Tunnel Magnetoresistance scan of a pristine 3D topological insulator

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Though the Fermi-surface of surface states of a 3D topological insulator (TI) has zero magnetisation, an arbitrary segment of the full Fermi surface has a unique magnetic moment consistent with the type of spin-momentum locking in hand. We propose a three-terminal set up which directly couples to the magnetisation of a chosen segment of a Fermi surface hence leading to a finite tunnel magnetoresistance (TMR) response of the non-magnetic TI surface states, when coupled to spin polarised STM probe. This multi-terminal TMR not only provides an unique signature of spin-momentum locking for a pristine TI but also provides a direct measure of momentum resolved out of plane polarisation of hexagonally warped Fermi surfaces relevant for $Bi_2Te_3$ which could be as comprehensive as spin resolved ARPES.

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**Introduction:** The two popular probes used to scan the surface states of TI are either ARPES or STM. Spin polarized ARPES provides a direct probe into the spin texture of surface states but the STM on the other hand primarily relies on the disorder induced quasi-particle interference patterns which provide indirect information about the spin texture of the Fermi surface. Hence an electrical transport probe which would work in the ballistic limit and directly couple to the spin texture like ARPES is missing at the moment. Engineering such a probe is of utmost importance for developing a clear understanding of possible application of TI in device physics (for e.g., in TI based spin transistors). Both theoretical and experimental attempts have been made in this direction using spin polarised STM (SPSTM) via tunnel magnetoresistance (TMR) scan. But these proposals intrinsically rely on explicitly breaking time reversal symmetry either by applying an external magnetic field or by magnetic doping. The reason being, spin texture of Fermi surfaces constrained by time reversal symmetry (TRS) do not couple to magnetization direction of SPSTM hence rendering the SPSTM useless unless TRS is broken externally. In this letter we propose a protocol using SPSTM tip which results in a large TMR between the TI and SPSTM in absence of any TRS breaking elements in the TI. We show that the angular distribution of the injected current from SPSTM into the TI surface changes as we change the direction of magnetisation of the STM though its magnitude remains unchanged. And this anisotropy in the in-plane angular distribution of injected current can be captured in a multi-terminal set up leading to a finite TMR defined within this multi-terminal setup. We show that, one can exploit this observation to directly probe spin textures of TI surface states using multi-terminal TMR and the results are shown to be as comprehensive as that from ARPES.

**Proposed set up:** The proposed set up comprises of two contact pads placed diametrically opposite to each other on the surface of the TI and electrons are injected from the SPSTM placed at the centre of the sample as shown in Fig. 1. The surface can be imagined to be divided into two halves by a line through the center of the sample perpendicular to the direction joining the two contacts, (for future reference, we mention that the angle made by this partitioning line with the $x$-axis is denoted by $\gamma$, see Fig. 1). Each contact measures the current flowing in the surface in its own half. We show that the total current $I_0 = I_L + I_R$ is insensitive to current anisotropy discussed above owing to zero magnetisation of Fermi surface but the $\Delta I = I_L - I_R$ is very sensitive to the current anisotropy and leads to a finite TMR response with the spin polarised STM which varies as a function of $\gamma$. Note that $\gamma$ can be changed simply by rotating the sample with respect to the tip about $z$-axis. We show that $\Delta I$ measured as a function of $\gamma$ leads to a direct reconstruction of in-plane spin texture in the momentum space.
i.e., we can extract the angle of spin-momentum locking ($\theta_L$) and the chirality; left chiral or right chiral from this study. Then we extend the calculation to include warping effects and show how a similar measurement can uniquely reconstruct the six-fold symmetric out-of-plane spin texture of the warped Fermi surface too.

