Probing surface states exposed by crystal terminations at arbitrary orientations of 3D topological insulators

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Topologically protected surface states appearing on a planar surface exposed by cleaving a crystal of 3D topological insulator (e.g., Bi2Se3, Bi2Te3, and Sb2Te3) are distinct from each other for different crystal terminations, characterized by the angle (θ) which, the normal to the surface makes with the crystal growth axis. The exposed planar surfaces for a given θ show a spin texture which is specific to the angle θ where only the θ = 0, π surfaces have a spin texture consistent with perfect spin-momentum locking while the θ ≠ 0, π surfaces deviate from it. This variety in spin texture arises due to the θ dependent contribution of orbital parity of the bulk Hamiltonian in construction of these surface states. In this article we show that, current due to spin polarized tunneling of electrons injected into the surface states may provide information unique to the surface corresponding to a given θ. Hence our study provides a proposal for experimentally probing and distinguishing these different surfaces by directly coupling to the spin textures of the surface states. We also show that the study of the spin textures for different surfaces put together acts like a hologram of the bulk band structure of the material.

I. INTRODUCTION

Topological insulators (TI) have been a very active subject of research in condensed matter physics since their inception. The discovery of strong 3D TI materials which have an insulating bulk and topologically protected metallic surface states has led to an ever increasing amount of studies since their discovery. These materials have taken the community by surprise as by now one believed that there was almost nothing exotic and interesting left to be explored within a free electron band theory. In contradiction, these materials were found to exhibit extraordinary properties, consistent with free electron theories. These properties were attributed to the topological aspect of the bands associated with these materials. A special feature of surface states in these materials is the presence of spin-momentum locking which has been studied by spin-resolved angle resolved photoemission spectroscopy (ARPES) or by scanning tunneling microscope (STM) via study of quasi-particle interference patterns induced by weak disorder potential. Also, such studies have been done in the presence of ferromagnetic contacts on the TI, which explicitly break time reversal symmetry (TRS). Due to strong coupling between spin and momentum in these systems, one gets an easy handle on manipulation of the former by manipulating the later and vice-versa which has led to an elevated hope for these materials to be one of the most promising future spintronics materials.

Though spin-resolved ARPES serves as an efficient probe for scanning the surface state spectrum, it does not provide a direct handle on electrical transport properties. On the other hand, STM does provide information regarding transport but only in the disordered limit as it relies on quasi-particle interference which is produced due to disorder-induced scattering and the information hence extracted is via an indirect probe for the spin-momentum locked spectrum. Hence, an electric transport probe which works in the ballistic regime and probes the spin texture more directly is desirable. Also, the technique of spin-polarized ARPES works very well as long as the spin-momentum locking is between a physical electron spin and its momentum, on the other hand if the locking is with a pseudo spin degree of freedom, then the expected success of spin-polarized ARPES in determining spin texture is a priori not clear. In this article we intend to study a situation where the surface state is represented by pseudo-spin-momentum locked spectrum in the ballistic limit. Very recently it was shown by two of the authors of the present article that a spin-polarized STM can be used to reconstruct the spin texture exactly by measuring current asymmetries in a multi-terminal set up in the ballistic limit. The proposal involved extraction of a finite tunnel magnetoresistance (TMR) response from the non-magnetic TI surface state by coupling a spin polarized STM to an arbitrary but finite segment of the Fermi surface of the surface state.

Band structure studies of 3D TI materials like Bi2Se3, Bi2Te3 and Sb2Te3 (or any other material with 3m space group) have shown that the low energy sector of the theory expanded around the centre of the Brillouin zone Γ are effectively spanned by states labeled by two quantum numbers. One being the fundamental quantum number which is the electron spin and the second one is a quantum number which emerges out of the parity inversion (P) symmetry of the unit cell which takes ±1 as its eigenvalue hence reducing the effective low energy theory to a four band model. For further reference, we refer to the space spanned by eigenstates of P as the orbital pseudo-spin space.

For the surface perpendicular to the crystal growth axis, the two sectors belonging to the spin and the parity are completely decoupled as far as dispersing degree of freedom are concerned, but this fact is true only for the surfaces corresponding to θ = 0 and π. In an elegant work by Zhang et al. the physics of surfaces oblique to the crystal growth axis was considered. It was shown that the dispersing modes form a new SU(2) degree of freedom constructed out the combination of spin and the parity. The exact composition of spin and par-
ity contribution depends directly on the angle $\theta$. Furthermore, unlike the top surface, the Fermi surface is no more circular but elliptic where the eccentricity again depends on the angle $\theta$. Such surfaces have been addressed experimentally but an extensive study is missing. Following the strategy developed in Ref. [28] we provide theoretical predictions for experiments to probe these textures using a spin polarized STM. Measurements of current asymmetries in a multi-terminal set-up gives rise to TMR signals, which could be used to uniquely identify the surface corresponding to a given $\theta$. We further show, how these transport measurements can be used to reconstruct the shape of the Fermi surface and then reconstruct the spin texture on the Fermi surface.

The rest of the paper is organized as follows: in Sec. II the geometry and the setup is discussed. In Sec. III, the low energy Hamiltonian for the surface states is discussed followed by discussions on degeneracy induced breaking of symmetries by surface states in Sec. IV and a discussion on their spin texture in Sec. V. In Sec. VI a model for a spin polarized STM is presented and the corresponding momentum resolved current is discussed. Current from STM injected into the TI surface is calculated to leading orders perturbatively in the weak tunnel coupling limit. In Secs. VII and VIII we discuss the strategy for identifying the $\theta$ corresponding to surfaces via a detailed study of tunneling current which carry unique fingerprints of the corresponding Fermi surfaces and its spin textures. We show that the spin textures for different surfaces can be used to extract fundamental parameters of the bulk Hamiltonian which effectively determine the surface dependent Fermi velocities for different $\theta$, hence acting as a hologram of the bulk. Finally the results are summarized in Sec. IX along with outlooks.

