf{k},\mathbf{p}}(z)$ , where the  $\phi_{\mathbf{k},\mathbf{p}}(\mathbf{r}_{\parallel})$ 's are considered to be plane waves. After an averaging over the random distribution of the tunneling centers  $\mathbf{R}_{i}^{S}$ , we obtain

$$\Gamma_{\mathbf{k}\mathbf{p}} = \frac{\pi v_0^2 n_{\mathrm{s}} C_{\mathrm{t}}}{\hbar A} \left[ \sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}}) \right] \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}), \quad (2)$$

where  $n_{\rm s} = N_{\rm S}/A$  is the roughness defect density of the interface, A is the surface area, and the overlap of the wave functions of the surface state and the metal in the tunneling region is  $C_{\rm t} = |\langle \xi_{\bf k}(z) | V_{\rm t}(z) | \xi_{\bf p}(z) \rangle|^2$ , which is presumed to be independent of the momentum of the electrons tunneling across the interface<sup>11</sup>. The tunneling potential is considered to be spin independent, so the spinor dependent part in Eq. (2) arises from the projection operator  $\frac{1}{2}[\sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\boldsymbol{p}})]$  which projects states to the upper band of the TI Hamiltonian<sup>7</sup>. The interface tunneling probability given by Eq. (2) is completely momentum randomizing, as considered by Zhang and Fert<sup>7</sup>. Here, we further consider the case of a smooth interface, in which the tunneling potential can be modeled by  $V_{\text{tun}}(\mathbf{r}) = v_c V_t(z)$  to be constant everywhere on the interface, and the tunneling probability becomes

$$\Gamma_{\mathbf{k}\mathbf{p}} = \frac{\pi v_{\mathrm{c}}^2 C_{\mathrm{t}}}{\hbar A} \left[ \sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}}) \right] (2\pi)^2 \delta(\mathbf{k}_{\parallel} - \mathbf{p}) \, \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}), \quad (3)$$

implying that the in-plane momentum  $\mathbf{k}_{\parallel}$  is conserved in the tunneling process. The rough and the smooth interface assumed are the extreme limits of the interface roughness model with a Gaussian distributed surface roughness potential. However, our main result is the modification of the transport scattering time as well as the IEE relaxation time due to the finite transmission time across the interface, which remains valid in either case; only the interface transmission time depends on the nature of the interface.

The second term on the right hand side of Eq. (1) denotes scattering between the state  $\mathbf{p}$  and  $\mathbf{p}'$  of the TI surface states due to defects or impurities close to the interface, with the scattering probability  $\Delta_{\mathbf{pp}'}$  given by the Fermi's Golden Rule as  $\Delta_{\mathbf{pp}'} = (2\pi/\hbar)|U_{\mathbf{pp}'}|^2 \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'})$ , where  $U_{\mathbf{pp}'}$  is the scattering matrix element between the state  $\mathbf{p}$  and  $\mathbf{p}'$  given by  $|U_{\mathbf{pp}'}|^2 = \langle |\langle \psi_{\mathbf{p}}(\mathbf{r})|V_{\mathrm{dis}}(\mathbf{r})|\psi_{\mathbf{p}'}(\mathbf{r})\rangle|^2 \rangle |\langle \chi_{\mathbf{p}}|\chi_{\mathbf{p}'}\rangle|^2$ . Here we model a short range, spin-independent disorder potential by  $V_{\mathrm{dis}}(\mathbf{r}) = u_0 \sum_{j=1}^{N_1} \delta(\mathbf{r}_{\parallel} - \mathbf{R}_j^{\mathrm{I}}) V_{\mathrm{d}}(z)$ , where  $\mathbf{R}_j^{\mathrm{I}}$ 's are the position of the  $N_{\mathrm{I}}$  impurities in the direction parallel to the surface, and  $V_d(z)$  represents an average value of the impurity potential due to the impurities near the interface. After averaging over the random impurity positions parallel to the surface, the scattering matrix element is evaluated to be  $|U_{\mathbf{pp}'}|^2 = (u_0^2 n_i C_d/A) \frac{1}{2} (1 + \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}')$ , where  $n_i = N_{\mathrm{I}}/A$  is the impurity concentration,  $C_d = |\langle \xi_{\mathbf{p}}(z)|V_d(z)|\xi_{\mathbf{p}'}(z)\rangle|^2$ , and  $|\langle \chi_{\mathbf{p}}|\chi_{\mathbf{p}'}\rangle|^2 = \frac{1}{2} (1 + \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}')$  where  $\chi_{\mathbf{p}}$  satisfies  $\mathbf{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}})\chi_{\mathbf{p}} = \chi_{\mathbf{p}}$ . So, we have

$$\Delta_{\mathbf{p}\mathbf{p}'} = \frac{\pi u_0^2 n_i C_d}{\hbar A} (1 + \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}') \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}). \tag{4}$$

Because the band-structure of the surface states is isotropic in the **p**-space within the considered energy range, the conservation of energy also implies conservation of the magnitude of momentum in the scattering process.

The solution to Eq. (1) can be obtained by considering  $\hat{f}_{\mathbf{k}} = \hat{f}_{\mathbf{k}}^0 + \delta \hat{f}_{\mathbf{k}}$  and  $\hat{g}_{\mathbf{p}} = \hat{g}_{\mathbf{p}}^0 + \delta \hat{g}_{\mathbf{p}}$ , where  $\hat{f}_{\mathbf{k}}^0 = f_{\text{FD}}(\epsilon_{\mathbf{k}})\sigma_0$ and  $\hat{g}_{\mathbf{p}}^0 = \frac{1}{2}[\sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}})]f_{\text{FD}}(\epsilon_{\mathbf{p}})$  are the equilibrium distribution functions for the metal and the TI surface states, respectively, where  $f_{\text{FD}}$  is the Fermi-Dirac distribution. We can write  $\delta \hat{f}_{\mathbf{k}} = (f_0 \sigma_0 + \mathbf{f} \cdot \boldsymbol{\sigma})\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathrm{F}})$  and  $\delta \hat{g}_{\mathbf{p}} = \hat{h}(\theta)\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathrm{F}})$ , which amounts to considering quasi-particle excitations at the Fermi energy  $\epsilon_{\mathrm{F}}$ . We consider  $f_0$  and  $\mathbf{f}$  are independent of the solid angle  $\Omega$  in the Fermi surface of the metal, and  $\hat{h}(\theta)$  is a function of the angle  $\theta = \tan^{-1}(p_y/p_x)$  in the Fermi surface of the TI surface state, reflecting the dispersion relations of the metal and the TI, respectively. Performing the summations over momentum by the following integrations:  $\Sigma_{\mathbf{k}} \rightarrow V \int N_{\mathbf{k}}(\epsilon_{\mathbf{k}}) d\epsilon_{\mathbf{k}} \int d\Omega/(4\pi)$  (where V = Ad is the volume of the metal, A is the surface area of the bilayer, and d is the thickness of the metal) and  $\Sigma_{\mathbf{p}} \rightarrow A \int N_{\mathbf{p}}(\epsilon_{\mathbf{p}}) d\epsilon_{\mathbf{p}} \int d\theta/(2\pi)$ (where  $N_{\mathbf{k}}(\epsilon_{\mathbf{k}})$  and  $N_{\mathbf{p}}(\epsilon_{\mathbf{p}})$  are the per spin density of states (DOS) of the metal and the TI surface states, respectively), and an integration over  $\epsilon_{\mathbf{p}}$  of Eq. (1) gives

$$\partial_{\mathrm{T}}\hat{h}(\theta) + v_{F} \,\boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \nabla_{\mathbf{R}}\hat{h}(\theta)) = \frac{1}{\tau_{\mathrm{t}}} [\boldsymbol{\sigma}_{0} + \boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\mathbf{p}})] (\boldsymbol{f}_{0}\boldsymbol{\sigma}_{0} + \boldsymbol{f} \cdot \boldsymbol{\sigma} - \hat{h}(\theta)) + \frac{1}{\tau_{\mathrm{p}}} \Big\langle (1 + \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}') (\hat{h}(\theta') - \hat{h}(\theta)) \Big\rangle_{\theta'}.$$
(5)

Here  $\langle ... \rangle_{\theta}$  denotes the average over the angle  $\theta$ ,  $\tau_t$  is the interface transmission time, and  $\tau_p$  is the momentum scattering time. In case of a rough interface with momentum randomizing tunneling, the interface transmission time is defined from Eq. (2) as

$$\frac{1}{\tau_{\rm t}} = \sum_{\mathbf{k}} \frac{\pi v_0^2 n_{\rm s} C_{\rm t}}{\hbar A} \delta(\epsilon_{\mathbf{k}} - \epsilon_{\rm F}) = \pi v_0^2 n_{\rm s} C_{\rm t} N_{\rm 3D} d/\hbar, \qquad (6)$$

with  $N_{3D}$  being the 3D DOS of the metal at the Fermi level. In case of a smooth interface, the interface transmission time is redefined from Eq. (3) as

$$\frac{1}{\tau_{\rm t}} = \sum_{\mathbf{k}} \frac{\pi v_{\rm c}^2 C_{\rm t}}{\hbar A} (2\pi)^2 \delta(\mathbf{k}_{\parallel} - \mathbf{p}_{\rm F}) \delta(\epsilon_{\mathbf{k}} - \epsilon_F) 
= \pi v_{\rm c}^2 C_{\rm t} N_{\rm 1D} d/\hbar,$$
(7)

where  $\mathbf{p}_{\rm F}$  is the Fermi momentum in the TI, and  $N_{1D}$  is the one-dimensional (1D) DOS of the metal at the Fermi level with the condition that the in-plane momentum is conserved, i.e.,  $\mathbf{p}_{\rm F}^2 + k_z^2 = \mathbf{k}_{\rm F}^2$ , with  $\mathbf{k}_{\rm F}$  being the Fermi momentum in the metal. So, for a smooth interface, tunneling is possible if the cross section of the 3D Fermi surface is larger than the 2D Fermi surface, i.e.,  $\mathbf{k}_{\rm F} > \mathbf{p}_{\rm F}$ . For large 2D Fermi surface, i.e.,  $\mathbf{p}_{\rm F} > \mathbf{k}_{\rm F}$ , there will be no tunneling  $(1/\tau_{\rm t} = 0)$  if the interface is smooth. From Eq. (4), we define the momentum scattering time as

$$\frac{1}{\tau_{\rm p}} = \sum_{\rm p} \frac{\pi u_0^2 n_{\rm i} C_{\rm d}}{\hbar A} \delta(\epsilon_{\rm p} - \epsilon_{\rm F}) = \pi u_0^2 n_{\rm i} C_{\rm d} N_{\rm F} / \hbar, \quad (8)$$

where  $N_{\rm F}$  is the 2D DOS of the TI surface states at the Fermi level.

