Transport theory for electrical detection of the spin-momentum locking of topological surface states

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Abstract

We provide a general transport theory for spin-polarized scanning tunneling microscopy (STM) through a doped topological insulator (TI) surface. It is found that different from the conventional magnetic substrate, the tunneling conductance through the tip-TI surface acquires an extra component determined by the in-plane spin texture, exclusively associated with the spin momentum locking. Importantly, this extra conductance unconventionally depends on the spatial azimuthal angle of the magnetized STM tip. By introducing a magnetic impurity to break the symmetry of rotation and local time reversal of the TI surface, we find that the measurement of the spatial resolved conductance can reconstruct the helical structure of spin texture, from which the spin-momentum locking angle can be extracted if the in-plane magnetization is induced purely by the spin–orbit coupling of surface Dirac electrons. Our theory offers an alternative way, differing from existing in-plane-current polarization probed in a multi-terminal setup or angle resolved photoemission spectroscopy, to electrically identify the helical spin texture on TI surfaces.

Keywords: topological insulator, spin-polarized transport, spin texture

Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)
quantitatively the polarization size because the applied current has parallel bulk and surface-state conduction paths and only that the fraction flowing in the surface channel contributes to the spin polarization arising from Dirac states [22].

Alternatively, it would be an effective approach to adopt the vertical transports through the TI substrate with a scanning tunneling microscopy (STM). STM as a powerful tool can probe the topological nature of the surface states by analyzing the quasi-particle interference (QPI) in Fourier-transform STM [4, 24–29], caused by scattering off impurities. The SML nature is manifested indirectly by the absence of backscattering between states of the opposite momentum and opposite spin. Nevertheless, these QPI patterns do not show any signature of the magnetic scattering even if the forbidden backscattering is lifted since the QPI reveals only the spin-conserving scattering. To extract the fingerprint of spin texture, the measurement of spin-polarized STM was suggested [24, 29–32]. One, however, can note that the most experiments only focus on the probing of the out-of-plane spin texture [33, 34] while the in-plane spin texture, vital for understanding the SML nature, receives no attention due to the complex physics in TIs. According to the existing theory, the spin-resolved STM conductance \( dI/dV \) links to the magnetization of tip and sample through [35–37]

\[
dI(r)/dV \propto \rho_{p}(r, eV) + |m_{\parallel}| M(r, eV)| \cos \theta.
\]

Here, \( \rho_{p}(r, eV) \) and \( m_{\parallel}|M(r, eV)| \) are, respectively, the charge and magnetization density of the tip (substrate), and \( \theta \) is the angle between the tip and sample magnetization. In equation (1), if polarizing the substrate \( M_{\parallel}(r, eV) = M_{\parallel}(r, eV)z \) along \( z \)-direction, perpendicular to the surface, the conductance is proportional only to the polar angle \( \theta \) of the tip magnetization, but independent of its azimuthal angle \( \varphi \). The situation, however, is radically changed if the substrate is the polarized TIs since the spin polarization \( M_{\parallel}(r, eV) \) can induce the extra in-plane components \( M_{\parallel}(r, eV) = (M_{\parallel}(r, eV), M_{\parallel}(r, eV)) \) due to the strong spin–orbit interactions [38, 39]. As a consequence, the total magnetization distorts from the primary \( z \)-axis and contributes an extra component of conductance. In this paper, we get insight into this new physics and modify the formula (1) to be suitable for the helical topological surface. It is found that the azimuthal-angle-dependent conductance has no analog in the conventional magnetic metal, from which one can electrically probe the in-plane spin texture in real space and further to extract the SML angle of pristine topological states.

### 2. Formulas for spin-polarized transports

To connect \( M_{\parallel}(r, eV) \) to conductance, we employ a typical experimental setup as shown in figure 1, where a spin-polarized STM tip is placed over a host surface of TIs, absorbed by a magnetic impurity at the original point \( (r = 0) \). The introduction of a magnetic impurity has twofold meanings: (1) Polarizing the spins of the topological surface states. Although the surface electrons have a specific spin orientation in momentum space, they have no net polarization in real space due to the presence of time-reversal symmetry. (2) Breaking the spatial rotation symmetry to cause a \( \varphi \) dependence of conductance.