II. EXPERIMENTAL GEOMETRY

In this section, the schematic of the setup is discussed along with setting up the conventions and notations which are used in the rest of the paper. A schematic diagram of the setup is shown in Fig. 1. The crystal growth axis is always taken along the $z$ direction, and an arbitrary surface denoted by $\Sigma(\theta)$ is exposed by taking a cut parallel to the $y$ direction, such that the normal to the surface makes an angle $\theta$ with the crystal growth axis. Momentum normal to the exposed surface is denoted by $k_z$. Since the cut is parallel to the $y$ axis, hence one of the in-plane momentum remains $k_y$ as we vary $\theta$. The other in-plane momentum orthogonal to $k_y$ is denoted by $k_1$ which is basically $k_x$ rotated by an angle $\theta$ about the $y$ axis as shown in Fig. 1. For convenience of the readers we have kept the coordinate system defining the surface same as in Ref. [29]. Two contact pads are placed on diagrammatically opposite sides of the exposed surface such that each contact collects the current injected in that half of the sample in which the contact pad is placed. An imaginary line which divides the sample into two halves is shown by the dashed line in Fig. 1. The angle it makes with the $k_1$ axis is denoted by $\gamma$. According to this convention the current collected in the left contact denoted by $I_L$ is the current that flows in the region covered by the range of angle from $\gamma$ to $\gamma + \pi$, whereas the current collected by the right contact $I_R$, is the one collected in the region spanned by angle ranging from $\gamma + \pi$ to $\gamma + 2\pi$. In this way, a strict sense of consistency is maintained in regard to what is $I_L$ and $I_R$. The current asymmetry $\Delta I$ is defined as the difference of the two, i.e, $\Delta I = I_L - I_R$ and the total current injected from the tip into the TI surface is denoted by $I_0 = I_L + I_R$.

III. MODEL

In this section we start with a brief review of the derivation of the surface states obtained in Ref. [29] which sets the stage for evaluating the tunneling current. The low energy Hamiltonian expanded around the $\Gamma$-point for 3D TI material like Bi$_2$Se$_3$ retained up to linear order in momentum is given by

$$\mathcal{H} = (-m_0z + v_zk_z\tau_y) \otimes 1_x + v_\parallel \tau_x \otimes (ky\sigma_x - k_x\sigma_y),$$ (1)

where the basis chosen is given by $(|+ \uparrow\rangle, |+ \downarrow\rangle, |- \uparrow\rangle, |- \downarrow\rangle)$. Following Ref. [11], we use the parameter values $v_z = 2.2$ eVÅ and $v_\parallel = 4.1$ eVÅ. We have chosen to work with $\sigma \otimes \tau$ representation as oppose to $\sigma \otimes \tau$ representation that appears in literature and its utility will be evident as we eventually proceed for calculating the spin texture on the Fermi surface. Here $\pm$ denotes the even and odd parity orbitals and the $\uparrow / \downarrow$ denotes the $z$-component of electron spin where $z$-axis is taken to be parallel to the crystal growth axis and $m_0$ denotes the bulk band gap. Solving the Hamiltonian for the surface states for a surface perpendicular to the $z$ axis leads to the well known spin-momentum locked Dirac Hamiltonian. These surface states are also eigenstates of the $\tau_x \otimes 1$ operator, where the positive eigenvalue corresponds to the top surface and the negative eigenvalue corresponds to the bottom surface. However, to get the surface Hamiltonian for an arbitrary surface $\Sigma(\theta)$ that is exposed by cleaving the crystal at an angle $\theta$ with the crystal growth axis, it is convenient to work with a local surface dependent frame of reference spanned by

![FIG. 1. A schematic of the set-up involving an arbitrarily cut surface of the TI, STM and the two contact pads. For more details we refer to the text in Sec.II](image)
where \( \mathbf{k}_1, \mathbf{k}_y, \mathbf{k}_3 \) axes (see Fig. 1), where \( \mathbf{k}_1, \mathbf{k}_y \) are the in-plane vectors. The rotation of the plane is always done about the \( \mathbf{k}_y \) axis and \( \mathbf{k}_3 \) is chosen to be perpendicular to the given surface. In such a frame, the Hamiltonian in Eq. (1) can be written as

\[
\mathcal{H} = -m_0 T_z + (v_3 k_3 + v_0 k_1) T_y + (v_1 k_y S_x - v_1 k_1 S_y) T_z, \tag{2}
\]

where \( S \) and \( T \) are pseudospins defined by surface dependent linear combinations of products of \( \tau \otimes I_\sigma \) and \( I_\tau \otimes \sigma \). They are given by

\[
T = \{ \alpha \tau_z \otimes I_\sigma + \beta \tau_y \otimes \sigma_y, \alpha \tau_y - \beta \tau_x \otimes \sigma_y, \tau_z \otimes I_\sigma \},
\]

and

\[
S = \{ \alpha I_\tau \otimes \sigma_x - \beta \tau_z \otimes \sigma_z, \alpha I_\tau \otimes \sigma_x + \beta \tau_z \otimes \sigma_z \}, \tag{3}
\]

where \( v_3 = \sqrt{(v_z \sin \theta)^2 + (v_z \cos \theta)^2} \), \( \alpha = v_z \cos \theta/v_3 \), and \( \beta = v_1 \sin \theta/v_3 \). Also \( v_0 = (v_1^2 - v_z^2) \sin \theta \cos \theta/v_3 \) and \( v_1 = v_x v_3/v_3 \). Both \( T \) and \( S \) independently satisfy the \( SU(2) \) algebra and they also satisfy \( [T_i, S_j] = 0 \) for all \( i, j \).

Using the topological boundary condition\(^29\) given in Ref. (29), the surface Hamiltonian is obtained as

\[
\mathcal{H}_{surf}(\theta) = v_1 k_y S_x - v_1 k_1 S_y, \tag{4}
\]

Explicitly writing down the surface Hamiltonian in Eq. (4) in our basis reveals that it is already in a block diagonal form (which was the reason for choosing the \( \tau \otimes \sigma \) representation) and now each block can be written in a \( \sigma \cdot B \) form where \( B \) can be thought of as an effective magnetic field acting on the spin degree of freedom belonging to the respective blocks. The block diagonal form of the surface Hamiltonian is given by

\[
\mathcal{H}_{surf}(\theta) = \left( \begin{array}{cc}
\sigma \cdot B_k^+ (\theta) & 0 \\
0 & \sigma \cdot B_k^- (\theta)
\end{array} \right), \tag{5}
\]

where

\[
B_k^\pm (\theta) = \{ v_1 k_y \alpha, -v_1 k_1, \pm v_1 k_y \beta \}. \tag{6}
\]