The solution for  $\hat{h}(\theta)$  is obtained by considering that the non-equilibrium distribution function for the surface states has a spinor form that is proportional to the upper band projection operator of the TI surface state Hamiltonian, i.e.,  $\hat{h}(\theta) =$  $h_0(\theta)[\sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\boldsymbol{p}})]$ , where  $h_0(\theta)$  is a scalar function times identity in spin space and can be written in terms of s- and p-wave components, i.e.,  $h_0(\theta) = h_s + \hat{\boldsymbol{p}} \cdot \boldsymbol{h}_a$ , with  $h_s$  and  $\boldsymbol{h}_a$ being independent of  $\theta$ . Taking trace of Eq. (5) in the spin space and integrating out the s- and p-wave components, we obtain

$$\partial_{\mathrm{T}}\mathbf{h}_{\mathrm{s}} + \frac{v_{\mathrm{F}}}{2}\nabla_{\mathbf{R}} \cdot \mathbf{h}_{\mathrm{a}} = \frac{2}{\tau_{\mathrm{t}}} \left(\frac{\mathbf{f}_{0}}{2} - \mathbf{h}_{\mathrm{s}}\right),\tag{9a}$$

$$\partial_{\mathrm{T}}\mathbf{h}_{\mathrm{a}} + v_{\mathrm{F}}\nabla_{\mathbf{R}}\mathbf{h}_{\mathrm{s}} = \frac{2}{\tau_{\mathrm{t}}}\left(\frac{\mathbf{f}}{2} \times \hat{\mathbf{z}}\right) - \left(\frac{2}{\tau_{\mathrm{t}}} + \frac{1}{2\tau_{\mathrm{p}}}\right)\mathbf{h}_{\mathrm{a}}.$$
 (9b)

The charge density n and the current density  $\mathbf{J}_{c}$  on the surface of the TI are given by

$$n = \frac{(-e)}{A} \sum_{\mathbf{p}} \operatorname{Tr}(\delta \hat{g}_{\mathbf{p}}) = -2eN_{\mathrm{F}} \mathbf{h}_{\mathrm{s}}, \qquad (10a)$$

$$\mathbf{J}_{\mathbf{c}} = \frac{(-e)}{A} \sum_{\mathbf{p}} \operatorname{Tr}(\mathbf{v}\delta\hat{g}_{\mathbf{p}}) = -eN_{\mathrm{F}}v_{\mathrm{F}}\mathbf{h}_{\mathrm{a}}.$$
 (10b)

The charge density  $n_{\rm M}$  and the spin density  $s_{\rm M}$  (in the unit of charge -e) in the metal are given by

$$n_{\rm M} = \frac{(-e)}{V} \sum_{\mathbf{k}} \operatorname{Tr}(\delta \hat{f}_{\mathbf{k}}) = -2eN_{\rm 3D} f_0, \qquad (11a)$$

$$\mathbf{s}_{\mathrm{M}} = \frac{(-e)}{V} \sum_{\mathbf{k}} \operatorname{Tr}(\boldsymbol{\sigma} \delta \hat{f}_{\mathbf{k}}) = -2eN_{\mathrm{3D}}\mathbf{f}.$$
 (11b)

We define the charge electrochemical potential  $\mu_0$  in the metal by the relation  $n_{\rm M} = 2e^2 N_{\rm 3D}\mu_0$ , where the factor of 2 is for spin degeneracy (as  $N_{\rm 3D}$  is the per spin DOS), and define the spin electrochemical potential  $\mu$  by the relation  $\mathbf{s}_{\rm M} = e^2 N_{\rm 3D} \mu$ . From Eq. (11) we obtain  $\mathbf{f}_0 = -\mu_0$  and  $\mathbf{f} = -e\mu/2$ . Using Eq. (10), the following diffusion equation in the TI is obtained from Eq. (9a),

$$\partial_{\mathbf{T}} n + \nabla_{\mathbf{R}} \cdot \mathbf{J}_{\mathbf{c}} = \frac{2}{\tau_{\mathbf{t}}} (e^2 N_{\mathbf{F}} \mu_0 - n).$$
(12)

Fourier transforming Eq. 9(b) to the frequency domain  $(\partial_T \rightarrow -i\omega)$  gives the charge current density in the TI,

$$\mathbf{J}_{\mathbf{c}} = \frac{1}{(1 - i\omega\tau_{\mathrm{tr}})} \left[ -\frac{v_{\mathrm{F}}^{2}\tau_{\mathrm{tr}}}{2} \nabla_{\mathbf{R}} n + e^{2} N_{\mathrm{F}} v_{\mathrm{F}} \frac{\tau_{\mathrm{tr}}}{\tau_{\mathrm{t}}} \left( \frac{\mathbf{\mu}}{2} \times \hat{\mathbf{z}} \right) \right], (13)$$

where  $\tau_{\rm tr}$  is the transport relaxation time defined as

$$\frac{1}{\tau_{\rm tr}} = \frac{1}{2\tau_{\rm p}} + \frac{2}{\tau_{\rm t}}.$$
 (14)

(The factor of 2 in  $2/\tau_t$  could be absorbed in the definition of  $\tau_t$  in Eq. (6)and (7) by redefining the DOS of the metal considering both the spins.) In absence of tunneling from the metal, the transport relaxation time in the TI is  $\tau_{tr}^0 = 2\tau_p$ , where the factor of 2 is due to the increasing attenuation of scattering with increasing scattering angle because of the helical spin-momentum locking in the TI, including elimination of direct backscattering where the spin components of the initial and final electronic states are orthogonal. The first term in the right hand side of Eq. (13) represents diffusion, with the diffusion constant  $D = v_F^2 \tau_{tr}/2$  being modified by the transmission rate across the interface through the redefined transport relaxation

time given by Eq. (14). The spin current density  $J_s$  through the interface (in the unit of charge current density) is given by

$$\mathbf{J}_{s} = \frac{(-e)}{A} \sum_{\mathbf{p},\mathbf{k}} \operatorname{Tr} \left[ \boldsymbol{\sigma} \Gamma_{\mathbf{k}\mathbf{p}} (\hat{f}_{\mathbf{k}} - \hat{g}_{\mathbf{p}}) \right]$$
  
$$= \frac{2}{v_{\mathrm{F}} \tau_{\mathrm{t}}} \left( e^{2} N_{\mathrm{F}} v_{\mathrm{F}} \frac{\boldsymbol{\mu}}{2} - \hat{\mathbf{z}} \times \mathbf{J}_{\mathrm{c}} \right).$$
(15)

Now we solve the non-equilibrium distribution function for the TI surface state under steady-state spatially-homogeneous conditions as per Zhang and Fert. The assumption of a slowly varying in position charge electrochemical potential in the metal with respect to the electrochemical potential (or equivalently the non-equilibrium charge density n) in the TI surface is valid since the metal has much higher conductivity than the TI surface. In the appendix, we show that under the assumption of a homogeneous charge electrochemical potential  $\mu_0$  in the metal, the charge density n and the charge current density  $\mathbf{J}_{c}$  in the TI surface becomes homogeneous in case of a short circuit between the two ends of the surface of the TI if either the applied spin electrochemical potential  $\mu$ in the metal or the applied spin current density  $J_s$  from the metal to the TI surface through the interface is assumed to be homogeneous. Under this homogeneous condition, we also show (in the appendix) that the applied position-independent charge electrochemical potential  $\mu_0$  in the metal will be balanced by a position-independent non-equilibrium charge density  $n = e^2 N_{\rm F} \mu_0$  (i.e., a position-independent electrochemical potential) in the TI. (Moreover, in case of spin pumping experiments, a purely spin electrochemical potential is applied in the metal, and both  $\mu_0$  and, thus, *n* vanish. However, what follows does not depend on these quantities vanishing.) The charge current density  $\mathbf{J}_c$  in the TI for a position-independent non-equilibrium charge density becomes

$$\mathbf{J}_{c} = \frac{e^{2} N_{F} v_{F} \tau_{p}}{4 \tau_{p} + \tau_{t}} (\mathbf{\mu}_{\parallel} \times \hat{\mathbf{z}}), \tag{16}$$

where  $\boldsymbol{\mu} = \boldsymbol{\mu}_{\parallel} + \boldsymbol{\mu}_{\perp} \hat{\boldsymbol{z}}$ , where  $\boldsymbol{\mu}_{\perp} = \boldsymbol{\mu} \cdot \hat{\boldsymbol{z}}$ . Substituting Eq. (16) into Eq. (15), we find the spin current density  $\boldsymbol{J}_s$  through the interface to be

$$\mathbf{J}_{\mathrm{s}} = \frac{e^2 N_{\mathrm{F}}}{4\tau_{\mathrm{p}} + \tau_{\mathrm{t}}} \left(1 + \frac{2\tau_{\mathrm{p}}}{\tau_{\mathrm{t}}}\right) \mathbf{\mu}_{\parallel} + \frac{e^2 N_{\mathrm{F}}}{\tau_{\mathrm{t}}} \mathbf{\mu}_{\perp} \hat{\mathbf{z}}.$$
 (17)

