Surface States of Topological Insulators

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We develop an effective bulk model with a topological boundary condition to study the surface states of topological insulators. We find that the Dirac point energy, the band curvature and the spin texture of surface states are crystal face-dependent. For a given face on a sphere, the Dirac point energy is determined by the bulk physics that breaks p-h symmetry in the surface normal direction and is tunable by surface potentials that preserve T symmetry. Constant energy contours near the Dirac point are ellipses with spin textures that are helical on the S/N pole, collapsed to one dimension on any side face, and tilted out-of-plane otherwise. Our findings identify a route to engineering the Dirac point physics on the surfaces of real materials.

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\[ \mathbb{Z}_2 \]

is joined to a TI with \( \mathbb{Z}_2 = -1 \). On the cleavage surface of Bi

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\[ \text{2} \]

\[ \text{2} \] Z

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Since the vacuum has p-h symmetry around for this eigenvalue problem. The spin and is localized on the surface. This midgap (001) equator represents the side faces perpendicular to the quintuple layers. For any face \( \Sigma(\theta) \), \( k_3 \perp \Sigma \) and \( k_2 = k_y \).

We first focus on the one dimensional quantum mechanics of (001) surface turning off the quadratic terms in Eq. (1). Notice that the two spin flavors are decoupled for this eigenvalue problem. The spin \( \uparrow \) states in \( \{ \tau, \sigma \} \) representation are determined by the following coupled Dirac equations

\[
\begin{pmatrix}
-\frac{m(z) - E}{v_x \partial_z} & -v_x \partial_z \\
v_x \partial_z & \frac{m(z) - E}
\end{pmatrix}
\begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix} = 0.
\]

The wave function \( \psi_\uparrow = (\psi_1, \psi_2)' \) is continuous across the surface, integrating Eq. (2) over the vicinity of the surface. This continuity condition leads to a nontrivial solution which is isolated in the middle of the bulk gap and is localized on the surface. This midgap (\( E = 0 \)) state has a simple and elegant exact solution,

\[
\psi_{k_3, \uparrow}(x, y, z) = \frac{1}{A} e^{i(k_x x + k_y y)} \phi(z) \begin{pmatrix} 1 \\ 0 \end{pmatrix}_\sigma \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_\tau,
\]

\[
\phi(z) = \begin{cases} 
e^{-\kappa z}, & z > 0 \quad \text{(TI)} \\
e^{\kappa_0 z}, & z < 0 \quad \text{(Vac)} 
\end{cases}
\]

where \( \kappa = m/v_x \), \( \kappa_0 = M/v_x \) and \( A \) is a normalization factor. \( \phi(z) \) is evanescent on both sides of the surface where the mass \( m_0 \) changes sign, analogous to Jackiw and Rebbi solution22 of a two-band Dirac model. The spin \( \downarrow \) solution can be obtained by \( \psi_\downarrow = T \psi_\uparrow \). This isolated midgap state at \( k_3 = 0 \) is identified as the Dirac point and at finite \( k_3 \) spreads into a perfect Dirac cone-the ideal topologically protected surface bands.

Surface state spin texture.— On the (001) surface, the midgap solution of the boundary problem at \( k_3 = 0 \) is determined by the operators \( \tau_\uparrow \) and is free under any rotation of the operators \( \sigma \). This \( \sigma \) algebra of the boundary problem can be generalized to any surface with \( \tau \) replaced by \( S_1 \) and \( \sigma \) by \( S_2 \). For an arbitrary crystal face \( \Sigma(\theta) \) defined in Fig. 1 the algebraic structure is

\[
\begin{align*}
S_1 &= \{ \alpha \tau_x + \beta \tau_y, \alpha \tau_y - \beta \tau_x, \tau_x \}, \\
S_2 &= \{ \alpha \sigma_x - \beta \sigma_y, \alpha \sigma_y + \beta \sigma_x \tau_z \},
\end{align*}
\]