Since \( |B_k^\pm (\theta)\rangle = |B_k^- (\theta)\rangle \), the energy dispersion resulting from Eq. (5) is two-fold degenerate. Also note that \( B_k^+ (\theta) \) and \( B_k^- (\theta) \) differ only in their z-component with an equal magnitude and opposite sign. This fact gives clear indications that, if we evaluate the expectation value of spin in an eigenstate of this Hamiltonian, its z-component may be zero regardless of the value of \( \theta \) as will be evident in the next section. The surface dependent energy dispersion (shown in Fig. (2)) has the form

\[
E_{k, \pm}(\theta) = \pm \sqrt{\frac{v_x^2 k_y^2}{v_1^2} + v_1^2 k_1^2} \tag{7}
\]

The surface Hamiltonian in Eq. (5) is a \( 4 \times 4 \) matrix, giving rise to the two degenerate Dirac-like dispersions, however it should be noted that one exposed surface of the TI has only one Dirac-like cone living on it. Actually one Dirac cone belongs to the top surface and the other one belongs to the bottom one. This suggests that an arbitrary state picked from the degenerate subspace of the eigenstates of \( \mathcal{H}_{surf}(\theta) \) does not represent the true surfaces states. The correct four component spinor describing the appropriate surfaces states are constructed in the following way.

The two eigenstates for each of the two blocks in Eq. (5) are given by

\[
\chi_{E+}^\pm (\mathbf{k}) = \left( \begin{array}{c}
\cos \frac{\theta_\pm}{2} \\
\sin \frac{\theta_\pm}{2} e^{i \phi_\pm}
\end{array} \right),
\]

and

\[
\chi_{E-}^\pm (\mathbf{k}) = \left( \begin{array}{c}
-\sin \frac{\theta_\pm}{2} \\
\cos \frac{\theta_\pm}{2} e^{i \phi_\pm}
\end{array} \right), \tag{8}
\]

where \( \chi_{E+}^\pm \) and \( \chi_{E-}^\pm \) are the positive and negative energy eigenstates respectively of the first block, and \( \chi_{E+} \) and \( \chi_{E-} \) are of the second block of Eq. (5). With this, it is straightforward to construct the eigenstates of the Hamiltonian in Eq. (5) as

\[
|E_{+}^\pm \rangle = \chi_{E+}^\pm (\mathbf{k}),
\]

and

\[
|E_{-}^\pm \rangle = \chi_{E-}^\pm (\mathbf{k}). \tag{9}
\]

In Eqs. (8) and (9), \( \theta_\pm^k \) and \( \phi_\pm^k \) are defined via the effective magnetic fields (Eq. (6)) as

\[
B_k^\pm = \{ |B_k^+| \sin \theta_\pm^k \cos \phi_\pm^k, \sin \theta_\pm^k \sin \phi_\pm^k, \cos \theta_\pm^k \}. \tag{10}
\]

The relation between \( \theta_\pm^k \) and \( \phi_\pm^k \) can be trivially seen from Eq. (8) as \( \theta_\pm^k = \pi - \theta_{E+}^k \) and \( \phi_\pm^k = \phi_{E+}^k \). From now on, we drop the \( \pm \) superscript on the \( \theta_\pm^k \) and \( \phi_\pm^k \) and write everything in terms of \( \theta^k \) and \( \phi^k \) denoted by \( \theta_\pm^k \) and \( \phi_\pm^k \).

The correct description of states on the surface of the topological insulator can now be constructed by taking appropriate linear combinations of the states from the two fold degenerate subspace discussed above. The coefficients of the linear combination are fixed by considering the fact that the surface...
state also has to be an eigenstate of $T_z$ operator. The surface states being an eigenstate of $T_z$ operator can be understood from the last terms in the expression for bulk Hamiltonian $H$ in Eq. (2) which finally induces the dispersing modes of the surface Hamiltonian. Under the above condition, the wavefunction for surface electron can be written as

$$
\Psi_{c,v}^{1(2)}(k) = \frac{1}{\sqrt{2}} \left( \psi_{E^+(E-)}^{1(2)}(k) + e^{i\theta} \psi_{E^+(E-)}^{1(2)}(k) \right) c_{k,v}^{1(2)},
$$

which, in turn, reads as

$$
\Psi_{c,v}^{1(2)}(k) = \frac{1}{\sqrt{2}} \left( e^{i\theta} \chi_{E^+(E-)}^{1(2)}(k) \right) c_{k,v}^{1(2)},
$$

$$
e^{i\theta} = \pm \frac{\sqrt{\alpha^2 v_1^2 k_y^2 + \beta v_1 k_1}}{\sqrt{\alpha^2 v_1^2 k_y^2 + v_1^2 k_1^2}} + i \frac{\beta v_1 k_1}{\sqrt{\alpha^2 v_1^2 k_y^2 + v_1^2 k_1^2}},
$$

where $1(2)$ in the superscript denotes top (bottom) surface, $c(v)$ in the subscript denotes conduction (valence) band, and $c_{k,v}^{1(2)}$ is the corresponding electron annihilation operator with momentum $k$ for the TI surface. From here onwards, we work only with the surface states corresponding to the positive eigenvalue of $T_z$ and belonging to the conduction band (i.e. $\Psi_{c,v}^{1(2)}(k)$).

IV. BREAKING OF $\tau_z$ SYMMETRY BY SURFACE STATES

We first note that the block diagonal form of the $H_{surf}(\theta)$ in Eq. (5) implies that $\tau_z$ is a conserved quantity (i.e., $[H_{surf}(\theta), \tau_z \otimes I_x] = 0$) for the surface Hamiltonian. At the same time the surface states also have a two fold degeneracy where the degenerate solutions are given in Eq. (9). Though each of these individual degenerate solutions do respect the $\tau_z$ symmetry, a linear combination of these solutions which is also a valid eigenstate of $H_{surf}(\theta)$ could break the $\tau_z$ symmetry spontaneously. This is indeed the case for the surface states and this is a direct consequence of the fact that the surface states have to be simultaneous eigenstates of $H_{surf}(\theta)$ and $T_z$ ($= \alpha \tau_x \otimes I_y + \beta \tau_y \otimes I_y$). As the operator $T_z$ lies on the $x$-$y$ plane in the $\tau$ space, the correct surface state are constructed as equal weight superposition of degenerate eigenstates of $\tau_z \otimes I_x$ with only a relative phase allowed between them (see Eq. (13)) hence breaking the $\tau_z$ symmetry of $H_{surf}(\theta)$.