We also have derived the diffusion equation in the TI, as well as the expressions for the charge and spin current densities, from a full quantum-mechanical kinetic equation based on non-equilibrium Keldysh Green's function, which is provided in the appendix. We note that the expression for the spin current density in Eq. (17) derived here differs from the one in the previous work of Zhang and Fert<sup>7</sup> on which we build, despite the fact that we started with the same physical assumptions as theirs. Equation (17) indicates that the spin current density is induced by both the in-plane ( $\mu_{\parallel}$ ) and out-of-plane ( $\mu_{\perp}$ ) components of the spin electrochemical potential. The coefficients for both terms are different from each other. Furthermore, the coefficient for the in-plane component in Eq. (17) differs from that provided by Zhang and Fert<sup>7</sup>. This difference becomes significant when the interface transmission time is comparable to or smaller than the momentum scattering time. The physical and practical significance of the difference will be addressed as part of the discussion below.

Now we consider the physical meaning of the coefficients in the expression of  $\mathbf{J}_s$  given in Eq. (17). It can be seen from Eq. (17) that the spin current density across the interface is directly proportional to the interface tunneling rate,  $1/\tau_t$ , if we consider pure out-of-plane component of the spin electrochemical potential (i.e.,  $\boldsymbol{\mu}_{\parallel} = 0$ ). In addition, in case of a pure in-plane component of the spin electrochemical potential (i.e.,  $\boldsymbol{\mu}_{\perp} = 0$ ) in both limits of  $\tau_p$ ,  $\tau_p \gg \tau_t$  and  $\tau_p \ll \tau_t$ , the spin current density across the interface also is proportional to the interface tunneling rate and, thus, depends on the barrier thickness, although the proportionality constant varies by a factor of 2 between these two limits. The spin current to charge current conversion efficiency is measured by the IEE length defined as  $\lambda_{\text{IEE}} \equiv |\mathbf{J}_c|/|\mathbf{J}_s|$ , which is found to be, in case of a pure in-plane spin-electrochemical potential,

$$\lambda_{\rm IEE} = \frac{\lambda_{\rm mf}}{\left(1 + \frac{2\tau_{\rm p}}{\tau_{\rm t}}\right)},\tag{18}$$

where  $\lambda_{\rm mf} \equiv v_{\rm F} \tau_{\rm p}$  is the mean free path in the TI. If the orientation of the spins in the spin current injected from the metal to the TI surface is purely out-of-plane, i.e.,  $\mu_{\parallel} = 0$ , from Eq. (16), there will be no charge current on the TI surface, because the spins of the carriers on the TI surface can only be oriented in-plane since we have assumed an ideal helical Dirac Hamiltonian for the TI surface states with spins locked to the momentum on the 2D surface. In a real TI system, there will be hexagonal warping present, and in the thin film of TI there can be an additional gap opening around the Dirac point, which will provide a non-vanishing out-of-plane component to the spins of the TI surface states. In these cases, the charge current on the TI surface will be non-zero and will depend on the degree of the non-idealities of the Hamiltonian if the injected spins are out-of-plane. However, the ideal model of linear Dirac cone dispersion for the TI surface states remains valid if the Fermi level lies away from the bulk bands, and away from the Dirac point in the thin TI films. In the experiment, the orientation of the spins in injected spin current through the interface is in-plane, so the IEE length is always less than the mean free path, i.e.,  $\lambda_{\text{IEE}} < \lambda_{\text{mf}}$ , because of the correction factor  $(1 + 2\tau_p/\tau_t)$  in Eq. (18) with non-zero and finite  $\tau_p$  and  $\tau_t$ . This correction factor can be viewed as a modification of the IEE relaxation time  $\tau_{\text{IEE}}$ , which is defined by  $\lambda_{\text{IEE}} \equiv v_{\text{F}} \tau_{\text{IEE}}$ . So, the IEE relaxation time can be written as

$$\frac{1}{\tau_{\text{IEE}}} = \frac{1}{\tau_{\text{p}}} + \frac{2}{\tau_{\text{t}}}.$$
 (19)

Physically, both Eq. (14) and Eq. (19) exhibit an additional momentum and spin relaxation term in the helically locked TI surface states due to exchange of electrons across the interface, apart from scattering within the TI, that modifies the transport relaxation time and the IEE relaxation time in the



FIG. 2. Variation of normalized transport relaxation time and normalized IEE relaxation time with the normalized transmission rate in our calculation and as calculated by Zhang and Fert<sup>7</sup>.

TI, respectively. (The relaxation is a result of injection (extraction) of electrons from (to) the TI with a tilted-in-p-space Fermi level to (from) the flat-in-k-space spin electrochemical potential  $\mu$  in the metal, which promotes injection and extraction of electrons of opposite spin and momentum.) We find that the effects of the interface on the relaxation times are directly related through the interface transmission rate as shown in Fig. 2. In Fig. 2, we have plotted the variation of relaxation times normalized with respect to the momentum scattering time (i.e., the normalized transport relaxation time  $\tau_{\rm tr}/\tau_{\rm p}$ and the normalized IEE relaxation time  $\tau_{\rm IEE}/\tau_{\rm p}$ ) with the normalized transmission rate  $\tau_p/\tau_t$ . It is clear from Eq. (12) that the interface conductance is proportional to  $2e^2 N_{\rm F}/\tau_{\rm t}$ , and, so the variation of the relaxation times with the transmission rate in Fig. 2 also shows the variation with the interface conductance. Zhang and Fert only pointed to a modification of the IEE relaxation rate due to the hybridization of the states of the TI and the metal (as well as the bulk of the TI) through modification of the momentum relaxation rate  $1/\tau_p$  (through the overlap integral  $C_d$  in Eq. (8)), which, of course, remains relevant to this work as well. We find that such hybridization also modifies the IEE relaxation rate through interface transmission characterized by the rate  $1/ au_{\mathrm{t}}$  (through the overlap integral  $C_t$  in Eq. (6) and (7)), with the resulting correction given by Eq. (18) becoming significant when the interface transmission rate  $1/\tau_t$  between the metal and the TI is comparable to or greater than the momentum relaxation rate  $1/\tau_{\rm p}$ . The hybridization of the states depend on the thickness and quality of the tunnel barrier. Our finding is important because an absence of a tunnel barrier between the TI and the metal will lead to a higher interface transmission rate (limited only by the Landauer-Buttikier formula in the case of an ideal interface<sup>12</sup>) and, thus, a lower IEE relaxation time  $\tau_{\text{IEE}}$  than when a tunnel barrier is present at the interface. This result could explain the experimental observation of a short  $\tau_{\text{IEE}}$  at an interface with a metal, such as in the interface between topological insulator  $\alpha$ -Sn/Ag or the Rashba 2DEG at Bi/Ag interface, but a longer  $\tau_{\text{IEE}}$  for Rashba 2DEG at STO/LAO oxide interface. In a recent experiment on the Edelstein magnetoresistance of the Rashba 2DEG at the Bi<sub>2</sub>O<sub>3</sub>/Cu interface<sup>13</sup>, a phenomenological model is used for the total relaxation time of spin states in the Rashba 2DEG/metal interface consisting of spin relaxation time at the interface and spin relaxation time out of the interface into the metal. Our theory gives an explanation of the phenomenological model that has been used to explain the Edelstein magnetoresistance of the Rashba 2DEG, in which the spin relaxation time at the interface is equivalent to the momentum scattering time on the TI surface in our model. (The momentum relaxation time is same as the spin relaxation time on the TI surface because of the spin-momentum locking on the TI surface.) The spin relaxation time out of the interface into the metal is equivalent to the interface tunneling time across the interface. Further experiments on TI/oxide interfaces compared to TI/metal interfaces will be of interest to see the effect of the interface transmission rate in the spin to charge current conversion efficiency on the TI surface.

In summary, we studied the spin-charge transport of a TI surface state coupled to a metal through a tunnel barrier and derived various parameters related to the transport, including the transport relaxation time ( $\tau_{tr}$  of Eq. (14)), the IEE relaxation time ( $\tau_{IEE}$  of Eq. (19)) and the spin-to-charge conversion efficiency ( $\lambda_{IEE}$  of Eq. (18)) of the bilayer when the metal has a pure spin bias. We found that the interface transmission rate plays a crucial role in determining the transport relaxation rate, the IEE relaxation rate, and the spin-to-charge conversion efficiency. In particular, we found that reducing the barrier thickness to the point that the interface transmission and the momentum relaxation rates are comparable reduces the spin-to-charge conversion efficiency. However, increasing the barrier thickness reduces the absolute spin injection. Thus, performance optimization will require careful barrier design.

