Protection of the surface states of a topological insulator: Berry phase perspective

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Hiroshima University Sophia University Sophia University Simon-Fraser University Ibaraki University Tsukuba University NIMS, Tsukuba The surface states of a topological insulator has a dual personality: extrovert and introvert

The topological insulator has a *dual* personality.

bulk ----- insulating surface ----- metallic topologically protected

Its metallic (gapless) surface state also has a *dual* personality.

introvert: staying on the surface; not penetrating into the bulk

extrovert:

inducing a fictitious magnetic field on *curved* surfaces; solenoid or magnetic monopole type (spin) Berry phase





What are the "defining properties" of the topological insulator?

- Existence of a protected gapless surface state cf. (a pair of) Dirac cones in graphene
- The bulk-surface correspondence





topological insulators

A chronological viewpoint:

spin Hall effect



3D

topological insulator







Topological insulators

Band "inversion" due to spin-orbit coupling



magnitude of the SOC

can be modeled by a Wilson-Dirac type effective (bulk) Hamiltonian

gap
$$\longrightarrow$$
 mass $m \rightarrow m(p) = m_0 + m_2 p^2$
Einstein Newtonian

The two bands get inverted by changing the *sign* of a mass term.

Bernevig et al., Science '07

2D example: how to characterize the bulk

 $m(\boldsymbol{p}) = m_0 + m_2 \boldsymbol{p}^2$

$$H = p_x \sigma_x + p_y \sigma_y + m(\mathbf{p})\sigma_z$$
$$= P_\mu(\mathbf{p})\sigma_\mu$$

 $n_{\mu}(\boldsymbol{p}) = \frac{P_{\mu}(\boldsymbol{p})}{\sqrt{P_{\mu}P_{\mu}}}$ The winding number (Chern number) $N_2 = -\frac{1}{8\pi} \int d^2 p \,\epsilon_{\mu\nu} \,\boldsymbol{n} \cdot [\partial_{p_{\mu}} \boldsymbol{n} \times \partial_{p_{\nu}} n],$ mapping: $\boldsymbol{p}
ightarrow n_{\mu}(\boldsymbol{p})$ $\mathbb{R}^2
ightarrow \mathbb{S}^2$ $p = |\boldsymbol{p}| \to \infty$ $p = |\mathbf{p}| o \infty$ p = 0 $\mathbf{n}(\mathbf{p}) o (0, 0, \operatorname{sgn}(m_2))$ $\mathbf{n}(\mathbf{p}) o (0, 0, \operatorname{sgn}(m_0))$ p = 0stereographic \rightarrow $\mathbb{S}^2 \rightarrow \mathbb{S}^2$ $\pi_2(\mathbb{S}^2) = 0, \pm 1, \pm 2, \cdots$ projection

$$V_2 = \frac{\operatorname{sgn}(m_2) - \operatorname{sgn}(m_0)}{2}$$

The bulk-edge correspondence



The Wilson-Dirac type (bulk) effective Hamiltonian

Zhang et al., Nature Phys. '09; Liu et al., PRB '10

Dirac equation in 3+1 D $H\psi = E\psi$ $H = m\gamma_0 + Ap_\mu\gamma_\mu \qquad 4 \times 4$ matrix Time-reversal symmetry $= m\tau_x + A\tau_y(p_x\sigma_x + p_y\sigma_y + p_z\sigma_z)$ preserved Two types of
Pauli matrices: $spin: \sigma_x, \sigma_y, \sigma_z$
orbital: τ_x, τ_y, τ_z • Two types of \mathbb{Z}_2 topological insulators • gamma matrices: $\{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu\nu}$ $\longrightarrow E = E(\mathbf{p}) = \pm \sqrt{m^2 + A^2 \mathbf{p}^2}$ Wilson term: a "spice" for the mass term $m \rightarrow m(\boldsymbol{p}) = m_0 + m_2 \boldsymbol{p}^2$ $= m_0 + m_2(p_x^2 + p_y^2 + p_z^2)$

m

The bulk-surface correspondence: 3D version



 $m_0/m_2 = -1$

 $m_0/m_2 = 1$





Zhang et al., Nature Phys. '09

Bulk-surface correspondence

Act I: The extrovert Finite-size Inducing a fictitious magnetic energy gap filed on *curved* surfaces The topological - sensitivity to the geometry of protection does not help. the sample spin connection cylindrical sample imaginary solenoid (TI nanowire) <u>spherical</u> sample effective monopole (TI nanoparticle)

Act II: The noninvasive metallic state

The surface stays *introvert* as a consequence of its *extroverted* character.