V. SPIN TEXTURE OF THE SURFACE STATES

Using the surface wavefunction given by Eq. (11) for an arbitrary surface termination characterized by the angle $\theta$ as described in Sec. III the spin texture in the momentum space is obtained by taking the expectation of the spin operators $\mathbf{I}_{2 \times 2} \otimes \sigma$ as

$$
\langle \Psi_{c,v} | \mathbf{I}_{2 \times 2} \otimes \sigma | \Psi_{c,v} \rangle = \frac{1}{2} \left( \langle \chi_{E^+}^c | \sigma | \chi_{E^+}^v \rangle + \langle \chi_{E^-}^c | \sigma | \chi_{E^-}^v \rangle \right).
$$

Note that the effective magnetic field for the two parity sectors are related as $B_x^+ = B_x^-$, $B_y^+ = B_y^-$, and $B_z^+ = -B_z^-$. This implies that $\langle \sigma^z \rangle$ should identically vanish for any arbitrary surface. The expectation value of the spin can be directly read off from the Hamiltonian as

$$
\langle \sigma(k) \rangle = \frac{B_x^+ + B_x^-}{2 |B_k|}.
$$

Hereafter, it is straightforward to obtain the expectation values of the spin operators as

$$
\langle \sigma_x \rangle = \frac{v_x v_y k_y \cos \theta}{v_3 \sqrt{v_1^2 k_y^2 + v_2^2 k_y^2}},
$$

$$
\langle \sigma_y \rangle = \frac{-v_x v_y k_z}{v_3 \sqrt{v_1^2 k_y^2 + v_2^2 k_y^2}},
$$

$$
\langle \sigma_z \rangle = 0.
$$
Note that the expectation values of the spin operators flip sign for valence band. Also, note that the spin on any arbitrary surface always lies in the x-y plane defined in a global coordinate system. Therefore, for an arbitrary surface, which is not parallel to the x-y plane, the spin can have a component perpendicular to the surface and this is a signature of absence of a perfect spin-momentum locking in contrary to the case for the θ = 0 and π surfaces. This becomes even more evident if the expectation value of spin is looked at in the local surface dependent coordinate system, where the surface is described by the $k_x, k_y$ plane and $k_z$ points perpendicular to the surface. In these local coordinates system $\langle \sigma_x \rangle_\theta = \langle \sigma_x \rangle \cos \theta$ and $\langle \sigma_z \rangle_\theta = \langle \sigma_z \rangle \sin \theta$.

Also, the magnitude of the spin $|\langle \sigma \rangle| = \sqrt{\langle \sigma_x \rangle^2 + \langle \sigma_y \rangle^2 + \langle \sigma_z \rangle^2}$ has a texture in the momentum space which depends on the surface. This is also an additional signature of imperfect spin-momentum locking. Interesting features that appear in the spin texture for an arbitrary surface of the TI are shown in Fig. (3). The third column of Fig. (3) shows that for an arbitrary surfaces the magnitude of the spin on the Fermi surface is not a constant.

The imperfection in the spin-momentum locking is better highlighted if one calculates the spin-momentum locking angle ($\theta_\ell$). It turns out that it is a constant for the surface perpendicular to the crystal growth axis, whereas for arbitrary surface, $\theta_\ell$ has a texture in the momentum space. Using the relation $\cos \theta_\ell(\bm{k}) = \langle \sigma \rangle(\bm{k}) \cdot \hat{k} / |\langle \sigma \rangle(\bm{k})|$, and the expressions in Eqs. (16a) and (16b), one can show that

$$\theta_\ell(\bm{k}) = \cos^{-1} \left( \frac{\sin^2 \theta \sin \delta_k \cos \delta_k}{\sqrt{\cos^2 \theta \sin^2 \delta_k + \cos^2 \delta_k}} \right),$$  \hspace{1cm} (17)

where $\delta_k$ parametrizes the momentum on the surface as $k_1 = k_x \cos \delta_k$ and $k_2 = k_y \sin \delta_k$ with $k_y$ being the magnitude of components of the momentum in the plane. As can be seen from Eq. (12) and Fig. 4 the spin always points perpendicular to the momentum for $\theta = 0$, however as one begins to take arbitrary surfaces, the spin-momentum locking angle begins to develop a dependence on the momentum. This ultimately leads to differences in the magnetization of half of the Fermi surfaces for different surfaces, which could reflect itself in the current asymmetry measurements using spin-polarized STM[23]. Hence such measurements carry fingerprints of the given surface and could help identify them. This will be discussed in details later in Secs. VII and VIII.

VI. PERTURBATIVE CALCULATION OF TUNNELING CURRENT FROM STM

In this section, we engineer a minimal model for a tunnel Hamiltonian which can be used to inject spin polarized electron for a magnetic STM tip into the TI surface. The key ingredient in this construction stems from the observation that $\tau_z$ is a conserved quantity. The diagonal blocks of $\mathcal{H}_{\text{surf}}(\theta)$ belonging to a +1 or −1 eigenvalues of $\tau_z$ have a spin degree of freedom associated with them, which points along $\mathbf{B}_{\mathbf{k}}$ and $\mathbf{B}_{\overline{\mathbf{k}}}$ respectively. Hence each STM electron injected into the TI surface state sees two independent channels given by $\tau_z = \pm 1$. Tunnel into each channel corresponding to $\tau_z = \pm 1$ will have a finite amplitude (call it $t^z_{\mathbf{k} \overline{\mathbf{k}}}$ and $t^z_{\overline{\mathbf{k}} \mathbf{k}}$). We note that the corresponding tunneling currents injected into each $\tau_z$ should not only be proportional to $|t^z_{\mathbf{k} \overline{\mathbf{k}}}|^2$ but also to the modulus squared of overlap of the STM electron spinor pointing along the polarization direction of the tip and that of a spinor which is pointing in the direction of $\mathbf{B}_k$. This could give rise to a finite TMR which is the central focus of this article. In a realistic situation, the relative phase between the two couplings $t^z_{\mathbf{k} \overline{\mathbf{k}}}$ and $t^z_{\overline{\mathbf{k}} \mathbf{k}}$ and their relative weights would depend on the microscopic details of overlap of the surface state wavefunction and the tip wavefunction and is expected to get randomized over several measurements. Hence, the physical results are obtained by averaging over the relative phase and relative weight of $t^z_{\mathbf{k} \overline{\mathbf{k}}}$ and $t^z_{\overline{\mathbf{k}} \mathbf{k}}$ at end of the calculation. An efficient way to implement the above consideration is to artificially expand the Hilbert space of the tip Hamiltonian to include a fictitious $\tau$ degree of freedom on the tip so that we have