We model the Hamiltonian of the spin-polarized STM tip as

\[
\hat{H}_{\text{tip}} = \sum_{k} \epsilon_{k}^\uparrow \hat{c}_{k}^\uparrow \hat{c}_{-k}^\downarrow + \sigma \hat{m}_{\parallel}, \quad \text{with } \hat{m}_{\parallel}, \text{the magnetization vector and } \sigma \text{ the vector of spin Pauli matrices, and the hybridized Hamiltonian between the tip and topological surface as}
\]

\[
\hat{H}_{\text{hyb}} = \int \int d\mathbf{r}_{1} d\mathbf{r}_{2} \psi_{\uparrow}^\dagger(\mathbf{r}_{1}, t) T(\mathbf{r}_{1}, \mathbf{r}_{2}) \psi_{\downarrow}(\mathbf{r}_{2}, t) + h.c.,
\]

where the quantum field operators \( \psi_{\uparrow}(\mathbf{r}, t) = \frac{1}{\sqrt{\mathcal{N}}} \sum_{k} c_{k,\uparrow}(t) e^{-i\mathbf{k} \cdot \mathbf{r}} \) with \( c_{k,\uparrow}(t) = (c_{\uparrow}(t), c_{\downarrow}^\dagger(t)) \) is the creation operator of electrons for the surface \((\eta = s)\) and tip \((\eta = t)\). We choose the spin-quantization axis of the surface electrons as the global reference axis. The tip-surface coupling is assumed to be spin independent \( T(\mathbf{r}_{1}, \mathbf{r}_{2}) = T_{0}(\mathbf{r}_{1}) \delta(\mathbf{r}_{2} - \mathbf{r}) \) for simplicity with \( \mathbf{r} \) being the in-plane spatial vector of tip measured from the impurity point. Here, the coupling between the tip and impurity is neglected since we focus on a large \( \mathbf{r} \). By introduction of unitary matrix \[ U = \begin{bmatrix} \cos(\theta/2) & e^{-i\phi(t)} \\ -e^{i\phi(t)} & \cos(\theta/2) \end{bmatrix}, \]

where \( \phi(t) \) is the spin flipping due to noncollinear arrangement between the magnetic moments of substrate and tip enters the tip-surface tunneling, which can be rewritten as

\[
\hat{H}_{\text{hyb}} = \int \int d\mathbf{r}_{1} d\mathbf{r}_{2} \gamma_{k,\uparrow}(\mathbf{r}_{1}, t) T(\mathbf{r}_{1}, \mathbf{r}_{2}) \gamma_{k,\downarrow}(\mathbf{r}_{2}, t) + h.c.,
\]

where the renormalized coupling matrix \( \tilde{T}(\mathbf{r}_{1}, \mathbf{r}_{2}) = T(\mathbf{r}_{1}, \mathbf{r}_{2})U^{-1} \) has a nondiagonal form in spin space. The current through the tip is calculated with \( I = -e \frac{\partial}{\partial t} \sum_{\alpha} \int d\mathbf{r}_{1} \langle \gamma_{\alpha,\uparrow}(\mathbf{r}_{1}, t) \gamma_{\alpha,\downarrow}(\mathbf{r}_{1}, t) \rangle \). Carrying out the equa-
tion of motion for non-equilibrium Green’s function on the Keldysh technique, we obtain the conductance as (see the supplemental material available at stacks.iop.org/JPhysCM/30/335404/mediala)

\[
I = -2e |T_0|^2 \sum_p \int \frac{d\omega}{2\pi} \text{Tr} \{ \text{Re} \{ g^R(r, r, \omega) U g^\omega_{p\ell}(\omega) U^{-1} \} \},
\]

(4)

\[
g^<(r, r, \omega) = g^<(r, r, \omega) U g^\omega_{p\ell}(\omega) U^{-1} \},
\]

(5)

where \(g^<(r, r, \omega)\) is the retarded (lesser) Green’s function of topological surface states in real-frequency space and \(g^\omega_{p\ell}(\omega)\) is the advanced (lesser) Green’s function of tip in momentum-frequency space. We assume a single \(\delta(r)\) impurity potential and so denote \(T_0 = \int d\mathbf{r}_1 e^{-ip\cdot \mathbf{r}} T_0(\mathbf{r}_1)\) independence of momentum. Compared to the previous derivation [40–42], an important difference is the matrix \(g(r, r, \omega)\) including the spin flipping processes when Dirac electrons travel on the topological surface.