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#### Appendix A: Derivation from quantum kinetic equation using Keldysh Green's function

The spin-charge dynamics of the TI surface states coupled to the metal through a tunnel barrier can be obtained from the quantum kinetic equation written in terms of the Keldysh Green's function. We follow the approach given by Kopnin *et. al.*<sup>14</sup> and Kopnin *et. al.*<sup>15</sup>. To start with, we consider the full system Hamiltonian

$$H_{\rm tot} = H_{\rm S} + H_{\rm D} + H_{\rm T} + H_{\rm M}.\tag{A1}$$

Here, the TI surface state Hamiltonian  $H_{\rm S}$  is given by

$$H_{\rm S} = \lambda \int d^2 \mathbf{R} \, a^{\dagger}_{\alpha}(\mathbf{R}) \big[ \epsilon_{\rm S}(\mathbf{R}) - \epsilon_{\rm F} \sigma_0 \big]_{\alpha\beta} a_{\beta}(\mathbf{R}), \qquad (A2)$$

where  $\epsilon_{\rm S}(\mathbf{R}) = -i\hbar v_{\rm F} \, \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \nabla_{\mathbf{R}})$ , **R** is the 2D position vector on the TI surface.  $a^{\dagger}_{\alpha}(\mathbf{R})$ ,  $a_{\beta}(\mathbf{R})$  are the creation and annihilation operators on the TI surface with the spin index  $(\alpha, \beta)$ , and these operators are normalized to the thickness  $\lambda$  of the TI surface states such that the equal time anticommutator satisfies  $\{a_{\alpha}(\mathbf{R}), a^{\dagger}_{\beta}(\mathbf{R}')\} = \lambda^{-1}\delta(\mathbf{R} - \mathbf{R}')\delta_{\alpha\beta}$ , and repeated spin indices will imply summation over them. The impurities on the TI surface are modeled by the disorder Hamiltonian  $H_{\rm D}$ which is

$$H_{\rm D} = \lambda \int d^2 \mathbf{R} \ a_{\alpha}^{\dagger}(\mathbf{R}) V_{\rm D}(\mathbf{R}) a_{\alpha}(\mathbf{R}), \tag{A3}$$

where  $V_{\rm D}(\mathbf{R}) = V_0 \Sigma_{j=1}^{N_{\rm I}} \delta(\mathbf{R} - \mathbf{R}_j^{\rm I})$  represents short ranged spin-independent disorder potential and the integration of the envelope function of the surface state of the TI over the surface normal direction is already included in the average value  $V_0$ . The coupling of the TI surface states to the metal through the tunnel barrier is described by a tunneling Hamiltonian  $H_{\rm T}$ , which captures the transmission of the electron in and out of the TI surface states as

$$H_{\rm T} = \lambda \int d^2 \mathbf{R} \int d^3 \mathbf{r} \left[ b^{\dagger}_{\alpha}(\mathbf{r}) T_{\alpha\beta}(\mathbf{r}, \mathbf{R}) a_{\beta}(\mathbf{R}) + a^{\dagger}_{\alpha}(\mathbf{R}) T^{\dagger}_{\alpha\beta}(\mathbf{R}, \mathbf{r}) b_{\beta}(\mathbf{r}) \right], \tag{A4}$$

where  $b_{\alpha}^{\dagger}(\mathbf{r})$ ,  $b_{\beta}(\mathbf{r})$  are the creation and annihilation operators in the metal satisfying the equal time anticommutator  $\{b_{\alpha}(\mathbf{r}), b_{\beta}^{\dagger}(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}')\delta_{\alpha\beta}$ ,  $\mathbf{r}$  is the 3D position vector in the metal, and the tunneling matrix obeys  $T_{\alpha\beta}^{\dagger}(\mathbf{R}, \mathbf{r}) =$  $T_{\beta\alpha}^{*}(\mathbf{r}, \mathbf{R})$ . The creation and the annihilation operators in the metal and on the TI surface anticommutes with each other, i.e.  $\{a_{\alpha}(\mathbf{R}), b_{\beta}^{\dagger}(\mathbf{r}')\} = 0$ . We consider the tunneling to be instantaneous, and also we will assume a spin conserving and site-to-site (local) tunneling at the interface, in which case the tunneling matrix can be written as  $T_{\alpha\beta}(\mathbf{r}, \mathbf{R}) =$  $t(\mathbf{R})\delta(\mathbf{r}_{\parallel} - \mathbf{R})\delta(z)\delta_{\alpha\beta}$ , where  $t(\mathbf{R})$  already includes the overlap of the envelope functions in the metal and the surface state of the TI. We consider the Hamiltonian in the metal given by

$$H_{\rm M} = \int d^3 \mathbf{r} \, b_{\alpha}^{\dagger}(\mathbf{r}) \left[ \epsilon_{\rm M}(\mathbf{r}) - \epsilon_{\rm F} \sigma_0 + U_{\rm M} \right]_{\alpha\beta} b_{\beta}(\mathbf{r}), \quad (A5)$$

where  $\epsilon_{\rm M}(\mathbf{r}) = \left[\frac{1}{2m}(-i\hbar\nabla_{\mathbf{r}})^2 + \epsilon_{\rm b}\right]\sigma_0$  with *m* being the effective mass of the conduction band in the metal and  $\epsilon_{\rm b}$  being the band offset of the bottom of the conduction band in the metal with respect to the Dirac point of the TI surface state, and  $U_{\rm M} = U_0 \sigma_0 + \mathbf{U}_{\rm s} \cdot \boldsymbol{\sigma}$  where  $U_0$  is any applied electrochemical potential in the metal and  $\mathbf{U}_{\rm s}$  is an applied spin potential in the metal.

We consider the following non-equilibrium Green's function defined in the Schwinger-Keldysh time contour

$$i(G_{\rm S})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2}) = \langle T_{\tau}a_{\alpha}(\mathbf{R}_{1},\tau_{1})a_{\beta}^{\dagger}(\mathbf{R}_{2},\tau_{2})\rangle,$$
  

$$i(G_{\rm T})_{\alpha\beta}(\mathbf{r}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2}) = \langle T_{\tau}b_{\alpha}(\mathbf{r}_{1},\tau_{1})a_{\beta}^{\dagger}(\mathbf{R}_{2},\tau_{2})\rangle,$$
  

$$i(G_{\rm M})_{\alpha\beta}(\mathbf{r}_{1},\tau_{1};\mathbf{r}_{2},\tau_{2}) = \langle T_{\tau}b_{\alpha}(\mathbf{r}_{1},\tau_{1})b_{\beta}^{\dagger}(\mathbf{r}_{2},\tau_{2})\rangle.$$
(A6)

Here  $G_S$  is the Green's function for the TI surface states,  $G_T$  is the mixed Green's function for tunneling, and  $G_M$  is the Green's function in the metal neglecting the back reaction of the TI surface states, i.e.  $G_M$  satisfies

$$(G_{\mathbf{M}})_{\alpha\gamma}^{-1}(\mathbf{r}_{1},\tau_{1})(G_{\mathbf{M}})_{\gamma\beta}(\mathbf{r}_{1},\tau_{1};\mathbf{r}_{2},\tau_{2}) = \hbar\delta(\mathbf{r}_{1}-\mathbf{r}_{2})\delta(\tau_{1}-\tau_{2})\delta_{\alpha\beta},$$
(A7)

where  $(G_M)^{-1}(\mathbf{r}, \tau) = i\hbar\partial_{\tau} - \epsilon_M(\mathbf{r}) + U_M$ . From the Heisenberg equation of motion for the creation and annihilation operators, the equation of motion for the mixed Green's functions can be derived as

$$(G_{\mathbf{M}})_{\alpha\gamma}^{-1}(\mathbf{r}_{1},\tau_{1})(G_{\mathbf{T}})_{\gamma\beta}(\mathbf{r}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2})$$
  
=  $\lambda \int d^{2}\mathbf{R}' T_{\alpha\gamma}(\mathbf{r}_{1},\mathbf{R}')(G_{\mathbf{S}})_{\gamma\beta}(\mathbf{R}',\tau_{1};\mathbf{R}_{2},\tau_{2}).$  (A8)

Equation (A7) and (A8) gives

$$(G_{\mathrm{T}})_{\alpha\beta}(\mathbf{r}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2}) = \frac{\lambda}{\hbar} \int \mathrm{d}\tau' \mathrm{d}^{2}\mathrm{R}' \mathrm{d}^{3}\mathrm{r}'$$
  

$$(G_{\mathrm{M}})_{\alpha\mu}(\mathbf{r}_{1},\tau_{1};\mathbf{r}',\tau')T_{\mu\nu}(\mathbf{r}',\mathbf{R}')(G_{\mathrm{S}})_{\nu\beta}(\mathbf{R}',\tau';\mathbf{R}_{2},\tau_{2}).$$
(A9)

The Dyson equation for the Green's function of the TI surface states can be written as

$$(G_{\mathbf{S}})_{\alpha\gamma}^{-1}(\mathbf{R}_{1},\tau_{1})(G_{\mathbf{S}})_{\gamma\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2})$$
  