$$\Psi_{\text{STM}} = \frac{1}{N} \int d\bm{k} \left( t^z_{\mathbf{k} \overline{\mathbf{k}}} \right) \otimes \left( \frac{\cos(\theta_\ell/2)}{\sin(\theta_\ell/2)} e^{i \phi_\ell} \right) e^{i \mathbf{k} \cdot \mathbf{r}} d\mathbf{k},$$  \hspace{1cm} (18)

where $N$ is a normalization constant and the angles $\theta_\ell$ and $\phi_\ell$ denote the polar and the azimuthal angles for the magnetization direction of the STM tip, respectively. The corresponding Hamiltonian for the STM tip is given by

$$\mathcal{H}_{\text{STM}} = \sum_{\mathbf{k}} e_{\mathbf{k}} d_{\mathbf{k} \uparrow}^\dagger d_{\mathbf{k} \uparrow}.$$  \hspace{1cm} (19)

For simplicity we have considered the STM to be described by a Hamiltonian of a one dimensional electron gas hence leading to a energy independent density of states (DOS) for electron of the tip. The tunnel Hamiltonian between the tip and surface can be written as

$$\mathcal{H}_{\text{tunn}} = J \langle \Psi_{\text{STM}}^\dagger(\mathbf{r} = 0) \Psi_{\mathbf{c}}(\mathbf{r} = 0) + \text{h.c.} \rangle,$$  \hspace{1cm} (20)
which in the momentum space looks like
\[
\mathcal{H}_{\text{tunn}} = J \sum_{k,k'} (z_k \chi_{k'}^\dagger d_{k',\uparrow} + \text{h.c}),
\]  
where \(J\) is the tunneling amplitude, \(z_k\) is the overlap of the four component spinors of the TI (Eq. (13)) and the STM (Eq. (18)).

The corresponding current operator is defined as
\[
\hat{I} = e \frac{d\hat{N}_{\text{STM}}}{dt} = \frac{ie}{\hbar} [\mathcal{H}, \hat{N}_{\text{STM}}],
\]
where \(\mathcal{H}\) is the sum of the TI, STM and the tunnel Hamiltonians. To leading order in perturbation theory, the expectation value of the current is given by
\[
\langle I \rangle = \frac{i}{\hbar} \int_{-\infty}^{0} dt' \langle g | [\mathcal{H}_{\text{tunn}}, \hat{I}(t')], \hat{I}(0) | g \rangle,
\]
where \(|g\rangle = |g\rangle_{\text{TI}} \otimes |g\rangle_{\text{STM}}\) is the product of ground state of the individual systems in a decoupled state where they both are maintained in equilibrium at two different Fermi energies, the difference of Fermi energies being the applied bias. The subscript \(I\) denotes the fact that the operators are in the interaction picture. Writing everything in the momentum space, it becomes visible that the total current can be written as a sum of momentum resolved currents:
\[
\langle I \rangle = \int \frac{dk}{N_1} \left[ \frac{e J^2}{\hbar^2} |z_k|^2 \int \frac{dk'}{N_2} \chi_{k,k'} \right],
\]
where
\[
\chi_{k,k'} = \int_{-\infty}^{\infty} dt' \text{Im} \left[ G_{\text{TI}}(k, 0; k, t') G^*_{\text{STM}}(k', 0; k', t') \right].
\]
\(G\) denotes the standard time ordered fermionic Green’s functions. \(N_1\) and \(N_2\) are normalization constants, which depend on the system sizes of the TI and the STM respectively. The time integral in Eq. (25) leads to a delta function \(\delta(e_k' - E_{k,+})\), which ensures energy conservation. The Green’s functions just give the difference of Fermi functions, and the \(\delta\) function in energy ensures appropriate conditions over \(k'\) in Eq. (24) for the evaluation of the integral over \(k'\), leading to a momentum resolved expression for current which reads as
\[
\langle I \rangle(k) = \frac{e J^2}{\hbar^2 N_2} |z_k|^2 \chi_k,
\]
where
\[
\chi_k = \int_{-\infty}^{\infty} dk' \chi_{k,k'},
\]
\[
= \hbar \rho_{\text{STM}} (n_F(E_k, \mu_{\text{TI}}, T_{\text{TI}}) - n_F(E_k, \mu_{\text{STM}}, T_{\text{STM}})),
\]
where \(n_F\) denotes the Fermi functions, and \(\rho_{\text{STM}} = (\hbar v_{\text{STM}})^{-1}\) is the constant DOS of the STM. Note that, the STM principle can have a parabolic spectrum, however since we limit ourselves to tiny bias windows, the spectrum can be safely linearized and the DOS kept constant.