Noninvasiveness protected by the Berry phase

Consider a lattice (tight-binding) realization of topological insulator

 A lattice model is "sparse", existing only on sites and links



Yet, in reality protected surface states appear only on macroscopic surfaces.

Why is the surface state noninvasive into the bulk?

KI & *Takane, arXiv:1211.2088*

Which is the genuine surface?

Protection of the surface states in topological insulators: Berry phase perspective

Act I: Extrovert

The property of inducing a fictitious magnetic field on *curved* surfaces

The cylindrical topological insulator

Effective Dirac Hamiltonian on the cylindrical surface:

spin Berry phase

$$H_{\text{surf}} = \begin{bmatrix} 0 & -ip_{z} + \frac{1}{R} \left(-i \frac{\partial}{\partial \phi} + \frac{1}{2} \right) \\ ip_{z} + \frac{1}{R} \left(-i \frac{\partial}{\partial \phi} + \frac{1}{2} \right) & 0 \end{bmatrix}$$

KI, Takane & Tanaka, Phys. Rev. B **84**, 195406 (2011)
bulk effective Hamiltonian: $H_{\text{bulk}} = m(p)\tau_{z} + \tau_{x}(p_{x}\sigma_{x} + p_{y}\sigma_{y} + p_{z}\sigma_{z})$
Surface eigenstates:
 $H_{\text{surf}}\alpha = E\alpha$
 $\alpha = \begin{bmatrix} \alpha_{+} \\ \alpha_{-} \end{bmatrix}$
 $|r+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ e^{i\phi} \end{bmatrix}$
 $|r-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -e^{i\phi} \end{bmatrix}$
 $|r-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -e^{i\phi} \end{bmatrix}$

Possible interpretation

If one chooses the base double-valued,

$$|\pm\rangle\rangle = e^{-i\phi/2}|\widetilde{\pm}\rangle\rangle$$

$$\begin{split} |\widetilde{\boldsymbol{r}}+\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\phi/2} \\ e^{i\phi/2} \end{bmatrix} \\ |\widetilde{\boldsymbol{r}}+\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\phi/2} \\ -e^{i\phi/2} \end{bmatrix} \end{split}$$

$$\alpha(\phi, z) = \begin{bmatrix} \alpha_{+}(\phi, z) \\ \alpha_{-}(\phi, z) \end{bmatrix} \qquad E = \pm \sqrt{p_{\phi}^{2} + p_{z}^{2}}$$

$$= e^{ip_{\phi}R\phi + ip_{z}z} \begin{bmatrix} \beta_{+} \\ \beta_{-} \end{bmatrix} \qquad |\alpha\rangle\rangle = \alpha_{+}|\widetilde{+}\rangle\rangle + \alpha_{-}|\widetilde{-}\rangle$$
orbital part
$$L_{z} = p_{\phi}R$$

Half-odd integral quantizationof the orbital angularmomentum $L_z = \pm \frac{1}{2}, \pm \frac{3}{2}, \cdots$ single-valued $|\alpha(\phi + 2\pi)\rangle\rangle = |\alpha(\phi)\rangle\rangle$ anti-periodic $\alpha(\phi + 2\pi) = -\alpha(\phi)$





Spin-to-surface locking

Gapped surface states on the cylinder



cf. case of a slab-shaped sample

• The surfaces are flat.

But there are two of them (two Dirac cones); one on the top and the other at the bottom.

• If the thickness is finite, the two Dirac cones *communicate* each other through the bulk



a system of infinitely large slab



The magnitude of the gap is determined by the *overlap* of the two wave functions.

 $\rightarrow \Delta E \propto e^{-\kappa N_z}$

exponential decay

Linder, Yokoyama & Sudbo, PRB '09; Lu et al., PRB '10

Physical interpretation of the result

Effective Dirac Hamiltonian on a cylindrical surface

spin Berry phase

$$H_{\text{surf}} = \begin{bmatrix} 0 & -ip_z + \frac{1}{R} \left(-i\frac{\partial}{\partial\phi} + \frac{1}{2} \right) \\ ip_z + \frac{1}{R} \left(-i\frac{\partial}{\partial\phi} + \frac{1}{2} \right) & 0 \end{bmatrix}$$

Effects of the Berry phase

An electron on the cylindrical surface behaves as if an *imaginary solenoid* pierces the cylinder.