-  $\int d^{2}\mathbf{R}' d\tau'(\Sigma_{\mathbf{S}})_{\alpha\gamma}(\mathbf{R}_{1},\tau_{1};\mathbf{R}',\tau')(G_{\mathbf{S}})_{\gamma\beta}(\mathbf{R}',\tau';\mathbf{R}_{2},\tau_{2})$   
=  $\frac{\hbar}{\lambda}\delta(\mathbf{R}_{1}-\mathbf{R}_{2})\delta(\tau_{1}-\tau_{2})\delta_{\alpha\beta},$  (A10)

where  $(G_S)^{-1}(\mathbf{R}, \tau) = i\hbar\partial_{\tau} - \epsilon_S(\mathbf{R}) + \epsilon_F\sigma_0$ , and  $\Sigma_S$  is the self energy due to tunneling and disorder, i.e.  $\Sigma_S = \Sigma_T + \Sigma_D$ . The self-energy for tunneling will be given by

$$(\Sigma_{\mathbf{T}})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2}) = \frac{\lambda}{\hbar} \int d^{3}\mathbf{r}' d^{3}\mathbf{r}''$$

$$T^{\dagger}_{\alpha\mu}(\mathbf{R}_{1},\mathbf{r}')(G_{\mathsf{M}})_{\mu\nu}(\mathbf{r}',\tau_{1};\mathbf{r}'',\tau_{2})T_{\nu\beta}(\mathbf{r}'',\mathbf{R}_{2}).$$
(A11)

For  $T_{\alpha\beta}(\mathbf{r}, \mathbf{R}) = t(\mathbf{R})\delta(\mathbf{r}_{\parallel} - \mathbf{R})\delta(z)\delta_{\alpha\beta}$ , we obtain

$$\begin{aligned} (\Sigma_{\mathrm{T}})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2}) \\ &= \frac{\lambda}{\hbar} t(\mathbf{R}_{1}) (G_{\mathrm{M}})_{\alpha\beta}(\mathbf{R}_{1},z_{1}=0,\tau_{1};\mathbf{R}_{2},z_{2}=0,\tau_{2}) t(\mathbf{R}_{2}). \end{aligned}$$

$$(A12)$$

The self energy for disorder is given by

$$\begin{aligned} &(\Sigma_{\mathrm{D}})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2})\\ &=\frac{\lambda}{\hbar}V_{\mathrm{D}}(\mathbf{R}_{1})(G_{\mathrm{S}})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{R}_{2},\tau_{2})V_{\mathrm{D}}(\mathbf{R}_{2}). \end{aligned}$$
(A13)

By analytical continuation from the Schwinger-Keldysh time contour to the real time axis, Eq. (A7-A13) can be

written in terms of Keldysh space Green's functions  $\check{G}_i$  (i = S,T,M) and self energies  $\check{\Sigma}_j$  (j = S,T,D)

$$\check{G}_{i} = \begin{pmatrix} G_{i}^{\mathsf{R}} & G_{i}^{\mathsf{K}} \\ 0 & G_{i}^{\mathsf{A}} \end{pmatrix}, \ \check{\Sigma}_{j} = \begin{pmatrix} \Sigma_{j}^{\mathsf{R}} & \Sigma_{j}^{\mathsf{K}} \\ 0 & \Sigma_{j}^{\mathsf{A}} \end{pmatrix},$$
(A14)

where  $G_i^{\mathbf{R},\mathbf{A},\mathbf{K}}$  ( $\Sigma_j^{\mathbf{R},\mathbf{A},\mathbf{K}}$ ) are the retarded, advanced and Keldysh Green's functions (self energies), all of which are 2 × 2 matrices in spin space with variables ( $\mathbf{R}_1, t_1; \mathbf{R}_2, t_2$ ) with  $t_1, t_2$ being real time variables. A function  $A(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2)$  can be Wigner transformed to  $\tilde{A}(\mathbf{R}, \mathbf{T}; \mathbf{p}, \omega)$  by doing a coordinate transformation to the center-of-mass coordinates ( $\mathbf{R}, \mathbf{T}$ ) and relative coordinates ( $\delta \mathbf{R}, \delta t$ ), and performing Fourier transforms of these relative coordinates to momentum and frequency variable ( $\mathbf{p}, \omega$ ). We define the modified Wigner transformed function in terms of momentum and energy ( $\mathbf{p}, \epsilon = \hbar\omega$ ) by  $A(\mathbf{R}, \mathbf{T}; \mathbf{p}, \epsilon) = \hbar \tilde{A}(\mathbf{R}, \mathbf{T}; \mathbf{p}, \omega)$ , which is related to  $A(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2)$  by

$$A(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2) = \int \frac{\mathrm{d}\epsilon}{2\pi} \frac{\mathrm{d}^2 \mathbf{p}}{(2\pi)^2} A(\mathbf{R}, \mathsf{T}; \mathbf{p}, \epsilon) e^{i(\mathbf{p}\cdot\delta\mathbf{R} - \frac{\epsilon}{\hbar}\delta\mathbf{t})}.$$

We use the lowest order gradient expansion to express the Wigner transform of a product function to the product of Wigner transformed function, which gives the following relation for the modified Wigner transformed functions

$$(AB)(\mathbf{R}, \mathsf{T}; \mathbf{p}, \epsilon) = \hbar A(\mathbf{R}, \mathsf{T}; \mathbf{p}, \epsilon) B(\mathbf{R}, \mathsf{T}; \mathbf{p}, \epsilon).$$
(A16)

The Keldysh component of the the Wigner transformed leftright subtracted Dyson equation, written in terms of the modified Wigner transformed Green's function and self energy, gives the quantum kinetic equation

$$\partial_{\mathbf{T}}G_{\mathbf{S}}^{\mathbf{K}} + \frac{1}{2} \{ \mathbf{v} \cdot \nabla_{\mathbf{R}}, G_{\mathbf{S}}^{\mathbf{K}} \} + \frac{i}{\hbar} \left[ \epsilon_{\mathbf{S}}(\mathbf{p}), G_{\mathbf{S}}^{\mathbf{K}} \right]$$

$$= -i \left[ \left( \Sigma_{\mathbf{S}}^{\mathbf{R}}G_{\mathbf{S}}^{\mathbf{K}} - G_{\mathbf{S}}^{\mathbf{K}}\Sigma_{\mathbf{S}}^{\mathbf{A}} \right) - \left( G_{\mathbf{S}}^{\mathbf{R}}\Sigma_{\mathbf{S}}^{\mathbf{K}} - \Sigma_{\mathbf{S}}^{\mathbf{K}}G_{\mathbf{S}}^{\mathbf{A}} \right) \right],$$
(A17)

where  $\epsilon_{\rm S}(\mathbf{p}) = \hbar v_{\rm F} \mathbf{\sigma} \cdot (\hat{\mathbf{z}} \times \mathbf{p})$  and  $\mathbf{v} = v_F (\mathbf{\sigma} \times \hat{\mathbf{z}})$ .

The self energy is due to disorder and tunneling from the metal. For the disorder potential  $V_{\rm D}(\mathbf{R}) = V_0 \Sigma_{j=1}^{N_{\rm I}} \delta(\mathbf{R} - \mathbf{R}_j^{\rm I})$ , from Eq. (A13) the disorder self energy becomes, after impurity averaging,

$$\check{\Sigma}_{\mathrm{D}}(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2) = \frac{\lambda V_0^2 n_{\mathrm{i}}}{\hbar} \delta(\mathbf{R}_1 - \mathbf{R}_2) \check{G}_{\mathrm{S}}(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2),$$
(A18)

and the Wigner transformed disorder self energy reads

$$\check{\Sigma}_{\mathrm{D}}(\mathbf{R},\mathrm{T};\mathbf{p},\epsilon) = \frac{\lambda V_0^2 n_{\mathrm{i}}}{\hbar} \int \frac{\mathrm{d}^2 \mathrm{p}'}{(2\pi)^2} \check{G}_{\mathrm{S}}(\mathbf{R},\mathrm{T};\mathbf{p}',\epsilon). \quad (A19)$$

We introduce the 2D quasi-classical Green's functions for the TI surface states defined as

$$\check{g}_{\mathbf{S}}(\mathbf{R}, \mathbf{T}; \mathbf{p}_{\mathbf{F}} \hat{\mathbf{p}}, \epsilon) = \frac{i\lambda}{\pi} \int d\xi_{\mathbf{S}} \,\check{G}_{\mathbf{S}}(\mathbf{R}, \mathbf{T}; \mathbf{p}, \epsilon), \qquad (A20)$$

where  $\xi_{\rm S} = \hbar v_{\rm F} p - \epsilon_{\rm F}$ , and the  $\xi_{\rm S}$  integration is performed near the Fermi surface. As the quasi-classical Green's function is peaked at the Fermi energy, the following *ansatz* holds

$$\check{G}_{\rm S}(\mathbf{R},{\rm T};\mathbf{p},\epsilon) = -\frac{i\pi}{\lambda}\check{g}_{\rm S}(\mathbf{R},{\rm T};{\rm p}_{\rm F}\hat{\mathbf{p}},\epsilon)\delta(\xi_{\rm S}). \tag{A21}$$

The disorder self-energy now can be written as

$$\check{\Sigma}_{\rm D}(\mathbf{R}, \mathrm{T}; \mathbf{p}, \epsilon) = -\frac{i}{\tau_{\rm p}} \langle \check{g}_{\rm S}(\mathbf{R}, \mathrm{T}; \mathbf{p}_{\rm F} \hat{\mathbf{p}}, \epsilon) \rangle, \qquad (A22)$$

where  $\langle ... \rangle$  denotes angular averaging in the **p** space and we define  $1/\tau_{\rm p} = \pi V_0^2 n_{\rm i} N_{\rm F}/\hbar$ .