The expression for the momentum resolved current can be rearranged explicitly to identify the contribution coming from the three different processes to the leading order as follows,
\[
I(k) = \frac{e J^2 \rho_{\text{STM}}}{2\hbar N_2} \left( \frac{|t_{z\uparrow}^s|^2}{2} M_1(k) + \frac{|t_{z\uparrow}^o|^2}{2} M_2(k) \right) \times \left( n_F(E_k, \mu_{\text{TI}}, T_{\text{TI}}) - n_F(E_k, \mu_{\text{STM}}, T_{\text{STM}}) \right).
\]

The first and the second term with the coefficients \(|t_{z\uparrow}^s|^2\) and \(|t_{z\uparrow}^o|^2\) respectively refer to the processes where the electron is injected into and then taken back from the Fermi energy and odd parity orbitals respectively, hence they come with their respective STM coupling strengths \(|t_{z\uparrow}^s|^2\) and \(|t_{z\uparrow}^o|^2\). The third term on the other hand refers to the process where the electron is injected into an even parity orbital but taken out from the odd parity orbital. The explicit form of the terms \(M_1(k)\), \(M_2(k)\) and \(M_1(k)\),
\[
M_1(k) = 1 + \cos \theta_s \cos \theta_k + \sin \theta_s \sin \theta_k \cos(\phi_s - \phi_k)
\]
\[
M_2(k) = 1 - \cos \theta_s \cos \theta_k + \sin \theta_s \sin \theta_k \cos(\phi_s - \phi_k)
\]
\[
M_{12}(k) = e^{-i\phi_z} [\sin \theta_k + \sin \theta_s \cos(\phi_s - \phi_k) + \cos \theta_s \sin(\phi_s - \phi_k)]
\]
sheds more light on the three processes described above. It is quite clear from Eq. (29) and Eq. (30) that \(M_1(k)\) and \(M_2(k)\) are nothing but the magnitude squared of the spinor overlaps of the spin part of the STM spinor and the ones representing the spins of the even and odd parity orbital sectors respectively. These two terms are later used to reconstruct the spin texture. The third term containing \(M_{12}(k)\) can be understood in terms of an interference term for a two path interferometer where even and odd parity orbital sectors define the two paths. As discussed in the beginning of section, to obtain a physical answer we need to average over the relative amplitude and phase of \(t_{z\uparrow}^{\uparrow}\). In order to do so, we use the parametrization, \(t_{z\uparrow}^{\uparrow} = \cos(\theta_o/2)\) and \(t_{z\uparrow}^{\downarrow} = e^{i\phi_o} \sin(\theta_o/2)\) where smallness of the tunneling amplitude is dumped into \(J\) (see Eq. (20)). This allows us to explore and perform an equal weight averaging over the full space of relative amplitudes of \(t_{z\uparrow}^{\uparrow}\) and \(t_{z\uparrow}^{\downarrow}\) and also an averaging over all possible relative phases (for \(\theta_o\), averaging is done from 0 to \(\pi\), and for \(\phi_o\), it is from 0 to \(2\pi\)). The momentum resolved current before averaging takes a form given by
\[
I(k) = \frac{e J^2 \rho_{\text{STM}}}{2\hbar N_2} \left[ 1 + \cos \theta_o \cos \theta_s \cos \theta_k + \sin \theta_s \sin \theta_k \cos(\phi_s - \phi_k) - \sin \theta_s \cos(\phi_s - \phi_k) \sin \theta_k \right.
\]
\[
+ \sin \theta_s \cos(\phi_s - \phi_k) + \cos \theta_s \sin(\phi_s - \phi_k)]
\]
\[
\times \left( n_F(E_k, \mu_{\text{TI}}, T_{\text{TI}}) - n_F(E_k, \mu_{\text{STM}}, T_{\text{STM}}) \right).
\]
Taking an average over $\theta_o$ and $\phi_o$, the momentum resolved current can be expressed as
\[
I(k) = eJ^2\frac{\rho_{\text{STM}}}{\hbar N_2} (1 + \sin \theta_o \sin \theta_k \cos(\phi_o - \phi_k)) \times (nF(E_k, \mu_{\text{TI}}, T_{\text{TI}}) - nF(E_k, \mu_{\text{STM}}, T_{\text{STM}})). \quad (33)
\]
Since in an realistic situation, the STM will never be fully polarized, one has to account for it by putting in a polarization factor defined by $p = (\rho_0^{\text{STM}} - \rho^x_{\text{STM}})/(\rho_0^{\text{STM}} + \rho^x_{\text{STM}})$ in the expression for current as
\[
I(k) = eJ^2\frac{\rho_{\text{STM}}}{\hbar N_2} ((1 + p) S_{\text{STM}} \cdot \langle \sigma \rangle(k)) \times (nF(E_k, \mu_{\text{TI}}, T_{\text{TI}}) - nF(E_k, \mu_{\text{STM}}, T_{\text{STM}})). \quad (34)
\]
where $S_{\text{STM}}$ is the unit vector which is pointing along the magnetization of the STM. $\rho_{\text{STM}} = (\rho_0^{\text{STM}} + \rho^x_{\text{STM}})/2$ is defined as the average DOS of the STM. Note that the current injected from the STM into each momentum mode indeed has a elegant TMR form\cite{23} once averaging is performed. Of course the contribution of the term $S_{\text{STM}} \cdot \langle \sigma \rangle(k)$ to $I(k)$ reduces to zero if we sum over all momentum modes due to TRS. On the other hand the value of $S_{\text{STM}} \cdot \langle \sigma \rangle(k)$ when summed over a finite segment of the Fermi surface of the TI surface is non zero. Based on this fact and following Ref.\cite{28} below we define a current asymmetry $\Delta I$ which successfully captures the TMR response and can be measured in a multi-terminal set-up shown in Fig. (1).

\[
\Delta I = I_L - I_R = \left( \int_{-\pi}^{\gamma+\pi} - \int_{\gamma+\pi}^{+2\pi} \right) d\delta k \int_0^\infty dk k I(k), \quad (35)
\]
where $k_1$ and $k_y$ are parametrized as $k_1 = k \cos \delta k$ and $k_y = k \sin \delta k$ and $I_L$ and $I_R$ are the current collected by the left and the right contact. This quantity essentially couples to the magnetization of half of the Fermi surface of the TI surface state where the chosen half of the Fermi surface depends on the choice of $\gamma$. This result gives a clear indication that, by studying the profile of the current asymmetry $\Delta I$ as a function of the magnetization direction of the STM electron and $\gamma$, one can reconstruct the Fermi surface and its spin texture for all surfaces corresponding to different values of $\theta$. To get rid of the dependencies on parameters like the system sizes, tunneling strength etc., one can always define a dimensionless measurable, the current asymmetry $\Delta I$ normalized by the total injected current $I_0$, as
\[
\frac{\Delta I}{I_0} = \left( \int_{-\pi}^{\gamma+\pi} - \int_{\gamma+\pi}^{+2\pi} \right) d\delta k \int_0^\infty dk k I(k). \quad (36)
\]