where \( \beta = \sqrt{(v_x \cos \theta)^2 + (v_\gamma \sin \theta)^2}, \quad \alpha = v_x \cos \theta/v_3 \) and \( \beta = v_\gamma \sin \theta/v_3 \). These new pseudospins satisfy \([S_1, S_2^\dagger] = 2i \sigma a \sigma e^{i\theta} S_h^a \). Rewritten in this new pseudospin basis, Eq. (1) reads

\[
\mathcal{H} = -m_0 S_1^2 + (v_3 k_3 + v_0 k_1) S_1^y \\
+ (v_0 k_y S_2^y - v_1 k_1 S_2^z) S_1^x,
\]

from which we can further explicitly demonstrate the surface state spin texture on \( \Sigma(\theta) \):

\[
\langle \sigma_x \rangle_\theta = \pm \frac{v_x v_0 k_y \cos \theta}{v_3 \sqrt{v_1^2 k_1^2 + v_0^2 k_y^2}},
\]

\[
\langle \sigma_y \rangle_\theta = \pm \frac{-v_3 v_1 k_y}{v_3 \sqrt{v_1^2 k_1^2 + v_0^2 k_y^2}},
\]

\[
\langle \sigma_z \rangle_\theta = 0,
\]

where \((+(-))\) denotes the conduction (valence) band. The electron real spin \((s)\) is proportional to but always smaller than \((\sigma)\) due to the SOC\[23\]. In the local coordinates, \( \langle \sigma_x \rangle_\theta = \langle \sigma_x \rangle_\theta \cos \theta \) and \( \langle \sigma_y \rangle_\theta = \langle \sigma_y \rangle_\theta \sin \theta \). Eq. (7) indicates that the surface state spin texture is rather different from face to face while its pseudospin \((S_2)\) has a universal structure on the elliptic constant energy contour near the Dirac point. Clearly, there is no spherical symmetry to guarantee that the spin and orbital structures are the same anywhere on a TI sphere. The crystal face-dependent spin texture is helical on the south and north poles, is compressed to a single dimension along the equator, and is tilted out-of-plane otherwise. The surface state anisotropy and spin textures for different faces are compared in Fig. 2.
In linear order C₃ symmetry upgrades to continuous rotational symmetry, consequently, the surface normal spin is zero along the TI equator. On the two poles, the mirror symmetry and the C₃ symmetry insure that the spin-momentum locking into the form of \( k_y \sigma_x - k_x \sigma_y \). \( \sigma_z \) decouples to any momentum in the linear order, taking into account all the four symmetries.

It’s interesting to point out that the surface band is the positive eigenstate of \( S^2 \) and the chiral counterpart is separated and localized on the opposite face. Thus the surface state Hilbert space is reduced by \( \text{P} \) and the translational symmetry, consequently, the surface normal spin \( \tau_n \) breaks \( \mathcal{P} \) symmetry. For a \( \tau_n \) potential, it simply modifies the mass term on the surface and it is not surprising that it does not affect the surface spectra.

### Dirac point energy and surface potentials

Among these six types: faces, as shown in Table I. We focus on potentials that preserve the surface spectra and the associated wave functions as well. We understand how localized surface potentials influence the Dirac point from the midgap to a nonzero energy cone a parabolic curvature described by Eq.(8) and shifts the Dirac point energy and surface potentials.

#### TABLE I: Summary of the influence of \( \mathcal{T} \) symmetry allowed momentum-independent surface potentials \( \Delta \bar{\sigma} r(\tau) \cdot 2 \tau n/m \) on the inversion symmetry, and the wave function continuity and the Dirac point energy of surface states. This \( \Delta \) represents different surface potentials and their corresponding energy scales: \( \Delta_{0} I, \Delta_{0} \tau_{x}, \Delta_{0} S^2 \) and \( \Delta_{0} S^2 S^2 \).