Model: We start with the generic Hamiltonian for the 3D TI surface state given by

$$\mathcal{H}_{TI} = \hbar v_F \sum_k \Psi_{TI}^*(\vec{k})(\sigma \times \vec{k})_z \Psi_{TI}(\vec{k}), \quad (1)$$

where $\Psi_{TI}(\vec{k}) = 1/\sqrt{2}(1, e^{i(\phi_k + \theta_L)})^T \hat{\epsilon}_\vec{k}^{\dagger}$ and $\hat{\epsilon}_\vec{k}$ is the annihilation operator with momentum $\vec{k}$. $\phi_k = \tan^{-1}(k_y/k_x)$ is the polar angle of the momentum vector. For Eq. (1), the spin-momentum locking angle $\theta_L$ is treated as interaction. De-composing the current in momentum space we obtain,

$$\chi_{(\vec{k}, \vec{k}')} = \int_0^\infty dt \Re \{ G_{TI}(\vec{k}, 0; \vec{k}, \tau) G_{STM}(\vec{k}', \tau; \vec{k}', 0) \}$$

has the Green’s functions, where $G$ denotes the standard time ordered Fermionic Green’s functions and the delta function ensures energy conservation. Hence we obtain a momentum resolved current given by

$$\langle I(\vec{k}) \rangle = \frac{e}{h} |z_k|^2 \chi_{\vec{k}}, \quad (4)$$

where $\chi_{\vec{k}} = \int_{-\infty}^{+\infty} d\vec{k}' \chi_{\vec{k}, \vec{k}'} \delta(\varepsilon_{STM}(\vec{k}') - \varepsilon_{TI}(\vec{k})).$ The total tunneling current is just a sum over $\langle I(\vec{k}) \rangle$ for all possible $\vec{k}$ living in the bias window.

The angular distribution of the injected current in real space is same as the angular distribution of momentum resolved current about the tunneling point. As a consistency check for this, we evaluate the expectation value of the current vector operator for a pristine TI surface $\hat{j}(\vec{r}) = (\sigma^x(\vec{r}), -\sigma^y(\vec{r}))$ at $\vec{r} = 0$ perturbatively to second order in tunnel Hamiltonian and obtain $\langle \hat{j}(\vec{r} = 0) \rangle = \int \hat{\epsilon}_\vec{k} \Psi_{STM}(\vec{k}) \hat{n}_\vec{k}$ which reconfirms our interpretations of $\langle I(\vec{k}) \rangle$ being the real space angular distribution of current about the injection point. Here $\hat{n}_\vec{k}$ is a unit vector pointing along $\vec{k}$. Owing to the azimuthally symmetric (in $k$-space) Fermi surface, $\langle \hat{j}(\vec{k}) \rangle$, turns out to be separable in its dependence on $|\vec{k}|$ and $\phi_k$ as $\langle \hat{j}(\vec{k}) \rangle = \hat{I}_{\phi_k} \hat{I}_{\phi_k}$ with

$$\hat{I}_{\phi_k} = \frac{1}{2} \sin \theta_{STM} \sin(\phi_{STM} - \phi_k). \quad (5)$$

It is clear from the above result that the total injected current which is obtained by summing over all possible momenta in the bias window leads to a current which is independent of the direction of STM tip magnetisation\cite{STM} (zero TMR) consistent with TRS in TI. But the current asymmetry defined as $\Delta I = I_L - I_R = (\int_{-\pi/2}^{\pi/2} - \int_{-\pi/2}^{\pi/2}) d\theta_{STM} \hat{I}_{\phi_k} \int d|\vec{k}| \hat{n}_\vec{k}$ which could be measured directly in the set up depicted in Fig.1 shows a finite TMR as function of $\gamma$ given by

$$\Delta I = \frac{4eJ^2}{hN_{STM}^2} F \cos(\phi_{STM} - \gamma) \sin \theta_{STM}, \quad (6)$$

where $F = \int_{-\infty}^{+\infty} dE E(n_F^{TI} - n_F^{STM})$ is obtained from the $|\vec{k}|$ integral by appropriately putting in the density of states, where $n_F(E, \mu, T)$ denotes the Fermi function.