**VII. IDENTIFYING THE SURFACE**

In this section, we show that the current asymmetry measurement $\Delta I$ could lead to a unique identification of the surface $\Sigma(\theta)$. The strategy for this identification is based on the observation that the expression for the $\langle \sigma_x \rangle$ in Eq.\ref{16a} has a momentum independent part which is proportional to $\cos \theta/v_3$. This observation implies that the $x$-component of magnetization for any finite segment of the Fermi surface also scales by this factor which depends only on the value of $\theta$. Hence this factor will show up in the expression for $\Delta I$ (note that $\Delta I$ is proportional to magnetization of half of the Fermi surface) provided we choose the STM magnetization along the $x$-direction. To see this fact more clearly we note that the momentum resolved tunneling current for the case of STM magnetized pointing along $x$ direction (obtained from Eq.\ref{34}) is given by
\[
I(k) \propto (1 + p \langle \sigma_x \rangle(k)). \quad (37)
\]
It is now obvious from Eq.\ref{33} that the current asymmetry $\Delta I$ in this situation has to be proportional to the $\langle \sigma_x \rangle$ averaged over half of the Fermi surface of the surface state, which in turn depends on the scale factor $\cos \theta/v_3$. To maximize the signal, orientation of the contact is taken to be such that it maximizes $\Delta I$ for the given magnetization direction of the STM tip. It can be shown that $\gamma = 0$ is the configuration\cite{28} that meets the criterion. Note that, changing the orientation of the contact (i.e., changing $\gamma$) on the surface must be done with respect to the orientation of the underlying lattice which is be to be held fixed. Hence changing the orientation of contact is not equivalent to rotating the sample about the $k_3$-axis.

A systematic measurement of the quantity $\Delta I$ as a function of $\theta$ while the STM magnetization points only along the $x$-direction should fit a function of the form $c \cos \theta/v_3$ where $c$ is a constant. Hence, for an arbitrary surface $\langle \sigma_x \rangle$, measurement of $\Delta I$ with the STM magnetization pointing along $x$-direction can be used to uniquely identify the value of $\theta$ for that particular surface. Also, to ensure that a possible variation in strength of the tunnel coupling $J$ used to probe surfaces with different $\theta$ does not spoil the proposed strategy for identifying the surface, one can always normalize $\Delta I$ by total injected current $I_0 = I_R + I_L$ resulting in a dimensionless quantity irrespective of the details of $J$. This fact is demonstrated in Fig. (7). The value $c$ appearing in the plot is given by the following relation,
\[
c = v_z \frac{\Delta I}{I_0} \bigg|_{\theta=0,\gamma=0}. \quad (38)
\]
Since, for the $\theta = 0$ surface, the spin momentum locking is perfect, it is straightforward to show that
\[
\frac{\Delta I}{I_0} \bigg|_{\theta=0,\gamma=0} = p \frac{2}{\pi}. \quad (39)
\]
Plugging Eq.\ref{39} in Eq.\ref{38}, one gets the value of $c$ as
\[
c = p \frac{2v_z}{\pi}. \quad (40)
\]

It can be seen that the current asymmetry measurement discussed above, can be exploited to extract the fundamental parameters of the bulk Hamiltonian. $\Delta I/I_0$ if experimentally measured could be fitted to a theoretically predicted functional...
FIG. 5. The data points show \( \Delta I/I_0 \) calculated for the STM tip being magnetized in the \( x \) direction \( (\theta_x = \pi/2, \phi_x = 0) \) and the ideal case \( p = 1 \), for the contact configuration corresponding to \( \gamma = 0 \). The solid line shows the continuous function \( c \cos \theta/v_3 \) which is the function followed by the current asymmetry as function of the surface.

The form given by

\[
\frac{\Delta I}{I_0} = p \frac{2v_z}{\pi} \frac{\cos \theta}{\sqrt{v_z^2 \cos^2 \theta + v_3^2 \sin^2 \theta}} \tag{41}
\]

which is just a two-parameter fit over the fundamental parameters \( v_z \) and \( v_3 \) of the bulk Hamiltonian. In conclusion, the set of measurements of the current asymmetries over different surfaces, acts like a hologram of the bulk. This is not possible with any set of measurements on a single surface.

VIII. RECONSTRUCTION OF SPIN TEXTURE

The objective of this section is to show how the current asymmetry measurements lead to a direct reconstruction of the spin textures of Fermi surfaces of arbitrary TI surface states. It was earlier shown in Ref. [38] that scanning \( \Delta I \) as a function of \( \gamma \) with a fixed chosen direction for magnetization of the STM tip for a perfectly spin-momentum locked \( \theta = 0 \) surface leads to a complete reconstruction of the spin texture on the Fermi surface. This was possible as the Fermi surface for the \( \theta = 0 \) surface has a perfect azimuthal symmetry in the momentum space. For an arbitrary surface \( (\theta \neq 0) \), we can see from Fig. 2 that the Fermi surface is elliptical. Also, the average spin associated with each momentum mode is not a constant as we move along the Fermi surface. Moreover, the spin-momentum locking angle is also skewed in the sense that the angle between the averaged spin and the corresponding momentum is not a constant as we move along the Fermi surface. The Fermi surface being elliptic and the spin momentum locking angle being not a constant make it necessary that we make a TMR scan over \( \gamma \) for at least two magnetizations directions of the STM spin for a unique reconstruction of the spin texture. This is so because, for a general \( \theta \), the \( x \)- and \( y \)-components of the spins have independent dynamics as we move along the Fermi surface and hence it requires two distinct measurements with different STM magnetizations to reconstruct them.