As usual, we define the charge density of TIs as [32]

\[
\rho(r, r, \omega) = -\frac{1}{2\pi} \text{Im} \{ g(r, r, \omega + i0^+) \} \quad \text{and its spin texture as}
\]

\[
\mathbf{M}(r, \omega) = -\frac{1}{2\pi} \text{Im} \{ \sigma g(r, r, \omega + i0^+) \} \].

(6)

Finally, we find in the zero-temperature limit the expression for conductance at bias \(eV\), which can be divided into two parties

\[
G(r) = G_0(r) + G_{\text{flip}}(r),
\]

with

\[
G_0(r) = \pi e |T_0|^2 \text{[} \rho(r, eV) \rho_\parallel + \mathbf{M}(r, eV) |m| \cos \theta\},
\]

(6)

\[
G_{\text{flip}}(r) = \pi e |T_0|^2 \text{[} \mathbf{M}(r, eV) |m| \sin \theta \cos \varphi_{\parallel} - \varphi_{\perp} \],
\]

(7)

where \(\varphi_{\perp}\) is the azimuthal angle of \(\mathbf{M}(r, eV)\). The conductance \(G_0(r)\) recovers the usual formula equation (1), which is azimuthal independent. The most interesting part is \(G_{\text{flip}}(r)\) in equation (7), which is an azimuthal dependent and contributed by spin-flipping Green’s function \(g_{\text{flip}}(r, r, \omega)\) when an electron is scattered off the magnetic impurity. Importantly, such dependence of the tunneling conductance on the azimuthal angle of the tip magnetization has no analog in the conventional magnetic metals.

3. Probing of spin texture in linear dispersion

In this section, we will demonstrate how the measurement of \(G_{\text{flip}}(r)\) with a spin-polarized STM reconstructs the spin texture of the TI surface states and then further determines its SML angle in the real space. It is easy to verify that the presence of magnetic impurities is strictly necessary since \(M_1||r, eV\) vanishes without the magnetic impurity.

To calculate \(M_1||r, eV\) in equation (7), we must first obtain the full Green’s function \(g(r, r, \omega)\) of Dirac electrons, which can be calculated with T-matrix approach [43–45].

\[
g(r, r, \omega) = g_0(0, \omega) + g_0(r, \omega) T(\omega) g_0(-r, \omega).
\]

(8)

This method takes into account the multiple scattering events of electrons off the impurity but ignores the scattering between impurities, which is justified for lightly doped case where the interactions among impurities can be ignored. Here, the impurity-free Green’s function \(g_0(r, \omega)\) is the Fourier transform of \(g_0(k, \omega) = \left[ \omega + i0^+ - H_{11}(k) \right]^{-1}\) with respect to the bare TI Hamiltonian \(H_{11}\), and the T-matrix is given by the Bethe–Salpeter equation \(T(\omega) = V_{im} - V_{im}V_{00}(0, \omega) V_{im}\). The impurity potential is assumed in the form of [39] \(V_{im} = (U_0 - U_\sigma z)\), consisting of a local scalar potential \(U_0\) and a local Heisenberg exchange magnetic potential \(U_\sigma\) polarized perpendicular to the surface, as indicated by the vertical red arrow in figure 1. The Hamiltonian of surface of TI’s is described by [24]

\[
H_{11}^0(\lambda) = \sum_k [\hbar v_F \sigma \cdot \mathbf{k}] + \frac{\lambda}{2} (k_+^2 + k_-^2) \sigma_z,
\]

(9)

where \(k_\pm = k_x \pm ik_y\) and \(\lambda\) is the strength of warping term. The warping term is to change the linear dispersion only at high energy but can be neglected at low energy.