Reconstructing spin texture: We will now demonstrate that the above expression can be directly exploited to uniquely identify the spin-momentum locking angle and the chirality. At this point it is important to note that all the in-plane angles like $\gamma$ and $\phi_{STM}$ are measured with respect to the positive direction of x-axis along the anti-clock wise direction. For the case of $\phi_{STM} = \pi/2$ observing a zero in $\Delta I$ at $\gamma = 0$ (see Fig.2) implies that the momentum modes pointing towards the left and right contact starting from the tip position have a locked-spin which is pointing perpendicular to the STM polarisation
pointing along y-axis (see Fig. 1) so that the injected current gets symmetrically distributed between left and right contact. Assuming a planar spin texture, it directly tells us that the spin momentum locking angle $|\theta_L| = \pi/2$. Of course this conclusion relies on the assumption that the Fermi-surface is circular in shape so that spin on each half can be added up symmetrically. Now we are left with two possibilities: the two oppositely directed momentum modes discussed above pointing towards left and right contact have a locked-spin either pointing parallel and anti-parallel to the $x$-axis or the other way round respectively. And this information is nothing but the spin chirality of the Fermi surface. To settle the chirality, we observe that $\Delta I$ is maximally negative for $\gamma = \pi/2$. This implies that maximal share of the injected current is flowing to the right contact (as depicted in Fig. 1) implying that the momentum mode pointing towards right starting form the tip position has a locked-spin which is parallel to the tip magnetisation direction. Hence the study of $\Delta I$ also implies that the momentum mode pointing along $x$-axis has a locked-spin pointing along $y$-direction hence reading out the spin chirality of the Fermi surface in hand. So its leads to conclusion that the spin-momentum locked spin is uniquely given by $\hat{\sigma}(k) = (-\sin \phi_y, \cos \phi_y)$. Hence our claim of reconstructing the Fermi-surface spin texture using the proposed three-terminal TMR data is clearly demonstrated. For an arbitrary spin-momentum locking angle $\theta_L$, $\Delta I \sim \sin(\gamma - \phi_{STM} + \theta_L)$; the maxima in its magnitude occurs at $\gamma = \phi_{STM} - \theta_L + \pi/2$ and hence the spin-momentum locking angle can be extracted. The sign of the first maxima of $\Delta I$ as we increase $\gamma$ form zero gives the chirality.

**TMR and $I_{L/R}$:** The next step is to recast $I_{L/R}$ or equivalently $\Delta I$ in an explicit TMR form which puts our idea on a firm footing and adds further transparency to the discussion above. Note that a net spin polarisation vector can be obtained by performing a vector sum of spin polarisations of each momentum mode living on half of the Fermi surface of TI surface states, where the Fermi surface bipartition is done along the line defining $\gamma$. This quantity for each half of the Fermi Surface

$$I_{L/R} = \frac{\pi J e^2 |\rho_{STM}|}{h} [1 \mp \frac{2p}{\pi} \hat{\rho} \cdot \hat{S}] V$$

where $\rho_{STM}$ is the spin averaged DOS of the tip, $p$ is the polarisation of the tip given by $(\rho_{STM} - \rho_{STM}^\parallel)/(|\rho_{STM}^\parallel + 1)$ and $V$ is the applied voltage bias between tip and TI. $\hat{S}$ and $\hat{S}_{STM}$ are unit vectors along $\hat{l}$ and magnetization direction of the tip. We see that indeed the left and right contact shows a standard TMR response[9] having opposite signs (due to TRS) with the magnetized STM and the pure magnetic response can be extracted form it simply by taking an antisymmetric combination of the two which is nothing but $\Delta I$. Hence spin-momentum locking together with multi-terminal set up leads to this exotic situation where large TMR response is extracted out of a non-magnetic material which is shown to be useful for characterising the material itself. This is the central finding of this letter. It is important to note that the expression for $I_{L/R}$ obtained above remains valid as long as there is well defined spin-momentum locking protected by time reversal symmetry independent of the spin-momentum locked spins being in plane or out of plane. This observation is crucial for application of Eq. (7) to the next case (warped case) where we have out of plane spin-momentum locking.