A \( \tau_z \) potential tunes the amplitudes of \( \psi_1 \) and \( \psi_2 \) in the same manner on the matter side but this gives no observable effect since \( \psi_1(z) = \psi_2(z) \) and \( \psi_{1,2}(z < 0) \rightarrow 0 \) are still valid. Similarly, a potential like \( \sigma_n \tau_y \) (\( \Delta_{0} \sigma_n \equiv \bar{\Delta} \cdot \bar{\sigma} \)) does nothing to the surface spectra and \( \psi_1/\psi_2 \); however,
it couples the two spin flavors and shifts their phase in an opposite way. Note that $\psi_1 = \psi_2$ is always true on the vacuum side since $M \rightarrow \infty$. The above results are summarized in Table I providing sufficient information to construct the surface state wave function and to engineer the Dirac point energy position.

On an arbitrary face $\Sigma(\theta)$, the types of surface potentials are the same but their combinations and the corresponding roles are rearranged. This can be fully understood by the fact that the spin-orbital structure $\tau \otimes \sigma$ on the south pole is replaced by a pseudospin-pseudospin structure $S_1(\theta) \otimes S_2(\theta)$ on $\Sigma(\theta)$. Note that the combination only occurs for potentials with the same parity.

Although the surface states solutions are stable in the presence of localized surface potentials that preserve $T$ symmetry, two terms play an essential role in determining the energy position of Dirac point

$$E_{\text{DP}} = \mu_{\text{DP}} + \frac{4m^2(\Delta_0 + \Delta_e)(m^2 - \Delta_0^2 + \Delta_e^2)}{4m^2(\Delta_0 + \Delta_e)k^2 - (m^2 - \Delta_0^2 + \Delta_e^2)}$$

which implies that $I$ and $\tau_x$ potentials (Table I) are able to tune the Dirac point from the midgap to the band edges $\pm m$ independently.

Discussions.—The interactions of the topologically protected bands with surface potentials provides a robust route to engineer and manipulate the topological surface states. In particular, an external surface potential can raise or lower the Dirac point to the middle of the bulk gap and providing experimental access to the topologically protected band. This goal could be achieved by surface oxidation [25], or by other possible chemical processes [29, 31] and interactions [32] on the surface. We also point out that the electrostatic gating [25, 31, 33–35], $E_{\text{eff}}(t_a)\alpha$ can act to Stark shift the TI surface state into the gap, with field strength determined by the penetration length of surface states. Typically, the screened field $\sim 100$ meV·nm$^{-1}$ are required for the surface states evanescent in a couple of quintuple layers. Our present results provide a framework to study the self-consistent band bending physics of real TI materials [9, 10, 25, 27] and mean-field models of surface state many-body interactions.

Our model is quite different from the fixed boundary condition (FBC) which arbitrarily clamps the surface state wavefunction to zero at the boundary. The FBC solution is insensitive to the mass inversion at the surface which topologically protects the surface bands, and consequently it provides no information about the energy of the symmetry protected degeneracy relative to the bulk bands or their interaction with surface-localized potentials. Furthermore FBC admits an infinite number of (physically spurious) solutions with nonzero energies for $k_1 = k_2 = 0$ that satisfy an (incorrect) surface boundary condition. By contrast TBC guarantees that there is only one isolated solution, i.e., the Dirac point of surface bands protected by the change of bulk topology. Moreover, TBC demonstrates that the energy position of Dirac point is tunable in the bulk gap via the symmetry allowed scalar terms and surface potentials.

On a non cleavage surface, dangling bonds and their reconstruction may add complexity to the surface state spectrum which can be modeled as surface potentials encoded in the parameters $\Delta_0$ and $\Delta_e$. The fingerprint of the novel spin texture near the Dirac point on non cleavage surfaces are determined by the bulk symmetries along with the topological stability of the surface spectrum and may be accessible in ARPES and STM experiments. On an equatorial face, Zeeman coupling or magnetic disorder coupled to the spin degree of freedom do not generally open a gap, and the diamagnetic susceptibility is anticipated to be unusually anisotropic. More spectacularly, there is intrinsic charge redistribution in the surface bands near the corners of a TI that connect different crystal faces with intrinsically different Dirac point energies.

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