We first consider the case of low energy where the warping term can be ignored. We plot the real-space distribution of the in-plane spin texture \(M_1||r, eV\) in figure 2(d) and the spin-flipping conductance \(G_{\text{flip}}(r)\) in figures 2(a)–(c) for different azimuthal angles \(\varphi_{\parallel}\) of the magnetized tip. For a fixed tip direction \(\varphi_{\parallel}\), \(G_{\text{flip}}(r)\) is spatially asymmetric, with two extremum points appearing at certain diameter (dashed white line) of a circle around the original point. The positive and negative maxima, respectively, correspond to the in-plane magnetization \(M_1||r, eV\) parallel and antiparallel to the polarized direction of the STM tip, as indicated by arrows, due to the spin selection of the tip. As one rotates the tip direction \(\varphi_{\parallel} = 0, \pi/4, \pi/2\), two extremum positions also rotate anticlockwise with the unchanged magnitude, indicating the in-plane magnetization \(M_1||r, eV\) being a concentric circle with the clockwise helicity. To accurately determine the orientation of \(M_1||r, eV\), we depict the dependence of \(G_{\text{flip}}(r)\) on \(\varphi_{\parallel}\) in figure 2(e), where the position of peak just corresponds to \(\varphi_{\parallel}\). We choose representative positions as indicated in figure 2(d): A and B with the same distance but different orientation, and B and C with the same orientation but different distance. It is found that the relative direction between \(r\) and \(M_1||r, eV\) always satisfies \(\Delta \varphi = |\varphi_{\parallel} - \varphi_{\perp}| = \pi/2\) as shown in figure 2(f), independent of the spatial direction (comparing points A and B) or of the spatial distance (comparing points B and C). One recall that the SML angle is defined as the relative azimuthal angle \(|\varphi_{\parallel} - \varphi_{\perp}| = \pi/2\) between the spin and momentum. Interestingly, \(\Delta \varphi = \pi/2\) in real space just reflects the SML angle in the momentum space. Therefore, the measurement of \(G_{\text{flip}}(r)\) can reap the in-plane spin texture in figure 2(d).

To understand the origin of relation \(|\varphi_{\parallel} - \varphi_{\perp}| = \pi/2\), we further derive the analytical formula with \(H_{11}^0(\lambda = 0)\), from which

\[
g_0(0, \omega) = \frac{1}{\hbar v_F} \sum_{\lambda} \ln \left( \frac{\omega - i0^+}{\Delta_{\parallel} + i0^+ - \sigma_z} \right) - i |\omega| \Theta (D_{\parallel} - |\omega|)
\]

and

\[
g_0(r, \omega) = -\frac{\omega}{2\pi v_F} \left\{ K_0(\xi) e^{i\varphi_{\parallel}} K_1(\xi) + e^{-i\varphi_{\parallel}} K_1(\xi) \right\}.
\]

(10)

Here, \(D_{\parallel}\) is the cutoff energy for the band width of surface states, \(\xi = -i |\mathbf{r}| \omega /\hbar v_F\), and \(K_n(\xi)\) is the Bessel functions of the \(n\)-th order. \(\varphi_{\parallel}\) in equation (10) arises from the Fourier
transform of momentum direction $\varphi_{\mathbf{k}}$. Substituting equations (8) and (10) into the definition of $\mathbf{M}$, we finally obtain the azimuthal angle of the in-plane magnetization as

$$\cos \varphi_M = M_\parallel / \sqrt{M_x^2 + M_z^2} = \sin \varphi_r,$$

and its magnitude $|\mathbf{M}_\parallel(r,eV)| = \varphi^{(r)}_{\parallel} K_0(\xi) K_1(\xi)$ with $A = 1 - 2g_0(0,\omega)U_0 - g_0(0,\omega)^2(U_2^2 - U_0^2)$. Thus, we obtain $|\varphi_M - \varphi_r| = \pi/2$, which corresponds to SML angle $|\varphi_M - \varphi_r| = \pi/2$ of the pristine TI in momentum space. Notice that though the in-plane magnetization in real space is induced by the impurity magnetism, it is purely caused by the spin–orbit effect. Consequently, the planar $\mathbf{M}_\parallel(r,eV)$ still contains the information of SML, but reflected through the spin-position locking.