**Warped case:** Next, we consider a hexagonal warping term in the Hamiltonian of the TI which leads to out of plane polarisation of the TI electrons given by

$$\mathcal{H}_{warp} = \sum_{\mathbf{k}} (\hat{\sigma} \times \hat{k})_z + \frac{\lambda}{2} (k_1^3 + k_3^3)\sigma^z.$$
The warping Hamiltonian give rise to a spin texture at the Fermi surface whose out-of-plane spin polarisation has a staggered structure in momentum space. The momentum space splits up into six symmetric regions with alternating signs of the out of plane magnetisation. It can be seen from Fig. 3 that as the chemical potential doping is increased, the conical band structure begins to warp as depicted in the contour plots. For the numerical plots, the parameter values are taken from Ref.[10].

Reconstructing out of plane spin texture: In this case we keep the SPSTM magnetization either parallel or anti-parallel to the z-axis. Electrons injected from spin polarised STM pointing along positive z-direction see six alternating regions with positive and negative out-of-plane polarization on the Fermi surface leading to alternating high and low overlap of the wavefunctions in momentum space. This leads to a high current density in three regions and low current density in the rest of the three. This pattern reverses itself as the STM magnetisation is reversed. This pattern of the current distribution is evaluated using Eq. (7) and is shown in Fig. 4. This current pattern can be measured by the same three-terminal current measurements setup defined above but there is a crucial difference. In the previous case rotating the orientation of the contacts (i.e. changing $\gamma$) was equivalent to rotating the sample about z-axis owing to azimuthal symmetry of the Fermi surface but in this case the contacts are to be engineered separately for each $\gamma$ while keeping the orientation of underlying lattice on the x-y plane fixed as the hexagonal warping of the spectrum is a direct reflection of the underlying lattice. Hence a minimal set up requires multiple samples with identical orientation of underlying lattice in the x-y plane with contact pads rotated with respect to each other. The three-fold symmetry of the lattice, which gives rise to the three fold symmetry of the out of plane spin polarization causes a periodicity of $2\pi/3$ in $\Delta I$ measured as a function of $\gamma$ (see Fig. 4). It can be seen from the figure that if the line partitioning the sample into two halves goes through the corners of the hexagonal pattern of the Fermi surface, then the asymmetry is extremal, on the other hand if it goes through the centre of the sides of the hexagon, the asymmetry is zero. A periodicity of $2\pi/3$ in $\Delta I$ as we vary $\gamma$ implies that there is a 3-fold symmetry in the texture. Three successive peaks (dips) turning into dips (peaks) as we flip the STM magnetization direction from positive z-axis to negative z-axis implies the presence of three regions with positive out-of-plane magnetisation and three others with negative. The symmetry in magnitude of the dip and peak indicates the up and down polarised patches being equal in length on the Fermi surface. This demonstrates that $\Delta I$ could be used for uniquely reconstructing the out of plane polarisation of the Fermi surface in the warped case.

Conclusion: We showed that the non-magnetic surface states of the TI show strong TMR response when subjected to the proposed multi-terminal measurement set up involving spin polarised STM. A detailed protocol of reconstruction of spin-momentum locked Fermi surface in absence and presence of warping purely based on TMR scan is laid down which seems to be as comprehensive as the ARPES approach. Also this proposal could take the STM based TI probes to new directions which work in ballistic limit and couple directly to the spin texture unlike existing STM approaches based on disorder induced quasiparticle interference patterns. At the end, we would like to point out that largely disorder free TI samples where the physics described above could be tested are already in place where ferromagnetic contact were planted on the TI surface to probe spin momentum locking signatures[11].

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