The TMR response in Eq. (34) is same for all surfaces irrespective of the details of the spin texture discussed above and this is attributed to the fact that the current asymmetry \( \Delta I \) couples to the magnetization density (per unit area) of the half of the Fermi surface \( i.e., \langle \sigma \rangle_{\text{half}} \) in the bias window which is defined as

\[
\langle \sigma \rangle_{\text{half}}(\gamma) = \int_0^\infty dk \int_{\gamma}^{\gamma+\pi} d\delta_k \langle \sigma \rangle(\gamma)(n_{F,\text{STM}}(\gamma) - n_{F,\text{STM}}). \tag{42}
\]

Presence of TRS forces the net magnetization over the full Fermi surface to be zero, which implies that the magnetization of the two halves of the Fermi surface are equal and opposite to each other, i.e., \( \langle \sigma \rangle_{\text{half}} = -\langle \sigma \rangle_{\text{half}}(\gamma + \pi) \). Since the current asymmetry basically couples to the difference in the magnetization of the two halves i.e. \( \Delta I \approx S_{\text{STM}} \cdot (\langle \sigma \rangle_{\text{half}}(\gamma) - \langle \sigma \rangle_{\text{half}}(\gamma + \pi)) \), it is easy to see that

\[
\Delta I \approx S_{\text{STM}} \cdot \langle \sigma \rangle_{\text{half}}(\gamma), \tag{43}
\]

which is the central relation connecting the current asymmetry to the spin texture and hence leading to its reconstruction. The magnetization of half of the Fermi surface, depends on two factors, \( \theta \) and \( \gamma \). These two factors uniquely fix the magnetization of the given segment of the Fermi surface. The strategy which is followed for the spin reconstruction is as follows: first, a TMR scan by varying \( \gamma \) is done for an STM magnetized in the \( x \) direction and the current asymmetry is plotted as a function of \( \gamma \). The sign of the asymmetry gives the handedness of the spin texture. However, unlike the \( \theta = 0 \) and \( \pi \) surfaces, this is not enough for reconstructing the spin texture on an oblique surface. On the \( \theta = 0 \) and \( \pi \) surfaces, reconstruction of one component of the spin is enough to reconstruct the entire spin texture owing to the perfect spin-momentum

FIG. 6. The panels show the magnetization of the half of the Fermi surface in the \( x \) direction (top), \( y \) direction (middle) and its magnitude (bottom) as a function of \( \gamma \) for three different surfaces corresponding to \( \theta = 0, \pi/4 \) and \( \pi/2 \).
locking and azimuthal symmetry of the spin texture in the momentum space. For reconstructing the magnitude of the spin another TMR scan by varying $\gamma$ is done but with the STM magnetization pointing in the $y$ direction. $\Delta I/I_0$ plotted for the case of STM spin pointing in the $x$-direction is shown in Fig. (7). The three panels at the top show the current distribution pattern at finite bias in the $k_1-k_y$ plane for three different surfaces $\Sigma(\theta)$ corresponding to $\theta = 0$, $\pi/4$ and $\pi/2$ as labeled in the plot. It can be seen that, as one moves from the $\theta = 0$ surface to an oblique surface, the anisotropy in current distribution pattern at finite bias in the $x$ direction, as it exactly mirrors the $x$-component of magnetization of half the Fermi surface as shown in Fig. (6). Hence such a measurement will indeed lead to reconstruction of $x$-component of the spin texture presented in Fig. (6).

These measurements however do not throw any light on the $y$-magnetization of the Fermi surface and hence one can not predict anything about the texture of the magnitude of the spin polarization of the surface based on the above measurement alone. For this one needs, as mentioned above, another similar set of measurements, but with the STM spin pointing in the $y$-direction. These results are presented in Fig. (8). The current asymmetry peak as a function of $\gamma$ for the STM polarized in the $y$ direction (Fig. (8) bottom) is shifted by $\pi/2$ compared to the case where the STM polarization is in the $x$ direction (Fig. (7) bottom). However, for oblique surfaces the asymmetry profile is not just a trivial shift of the curve by $\pi/2$. Two differences are to be noted here, firstly, the asymmetry does not go down as one goes to a more and more oblique surface and secondly, the curve flattens out more and more near the peak as one goes to a more and more oblique surface. The first point implies that magnitude of the spin polarization does not go down as $\theta$ is increased, and the second, points towards an elliptical Fermi surface. This can be understood as follows: from Eq. (16b) one can see that on the Fermi surface, $\langle \sigma_y(k) \rangle$ is directly proportional to $k_1$. For a wide range of angles near the peak, $k_1$ is high enough to flatten out the peak of the current asymmetry. This already suggests an extended structure of the Fermi surface in the $k_1$ direction. Complimenting this is also the observation that as $\theta$ is increased the fall of the asymmetry’s magnitude towards $0$ gets sharper. This also indicates that the Fermi surface is less extended in the $k_y$ direction compared to the $k_1$ direction. These two observations uniquely identify the conic section of the Fermi surface to be an ellipse. Another information that can be extracted is about the Fermi velocities perpendicular and parallel to the crystal growth axis ($v_\parallel$ and $v_\perp$, respectively). As one goes to a more and more oblique surface, one expects that the contribution of $v_\parallel$ to the Fermi velocity in $k_1$ direction to increase. So the observation that as $\theta$ is increased the Fermi surface gets more elliptical and extended in the $k_1$ direction points to the fact that $v_\parallel < v_\perp$ as the semi-axes of the Fermi surface in the $k_1$ and $k_y$ directions are proportional to $v_\perp^{-1}$ and $v_\parallel^{-1}$ respectively. Coming back to the spin texture, one can conclude that all the surfaces are devoid of any spin polarization in the $z$ direction as one never finds any current asymmetry, if the STM is spin polarized in the $z$ direction. Hence in this section we have shown, how the current asymmetry can uniquely reconstruct the spin texture $\langle \sigma_x(k) \rangle$ and $\langle \sigma_y(k) \rangle$ and provide clear indication of change of Fermi surface from a circular (for $\theta = 0$ surface) shape to an ellipse (for $\theta \neq 0$ surface) like shape.
IX. CONCLUSION

In this article we have developed a tunnel Hamiltonian approach for injection of spin polarized electrons from a magnetized STM into the surface which is exposed by cleaving a crystal of a 3D TI material like Bi$_2$Se$_3$ at a given angle $\theta$ with respect to the crystal growth axis. We apply this tunnel Hamiltonian approach to demonstrate that electrical transport in the linear response regime carries unique signatures of the surface corresponding to a given $\theta$. Our proposal also provides a strategy to exploit the three terminal TMR scan to determine the unconventional spin-momentum locking textures for the $\theta \neq 0, \pi$ surfaces. Hence, though conventionally x-ray spectroscopy is used to identify different crystal surfaces, in this case one can use an electrical transport probe as an alternative. We also show that a complete set of current asymmetry measurements over different surfaces does act as a hologram of the bulk band-structure.

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