With equation (11), we can further rewrite

$$\mathbf{M}_\parallel(r,eV) = |\mathbf{M}_\parallel(r,eV)| \mathbf{x} \times \hat{U}_z,$$  

where $\hat{U}_z$ is the unit vector along $z$-direction. Obviously, $\mathbf{M}_\parallel(r,eV)$ is perpendicular to $r$, showing a consequence of the Dzyaloshinskii–Moriya interaction caused by the helical spin structure of Dirac surface states on TIs. Therefore, the measurement of $\mathbf{M}_\parallel(r,eV)$ not only provides a way to extract the pristine SML angle, but also the strength of the DM interaction. In addition, due to $\mathbf{G}_{\text{flip}}(r) \propto \cos(\varphi_r - \varphi_M + \pi/2)$, rotating the tip has equal role with the rotation of spatial position around the impurity, which is helpful in realistic measurement.

As for the magnitude of $\mathbf{M}_\parallel(r,eV)$ at a certain point $r$, we can determine it by rotating the tip direction, namely, $|\mathbf{M}_\parallel(r,eV)| = \text{Max}[G_{\text{flip}}(r,\varphi_r)] - \text{Min}[G_{\text{flip}}(r,\varphi_r)]/B$ with $B = 2\pi e [T_0] \mathbf{m}_r$.

4. Probing of spin texture in warping dispersion

For the case of high energy where a finite $\lambda$ plays a visible role, the magnetization density $\mathbf{M}_\parallel(r,eV)$ is demonstrated in figure 3(d). Compared to figure 2(d), introduction of the warping term greatly modifies the surface magnetism, i.e. not only modifying $\mathbf{M}_\parallel(r,eV)$ but also making $\mathbf{M}_\parallel(r,eV)$ deviate from the circular structure or $|\varphi_M - \varphi_r| \neq \pi/2$. Specifically, there appear the helical spin structures alternating clockwise and anticlockwise with six low intense centers. A main reason for this change of the spin texture is that the warping term generates an additional in-plane magnetization $\mathbf{M}_\parallel(r,eV)$, which can be regarded as the contribution of antiferromagnetic Ruderman–Kittel–Kasuya–Yosida interaction along the line joining the impurity and the magnetic tip [39]. In this situation, $\mathbf{M}_\parallel(r,eV)$ has a complex dependence on the spatial direction. When we scan the tip over the whole surface with a fixed tip azimuthal angle, e.g. $\varphi_r = 0$ in figure 3(a), the alternating positive and negative maxima of the conductance along the radial direction reflect the corresponding change of spin structure in figure 3(d). With the tip rotating from figures 3(a)–(c), the extremum points also rotate anticlockwise. Unlike the case without the warping term in figures 2(a)–(c), the structure of extremum regime from figures 3(a)–(c) is changed, indicating the spin texture deviating from the concentric circle. Even so, one still can exactly determine the direction of magnetization.
at an arbitrary point only by rotating the tip direction around the z-axis. For example, to determine the direction $\phi_M$ of magnetization in points A, B, and C labeled in figure 3(d), one can plot $G_{\text{flip}}(r)$ versus $\phi_t$ as shown in figure 3(e), where $\phi_M$ is equal to the size of $\phi_t$ at the conductance peak.

From discussions in figure 2, we are known that the direction difference $\Delta \phi = |\phi_r - \phi_M|$ between $r$ and $M_{\|}(r,eV)$ can characterize the SML angle well. In figure 3(f), we depict $\Delta \phi$ as a function of spatial direction $\phi_r$ for different values of $\lambda$. With the increase of $\lambda$, the deviated amplitude becomes larger but at the same time the oscillating period of $2\pi/3$ remains unchanged. The change of $\phi_M$ is remarkable along the directions of $\phi_r = n\pi/6$ with $n = 0, 2, 4, 6, 8, 10$ due to the strong out-of-plane magnetization, which corresponds to the center of the sides of the hexagon of Fermi surface. By contrast, for $\phi_r = n\pi/6$ with $n = 1, 3, 5, 7, 9, 11$ corresponding to the corners of the hexagon of Fermi surface, the perfect pristine SML angle $\Delta \phi = \pi/2$ (or $M_{\|}(r,eV) \perp r$) is still abided by due to the vanishing out-of-plane magnetization.