To calculate the tunneling self energy, we first consider the interface being rough which can be modeled by a random distribution of tunneling centers  $\mathbf{R}_i^{\text{S}}$  with  $t(\mathbf{R}) = t_0 \sum_{i=1}^{N_{\text{S}}} \delta(\mathbf{R} - \mathbf{R}_i^{\text{S}})$ . Then, averaging over the tunneling centers, the tunneling self energy is given by

$$\check{\Sigma}_{\mathrm{T}}(\mathbf{R}_{1}, t_{1}; \mathbf{R}_{2}, t_{2}) = \frac{\lambda t_{0}^{2} n_{\mathrm{s}}}{\hbar} \delta(\mathbf{R}_{1} - \mathbf{R}_{2}) \check{G}_{\mathrm{M}}(\mathbf{R}_{1}, z_{1} = 0, t_{1}; \mathbf{R}_{2}, z_{2} = 0, t_{2}),$$
(A23)

and after the Wigner transform it becomes

$$\check{\Sigma}_{\mathrm{T}}(\mathbf{R},\mathrm{T};\mathbf{p},\epsilon) = \frac{\lambda t_0^2 n_{\mathrm{s}}}{\hbar} \int \frac{\mathrm{d}^3 \mathrm{k}'}{(2\pi)^3} \check{G}_{\mathrm{M}}(\mathbf{R},z=0,\mathrm{T};\mathbf{k}',\epsilon),$$
(A24)

where  $\tilde{G}_{\rm M}(\mathbf{r}_{\parallel}, z, {\rm T}; \mathbf{k}, \epsilon)$  is the Wigner transform with respect to the 3D position and time coordinates. Now, we consider the 3D quasi-classical Green's functions for the metal defined as

$$\check{g}_{\mathrm{M}}(\mathbf{r},\mathrm{T};\mathbf{k}_{\mathrm{F}}\hat{\mathbf{k}},\epsilon) = \frac{i}{\pi} \int \mathrm{d}\xi_{\mathrm{M}} \,\check{G}_{\mathrm{M}}(\mathbf{r},\mathrm{T};\mathbf{k},\epsilon),\qquad(\mathrm{A25})$$

where  $\xi_{\rm M} = \hbar^2 k^2 / (2m) + \epsilon_{\rm b} - \epsilon_{\rm F}$ ,  $k_{\rm F}$  is the Fermi momentum in the metal and the  $\xi_{\rm M}$  integration is performed near the Fermi surface. Since the quasi-classical Green's function is peaked at the Fermi energy, the Green's function satisfies following *ansatz* 

$$\hat{G}_{\mathrm{M}}(\mathbf{r},\mathrm{T};\mathbf{k},\epsilon) = -i\pi\check{g}_{\mathrm{M}}(\mathbf{r},\mathrm{T};\mathrm{k}_{\mathrm{F}}\hat{\mathbf{k}},\epsilon)\delta(\xi_{\mathrm{M}}).$$
 (A26)

So the tunneling self-energy can be written as

$$\check{\Sigma}_{\mathrm{T}}(\mathbf{R},\mathrm{T};\mathbf{p},\epsilon) = -\frac{i}{\tau_{\mathrm{t}}} \langle \check{g}_{\mathrm{M}}(\mathbf{R},z=0,\mathrm{T};\mathbf{k}_{\mathrm{F}}\hat{\mathbf{k}},\epsilon) \rangle, \quad (A27)$$

where  $\langle ... \rangle$  denotes angular averaging in the **k** space and we define  $1/\tau_t = \pi t_0^2 n_s N_{3D} \lambda/\hbar$ .

In case of a smooth interface, the tunneling can be modeled by  $t(\mathbf{R}) = t_c$  being constant, and the Wigner transform tunneling self energy will be

$$\begin{split} \check{\Sigma}_{\mathrm{T}}(\mathbf{R},\mathrm{T};\mathbf{p},\epsilon) &= \frac{\lambda t_{\mathrm{c}}^2}{\hbar} \int \frac{\mathrm{d}k_z'}{2\pi} \check{G}_{\mathrm{M}}(\mathbf{R},z=0,\mathrm{T};\mathbf{p},k_z',\epsilon) \\ &= \frac{\lambda t_{\mathrm{c}}^2}{\hbar} \int \frac{\mathrm{d}^3 \mathbf{k}'}{(2\pi)^3} \check{G}_{\mathrm{M}}(\mathbf{R},z=0,\mathrm{T};\mathbf{k}_{\parallel}',k_z',\epsilon) (2\pi)^2 \delta(\mathbf{k}_{\parallel}'-\mathbf{p}), \end{split}$$
(A28)

where the in-plane momentum conservation holds. Using the *ansatz* Eq. (A26) for the Green's function and assuming that the 3D quasi-classical Green's function is isotropic in the  $\mathbf{k}$ 

space, i.e. independent of the solid angle in the **k** space, because of the isotropy of the Fermi surface in the metal, we obtain same relation for the tunneling self energy as Eq. (A27) with a redefined tunneling time given by  $1/\tau_t = \pi t_c^2 N_{1D} \lambda / \hbar$ .

In the quasi-classical limit, the Fermi energy is the largest energy scale, so the lowest order solution to the Green's function  $G_S^K$  is given by the one that commutes with the term  $\epsilon_S(\mathbf{R})$ in the commutator in Eq. (A17). Also, the normalization condition satisfied by the Keldysh Green's function  $\check{G}_S$  allows one to write the retarded/advanced Green's functions of the TI surface states to be obtained from the upper band projector of the surface state Hamiltonian<sup>16</sup>, i.e.

$$G_{\mathbf{S}}^{\mathbf{R},\mathbf{A}}(\mathbf{p},\epsilon) = \frac{1}{2\lambda} \frac{\sigma_0 + \mathbf{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}})}{\epsilon - \xi_{\mathbf{S}} \pm i0^+}.$$
 (A29)

The retarded/advanced quasi-classical Green's functions and the disorder self energies are then given by,

$$g_{\mathsf{S}}^{\mathsf{R},\mathsf{A}} = \pm \frac{1}{2} [\sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\boldsymbol{p}})], \ \Sigma_{\mathsf{D}}^{\mathsf{R},\mathsf{A}} = \mp \frac{i}{2\tau_{\mathsf{p}}} \sigma_0.$$
(A30)

We consider the following *ansatz* for the Keldysh component  $g_{\rm S}^{\rm K}(\hat{\mathbf{p}},\epsilon) = g_{\rm S}'(\hat{\mathbf{p}},\epsilon)[\sigma_0 + \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}})]$ , which means that the spin and momentum is locked for the TI surface states even in the non-equilibrium situation. In the diffusive limit, we can expand  $g_{\rm S}'(\hat{\mathbf{p}},\epsilon)$  in spherical harmonics<sup>16,17</sup>, i.e.,  $g_{\rm S}'(\hat{\mathbf{p}},\epsilon) = g_{\rm s}(\epsilon) + \hat{\mathbf{p}} \cdot \mathbf{g}_{\rm a}(\epsilon)$ , and solve the kinetic equation Eq. (A17). The charge density n on the surface of the TI will be obtained from  $g_{\rm S}^{\rm K}(\hat{\mathbf{p}},\epsilon)$  by<sup>18</sup>

$$n = \frac{eN_{\rm F}}{2} \int \mathrm{d}\epsilon \frac{\mathrm{Tr}}{2} [\langle g^{\rm K}(\hat{\mathbf{p}},\epsilon) \rangle] = \frac{eN_{\rm F}}{2} \int \mathrm{d}\epsilon \; \mathrm{g}_{\rm s}(\epsilon), \quad (A31)$$

and the current density  $\mathbf{J}_{c}$  is given by

$$\mathbf{J}_{c} = \frac{eN_{F}}{2} \int \mathrm{d}\epsilon \frac{\mathrm{Tr}}{2} [\langle \mathbf{v}g^{\mathrm{K}}(\hat{\mathbf{p}}, \epsilon) \rangle] = \frac{eN_{F}}{2} \int \mathrm{d}\epsilon \ \frac{v_{F}}{2} \mathbf{g}_{\mathrm{a}}(\epsilon).$$
(A32)

The retarded/advanced Green's functions of the metal is given by

$$G_{\mathbf{M}}^{\mathbf{R},\mathbf{A}}(\mathbf{k},\epsilon) = \frac{1}{\epsilon - \xi_{\mathbf{M}} \pm i0^{+}} \sigma_{0}, \qquad (A33)$$

so the retarded/advanced quasi-classical Green's functions and the tunneling self energies are obtained to be

$$g_{\mathrm{M}}^{\mathrm{R,A}} = \pm \sigma_0, \ \Sigma_{\mathrm{D}}^{\mathrm{R,A}} = \mp \frac{i}{\tau_{\mathrm{t}}} \sigma_0.$$
 (A34)