Another important feature for the TI with the warping term is the out-of-plane spin texture $M_z(r,eV)$ as shown in figure 4(a), which exhibits a typical hexagonal structure as in the momentum space. To probe its complex spin texture, we can set $\theta_t = 0$, $\lambda = 0.25$, and $eV = 0.6$. The rest of parameters refer to data used in figure 2.
$M_s(r, eV)$. In this case, we keep the spin-polarized STM magnetization either parallel or antiparallel to the $z$-axis and define the magnetoresistance (MR) effect as

$$MR(r) = \frac{G_0(r, \varphi_\perp = 0) - G_0(r, \varphi_\parallel = \pi)}{G_0(r, \varphi_\perp = 0) + G_0(r, \varphi_\parallel = \pi)}. \quad (13)$$

We depict $MR(r)$ in figure 4(b), which exhibits six regions with the alternating high and low conductance density, completely reconstituting the spatial pattern of spin texture $M_s(r, eV)$ in figure 4(a).

5. Discussions

The SML nature is related to the in-plane electronic transports and the electrical detection for it is usually carried out by the measurement of the spin-polarized conductance along the TI surface in a lateral spin valve geometry [19–22]. Although some progress has made, it was shown that the detection efficiency is low due to the unavoidable disturbance from the bulk states (bulk spin Hall effect or bulk channel shunting), the short spin-relaxation length, and the reflection of contacts. Moreover, they also can not exactly identify the SML angle. Instead, we here propose the method with the spin-polarized STM setup circumventing these problems by using the vertical transport probe. We find that when the tip magnetization is orientated along the TI surface, there exists a conductance component $G_{\text{tip}}(r)$ depending on the azimuthal angle of the tip, which has no analog in the conventional magnets and confirms the presence of the SML nature of surfaces. Due to the linear dependence on $G_{\text{tip}}(r)$, the magnitude of the in-plane spin texture can be directly extracted from the maximum of $G_{\text{tip}}(r)$ and its direction is determined by rotating the tip around the $z$-axis. Also, the out-of-plane spin texture can be mapped if the tip magnetization is polarized perpendicular to the surface. Therefore, the measurement of the spatial resolved conductance with the spin-polarized STM provides a direct method to reconstruct the spin texture of surface states, from which the SML angle can be further extracted.

Experimentally, the magnetic tip should be moved laterally nearby the adatom in a moderate range. If the STM tip is positioned just above the impurity, the azimuthal-angle dependence vanishes due to the lack of spin flipping. Note that $G_{\text{tip}}(r)$ stems from the SML-induced spin flipping in the process of transmission of surface electron. The ideal choice is $r = 2 \sim 5$ nm. Of course, the TI surface should be diluted doping so that the interaction between the magnetic impurities can be ignored safely. The magnetic tip can be prepared by coating the antiferromagnetic Cr on the tungsten tips where the magnetization of the tip can be controlled by the Cr thickness, either in plane ($\sim$30 nm) or out of plane ($\sim$5 nm) [37, 46]. The spin polarization of the impurity can be exerted using another spin-polarized STM or a weak external magnetic field. In order to probe the SML angle, we should shift the Fermi level around the Dirac point where the warping effect is negligible. This can be achieved through the nonmagnetic doping or gate control [47]. When shifting the Fermi level to the high energy, we can extract the warping parameter $\lambda$ from the spatial dependence of the in-plane magnetization in figure 3(f), which has not reported experimentally.

In measurement, the magnetic impurity must be polarized along $z$-axis. If the polarization of magnetic impurity deviates from the $z$-axis (or not perpendicular to the TI surface), the in-plane magnetization is not exclusively associated with the spin momentum locking since it can also directly stem from the tiled impurity magnetization. This case will cause unnecessary difficulty for extracting the in-plane spin texture of the surface states. Relatively speaking, the tiled impurity magnetization does not affect the information of the out-of-plane spin texture since it only modifies the background of the spin texture but does not affect the spin pattern due to the rotated symmetry structure.

In conclusion, employing the nonequilibrium Green’s function, we present a general theory for the spin polarized transports of Dirac electrons through a spin-polarized STM. In order to extract the quantitative information about the spin texture, we need to break the symmetry of rotation and time reversal with a typical impurity model. It is found that the conductance is modified by an extra component exclusively associated with the xy-plane spin texture, which exhibits an unconventional dependence on the azimuthal angle of the tip magnetization. The analysis of the azimuthal angle dependent conductance provides a direct method of the measurement of the local in-plane spin texture of the Dirac electrons on the TI surface.

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