We consider the effect of the applied charge and the spin potential in the metal through the Keldysh component of the Green's function in the metal  $g_M^K(\hat{\mathbf{k}}, \epsilon)$ , which is considered to be independent of solid angle in the  $\mathbf{k}$  space because of the isotropy of the Fermi surface in the metal. From Eq. (A27), the tunneling self energy only depends on  $g_M^K(z = 0, \hat{\mathbf{k}}, \epsilon)$ , so we only consider  $g_M^K(\hat{\mathbf{k}}, \epsilon)$  at the interface z = 0, but will write  $g_M^K(\hat{\mathbf{k}}, \epsilon)$  instead for brevity. The Keldysh component of the Green's function in the metal can be written as  $g_{\rm M}^{\rm K}(\hat{\mathbf{k}},\epsilon) = [\mathbf{g}_{\rm M}^0(\epsilon)\sigma_0 + \boldsymbol{\sigma} \cdot \mathbf{g}_{\rm M}(\epsilon)]$ . Further, the quantities charge and spin densities in the metal, and the corresponding charge and spin electrochemical potential in the metal will refer to the values at the interface and not be explicitly written afterwards. The charge density  $n_{\rm M}$  in the metal is given by

$$n_{\rm M} = \frac{eN_{\rm 3D}}{2} \int \mathrm{d}\epsilon \frac{\mathrm{Tr}}{2} [\langle g_{\rm M}^{\rm K}(\hat{\mathbf{k}},\epsilon) \rangle] = \frac{eN_{\rm 3D}}{2} \int \mathrm{d}\epsilon \ g_{\rm M}^{0}(\epsilon), \tag{A35}$$

and the spin density  $\mathbf{s}_{\mathrm{M}}$  (in the unit of charge -e) is obtained from

$$\mathbf{s}_{\mathrm{M}} = \frac{eN_{\mathrm{3D}}}{2} \int \mathrm{d}\epsilon \frac{\mathrm{Tr}}{2} [\langle \boldsymbol{\sigma} g_{\mathrm{M}}^{\mathrm{K}}(\hat{\mathbf{k}}, \epsilon) \rangle] = \frac{eN_{\mathrm{3D}}}{2} \int \mathrm{d}\epsilon \; \mathbf{g}_{\mathrm{M}}(\epsilon). \tag{A36}$$

As we have defined in the main text, the charge electrochemical potential  $\mu_0$  and the spin electrochemical potential  $\mu$  in the metal are given by  $n_{\rm M} = 2e^2 N_{\rm 3D}\mu_0$  and  $\mathbf{s}_{\rm M} = e^2 N_{\rm 3D}\mu$ . So, we obtain the following relations for  $\mu_0$  and  $\mu$  in terms of the quasi-classical Green's functions

$$\mu_0 = \frac{1}{4e} \int d\epsilon \ \mathbf{g}_{\mathbf{M}}^0(\epsilon), \ \mathbf{\mu} = \frac{1}{2e} \int d\epsilon \ \mathbf{g}_{\mathbf{M}}(\epsilon).$$
(A37)

After doing  $\xi_s$  integration of the Eq. (A17), and using Eqs. (A27) and Eq. (A30), we obtain

$$\partial_{\mathrm{T}}g_{\mathrm{S}}^{\mathrm{K}} + \frac{1}{2}v_{\mathrm{F}}\left\{\boldsymbol{\sigma} \times \hat{\boldsymbol{z}} \cdot \nabla_{\mathbf{R}}, g_{\mathrm{S}}^{\mathrm{K}}\right\} + iv_{\mathrm{F}}p_{\mathrm{F}}[\boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\mathbf{p}}), g_{\mathrm{S}}^{\mathrm{K}}]$$

$$= -\frac{g_{\mathrm{S}}^{\mathrm{K}}}{\tau_{\mathrm{p}}} + \frac{\langle g_{\mathrm{S}}^{\mathrm{K}} \rangle}{\tau_{\mathrm{p}}} + \frac{1}{2\tau_{\mathrm{p}}}\left\{\boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\mathbf{p}}), \langle g_{\mathrm{S}}^{\mathrm{K}} \rangle\right\}$$

$$- \frac{2g_{\mathrm{S}}^{\mathrm{K}}}{\tau_{\mathrm{t}}} + \frac{1}{2\tau_{\mathrm{t}}}\left\{\sigma_{0} + \boldsymbol{\sigma} \cdot (\hat{\boldsymbol{z}} \times \hat{\mathbf{p}}), \langle g_{\mathrm{M}}^{\mathrm{K}} \rangle\right\}.$$
(A38)

Now using the *ansatz* for  $g_{\rm S}^{\rm K}$ , after taking trace of Eq. (A.38) and integrating out the s- and p-wave components, we obtain

$$\partial_{\mathrm{T}}\mathbf{g}_{\mathrm{s}} + \frac{1}{2}v_{\mathrm{F}}\nabla_{\mathbf{R}} \cdot \mathbf{g}_{\mathrm{a}} = \frac{2}{\tau_{\mathrm{t}}} \left(\frac{\mathbf{g}_{\mathrm{M}}^{0}}{2} - \mathbf{g}_{\mathrm{s}}\right),\tag{A39a}$$

$$\partial_{\mathrm{T}}\mathbf{g}_{\mathrm{a}} + v_{\mathrm{F}}\nabla_{\mathbf{R}}\mathbf{g}_{\mathrm{s}} = \frac{2}{\tau_{\mathrm{t}}} \left(\frac{\mathbf{g}_{\mathrm{M}}}{2} \times \hat{\mathbf{z}}\right) - \left(\frac{2}{\tau_{\mathrm{t}}} + \frac{1}{2\tau_{\mathrm{p}}}\right) \mathbf{g}_{\mathrm{a}}, \quad (A39b)$$

which is equivalent to Eq. (9) in the main text. After  $\epsilon$  integration of Eq. (A39a) and using the Eq. (A31), (A32) and (A37), we obtain the diffusion equation in the TI i.e. Eq. (12) in the main text. Similarly, after  $\epsilon$  integration of Eq. (A39b), the current density  $\mathbf{J}_c$  is obtained to be the same as Eq. (13) in the main text.

The spin current density across the interface (in the unit of electron charge per unit area per unit time) will be given by  $\mathbf{J}_{\mathbf{s}} = -e\lambda d\mathbf{s}/dt = -e\lambda(i/\hbar)[H_{\mathrm{T}},\mathbf{s}]$  by the Heisenberg equation of motion, where  $\mathbf{s} = \langle a_{\alpha}^{\dagger}(\mathbf{R},t)\boldsymbol{\sigma}_{\alpha\beta}a_{\beta}(\mathbf{R},t)\rangle$ . Applying the equation of motion to the operators, we obtain

$$\mathbf{J}_{s} = \frac{-e\lambda}{\hbar} \int d^{3}\mathbf{r} \operatorname{Tr} \left[ \boldsymbol{\sigma} \Big( G_{Tc}^{<}(\mathbf{R}, t; \mathbf{r}, t) T(\mathbf{r}, \mathbf{R}) - T^{\dagger}(\mathbf{R}, \mathbf{r}) G_{T}^{<}(\mathbf{r}, t; \mathbf{R}, t) \Big) \right].$$
(A40)

Here, the complex conjugate tunneling Green's function  $(G_{\text{Tc}})_{\alpha\beta}(\mathbf{R}, t_1; \mathbf{r}, t_2) = (G_{\text{T}})^*_{\beta\alpha}(\mathbf{r}, t_2; \mathbf{R}, t_1)$ , and  $G^<_{\text{Tc}}, G^<_{\text{T}}$  are the corresponding lesser Green's function. From Eq. (A9), we obtain for the complex conjugate tunneling Green's function

$$(G_{\mathrm{Tc}})_{\alpha\beta}(\mathbf{R}_{1},\tau_{1};\mathbf{r}_{2},\tau_{2}) = \frac{\lambda}{\hbar} \int d\tau' d^{2}\mathbf{R}' d^{3}\mathbf{r}'$$
  

$$(G_{\mathrm{S}})_{\alpha\mu}(\mathbf{R}_{1},\tau_{1};\mathbf{R}',\tau')T^{\dagger}_{\mu\nu}(\mathbf{R}',\mathbf{r}')(G_{\mathrm{M}})_{\nu\beta}(\mathbf{r}',\tau';\mathbf{r}_{2},\tau_{2}).$$
(A41)

We write Eq. (A9), (A41) and (A11) in a simpler form as  $G_{\rm T} = \frac{\lambda}{\hbar}G_{\rm M}TG_{\rm S}$ ,  $G_{\rm Tc} = \frac{\lambda}{\hbar}G_{\rm S}T^{\dagger}G_{\rm M}$  and  $\Sigma_{\rm T} = \frac{\lambda}{\hbar}T^{\dagger}G_{\rm M}T$ , where the integrations over the internal variables are implicit. Then, from Eq. (A40),  $\mathbf{J}_{\rm s}$  can be written as

$$\mathbf{J}_{\mathrm{s}} = \frac{-e\lambda}{\hbar} \operatorname{Tr} \left[ \boldsymbol{\sigma} \left( G_{\mathrm{Tc}}^{<} T - T^{\dagger} G_{\mathrm{T}}^{<} \right) \right].$$
(A42)

By using Langreth rule<sup>19</sup> for the lesser function of product of three functions, which is given by

$$(ABC)^{<} = A^{R}B^{R}C^{<} + A^{R}B^{<}C^{A} + A^{<}B^{A}C^{A},$$
(A43)

 $G_{\text{Tc}}^{<}, G_{\text{T}}^{<}$  can be written as

$$G_{\rm T}^{<} = \frac{\lambda}{\hbar} \bigg[ G_{\rm M}^R T G_{\rm S}^{<} + G_{\rm M}^{<} T G_{\rm S}^A \bigg], \tag{A44a}$$

$$G_{\rm Tc}^{<} = \frac{\lambda}{\hbar} \bigg[ G_{\rm S}^R T^{\dagger} G_{\rm M}^{<} + G_{\rm S}^{<} T^{\dagger} G_{\rm M}^A \bigg]. \tag{A44b}$$

Here we have used the fact that the instantaneous tunneling T is neither retarded nor advanced and diagonal in Keldysh space, i.e.  $T^R = T^A = T$  and  $T^{<} = T^{>} = 0$ , and similarly for  $T^{\dagger}$ . Inserting Eq. (A44a) and (A44b), and using the relation for  $\Sigma_{\rm T}$ , Eq. (A42) is written as

$$\mathbf{J}_{\mathrm{s}} = \frac{-e\lambda}{\hbar} \operatorname{Tr} \left[ \boldsymbol{\sigma} \left( G_{\mathrm{S}}^{R} \Sigma_{\mathrm{T}}^{<} + G_{\mathrm{S}}^{<} \Sigma_{\mathrm{T}}^{A} - \Sigma_{\mathrm{T}}^{R} G_{\mathrm{S}}^{<} - \Sigma_{\mathrm{T}}^{<} G_{\mathrm{S}}^{A} \right) \right].$$
(A45)

Now the lesser functions in Eq. (A45) can be written in terms of retarded, advanced and Keldysh component as  $G_{\rm S}^{<} = \frac{1}{2}[G_{\rm S}^{K} - G_{\rm S}^{R} + G_{\rm S}^{A}]$  and  $\Sigma_{\rm T}^{<} = \frac{1}{2}[\Sigma_{\rm T}^{K} - \Sigma_{\rm T}^{R} + \Sigma_{\rm T}^{A}]$ . In the calculation of non-equilibrium quantities, only the Keldysh component is important<sup>18</sup>, so  $\mathbf{J}_{\rm s}$  is given by

$$\mathbf{J}_{s} = \frac{-e\lambda}{\hbar} \frac{\mathrm{Tr}}{2} \bigg[ \boldsymbol{\sigma} \Big( G_{S}^{R} \boldsymbol{\Sigma}_{T}^{K} + G_{S}^{K} \boldsymbol{\Sigma}_{T}^{A} - \boldsymbol{\Sigma}_{T}^{R} G_{S}^{K} - \boldsymbol{\Sigma}_{T}^{K} G_{S}^{A} \Big) \bigg].$$
(A46)

The above equation Eq. (A46) is written in coordinate representation and the product of two functions implies integration over the internal coordinate. The Eq. (A46) can be written in terms of the modified Wigner transformed function in which the transformation of the product of two functions will be given by Eq. (A16). So, in terms of the modified Wigner transformed functions,  $J_s$  can be written as

$$\mathbf{J}_{\mathrm{s}} = -e\lambda \int \frac{\mathrm{d}\epsilon}{2\pi} \frac{\mathrm{d}^{2}\mathbf{p}}{(2\pi)^{2}} \frac{\mathrm{Tr}}{2} \bigg[ \mathbf{\sigma} \Big( G_{\mathrm{S}}^{R} \Sigma_{\mathrm{T}}^{K} + G_{\mathrm{S}}^{K} \Sigma_{\mathrm{T}}^{A} - \Sigma_{\mathrm{T}}^{R} G_{\mathrm{S}}^{K} - \Sigma_{\mathrm{T}}^{K} G_{\mathrm{S}}^{A} \Big) \bigg].$$
(A47)

Using Eqs. (A21), (A27), (A30) and (A34), the above equation Eq. (A48) can be written in terms of the quasi-classical Green's functions as

$$\begin{split} \mathbf{J}_{s} &= \frac{eN_{\mathrm{F}}}{2} \int \mathrm{d}\epsilon \int \frac{\mathrm{d}\theta}{2\pi} \frac{\mathrm{Tr}}{2} \bigg[ \mathbf{\sigma} \Big( -\frac{2g_{\mathrm{S}}^{\mathrm{K}}}{\tau_{\mathrm{t}}} \\ &+ \frac{1}{2\tau_{\mathrm{t}}} \big\{ \sigma_{0} + \mathbf{\sigma} \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{p}}), \langle g_{\mathrm{M}}^{\mathrm{K}} \rangle \big\} \Big) \bigg] \end{split}$$
(A48)

It is clear from Eq. (A48) that the spin current density across the interface will be obtained from taking trace over the spin Pauli matrices of the tunneling term, i.e. the last two terms in Eq. (A38). Now, using the *ansatz* for  $g_{\rm S}^{\rm K}$  and  $g_{\rm M}^{\rm K}$ , and using the definitions for  $J_{\rm c}$  and  $\mu$  from Eqs. (A32) and (A37), we get the same equation for  $J_{\rm s}$ , i.e. Eq. (15) in the main text.

### Appendix B: Solution of diffusion equation in the TI with different boundary conditions in the metal

We consider an one-dimensional problem to solve the diffusion equation in the TI analytically. The transport direction is taken to be in the x direction, while we consider an in-plane spin electrochemical potential in the metal with only the y component of spin, i.e.  $\mu = \mu_y \hat{y}$ . Then the charge current density on the TI surface is given by  $\mathbf{J}_c = \mathbf{J}_c \hat{x}$ , and the spin current density across the interface will have only y component, i.e.  $\mathbf{J}_s = \mathbf{J}_s \hat{y}$ . The continuity equation in the TI, i.e. Eq. (12) becomes

$$\partial_{\mathrm{T}}n + \partial_x \mathbf{J_c} = \frac{2}{\tau_{\mathrm{t}}} (e^2 N_{\mathrm{F}} \mu_0 - n),$$
 (B1)

and from Eq. (13) we obtain the charge current density  $J_c$  in the TI to be

$$\mathbf{J}_{\mathbf{c}} = \frac{1}{(1 - i\omega\tau_{\mathrm{tr}})} \left[ -\frac{v_{\mathrm{F}}^2 \tau_{\mathrm{tr}}}{2} \partial_x n + e^2 N_{\mathrm{F}} v_{\mathrm{F}} \frac{\tau_{\mathrm{tr}}}{\tau_{\mathrm{t}}} \frac{\mu_y}{2} \right].$$
(B2)

Then, from Eq. (15), the spin current density  $J_s$  is given by

$$\mathbf{J}_{\mathrm{s}} = \frac{2}{v_{\mathrm{F}}\tau_{\mathrm{t}}} \left( e^2 N_{\mathrm{F}} v_{\mathrm{F}} \frac{\mu_y}{2} - \mathbf{J}_c \right). \tag{B3}$$

We assume that  $\mu_0$  and  $\mu_y$  in the metal to be homogeneous. In the steady state, Eq. (B1) and (B2) give the differential equation  $\partial_x^2 n' = n'/l^2$  for the new variable  $n' = (n - e^2 N_{\rm F} \mu_0)$ , where the characteristic length l is given by  $l = v_{\rm F} \sqrt{\tau_{\rm tr} \tau_{\rm t}}/2$ . The solution to n' is given by  $n'(x) = A_+ e^{x/l} + A_- e^{-x/l}$ . In case of a short circuit between the two ends of the surface of the TI, we apply the boundary condition that the electrochemical potential in the TI at the two ends to be same, i.e. n'(+L/2) = n'(-L/2), and the current going into the TI surface to be same as the current coming out of the TI surface (as there is no current leaking out through the metal), i.e.  $J_{\rm c}(+L/2) = J_{\rm c}(-L/2)$ . The condition n'(+L/2) = n'(-L/2) gives  $A_+ = A_- = A$  and the current density  $J_{\rm c} = -(v_{\rm F}^2 \tau_{\rm tr}/2l)A(e^{x/l} - e^{-x/l}) + J_0$ , where  $J_0$ 

 $e^2 N_{\rm F} v_{\rm F} \tau_{\rm tr} \mu_y / 2\tau_{\rm t}$ . Now the condition  $J_{\rm c}(+L/2) = J_{\rm c}(-L/2)$ is true only if A = 0, i.e. n' = 0 which implies  $n = e^2 N_{\rm F} \mu_0$ . So the charge density n in the TI becomes homogeneous and balances any charge potential in the metal, and the charge current density  $J_{\rm c}$  in the TI becomes homogeneous and is given by  $J_{\rm c} = J_0$ . As both  $\mu_y$  and  $J_{\rm c}$  are homogeneous, so the current density  $J_{\rm s}$  through the interface also becomes homogeneous and is given by  $J_{\rm s} = J_0 / v_{\rm F} \tau_{\rm HE}$ .

Next we assume  $\mu_0$  in the metal and  $J_s$  across the interface to be homogeneous. From Eq. (B1), (B2) and (B3), we obtain a new differential equation  $\partial_x^2 n' = n'/l'^2$ , where the length l' is given by  $l'^2 = 2l^2 \tau_{\text{IEE}}/\tau_{\text{tr}}$  ( $\tau_{\text{IEE}}$  is given by Eq. (19)). The solution to n' will be given by  $n'(x) = A_+ e^{x/l'} + A_- e^{-x/l'}$ . As discussed in the previous paragraph,

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for short circuit case the boundary condition n'(+L/2) = n'(-L/2) gives  $A_+ = A_- = A$  and the current density  $J_c = -(v_F^2 \tau_{IEE}/l')A(e^{x/l'} - e^{-x/l'}) + v_F \tau_{IEE}J_s$ . As the spin current density across the interface is assumed to be homogeneous, the condition  $J_c(+L/2) = J_c(-L/2)$  is true only if A = 0, which implies  $n = e^2 N_F \mu_0$ , so the charge density n is homogeneous. The current density  $J_c$  in the TI becomes homogeneous and is given by  $J_c = v_F \tau_{IEE}J_s$ . As both  $J_c$  and  $J_s$  are homogeneous, the spin electrochemical potential  $\mu_y$  in the metal turns out to be constant as well. Hence, either with a homogeneous condition for  $\mu_y$  or  $J_s$ , the solution for short circuit condition gives a homogeneous solution for n and  $J_c$  in the TI.

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