Electrons on a curved surface of topological insulator exhibits an "active" property reflecting its *geometry*.

Act I-B: The spherical topological insulator

KI, Yoshimura, Takane & Fukui, Phys. Rev. B 86, 235119 (2012)

Effective Dirac Hamiltonian on a spherical surface

 $H_{
m bulk}$

$$H_{\text{surf}} = \frac{A}{R} \begin{bmatrix} 0 & -\partial_{\theta} + \frac{i\partial_{\phi}}{\sin\theta} - \frac{\cot\theta}{2} \\ \partial_{\theta} + \frac{i\partial_{\phi}}{\sin\theta} + \frac{\cot\theta}{2} & 0 \end{bmatrix}$$

Surface states on the sphere:

$$|\alpha\rangle\rangle = \alpha_{+}|+\rangle\rangle + \alpha_{-}|-\rangle$$

$$H_{\rm surf} \boldsymbol{\alpha} = E \boldsymbol{\alpha}$$

Half-odd integral quantization:

$$m = \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}, \cdots$$

Bulk effective Hamiltonian:

$$H_{\text{bulk}} = m(\boldsymbol{p})\tau_x + A\tau_y(p_x\sigma_x + p_y\sigma_y + p_z\sigma_z)$$

$$(-|-\rangle) \qquad \boldsymbol{\alpha} = \begin{bmatrix} \alpha_+ \\ \alpha_- \end{bmatrix}$$

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$$(-|$$

 $|\boldsymbol{\alpha}(\theta,\phi+2\pi)\rangle\rangle = |\boldsymbol{\alpha}(\theta,\phi)\rangle\rangle$

Physical interpretation:

A (fictitious) magnetic monopole is induced at the center of the sphere!

Effective Dirac Hamiltonian in the single-valued basis

$$\mathcal{H}_{\rm sv} = \frac{A}{R} \begin{bmatrix} 0 & -\partial_{\theta} + \frac{i\partial_{\phi}}{\sin\theta} - \frac{1}{2}\cot\frac{\theta}{2} \\ \partial_{\theta} + \frac{i\partial_{\phi}}{\sin\theta} - \frac{1}{2}\tan\frac{\theta}{2} & 0 \end{bmatrix}$$

induced Berry phase vector potential associated with a magnetic monopole (+ Dirac string)

The surface Dirac equation:

$$H_{\rm surf} \left[\begin{array}{c} \alpha_+ \\ \alpha_- \end{array} \right] = E \left[\begin{array}{c} \alpha_+ \\ \alpha_- \end{array} \right]$$

$$\begin{cases} g = -2\pi & \text{for } \alpha_+ \\ g = 2\pi & \text{for } \alpha_- \end{cases}$$

Dirac string on $+\hat{z}$

A pair of magnetic monopole with an opposite magnetic charge: $g = \pm 2\pi$ is induced at the origin



Act II: Unification of the two aspects: the extrovert and the introvert

"The noninvasive metallic state"

Consider a lattice (tight-binding) realization of topological insulator

 A lattice model is "sparse", existing only on sites and links



Yet, in reality protected surface states appear only on macroscopic surfaces.

Why is the surface state noninvasive into the bulk?

KI & *Takane, arXiv:1211.2088*

Where is the genuine surface?

Why is the surface state not penetrating into the bulk?

Answer: because of the Berry phase π



Recall that the *cylindrical* surface state is gapped by the spin-to-surface locking.

A flux tube penetrating the system may *awaken* the invasive nature of surface state.

Invasion of the metallic surface state

deeply into the bulk along a flux tube

 $\Phi = 0.7\pi \qquad \Phi = 0.9\pi \qquad \Phi = 0.95\pi \qquad \Phi = \pi$

invasiveness of the surface state

Analytic treatments: hyperbolic "drain" geometry

$$\begin{aligned}
& \nabla = e_{\xi}\partial_{\xi} - \frac{1}{\eta(\theta) - \xi}e_{\theta}\partial_{\theta} + \frac{1}{r(\xi,\theta)}e_{\phi}\partial_{\phi} \quad \begin{cases} x = r\cos\phi\\ y = r\sin\phi\\ z = \xi\cos\theta + R\sqrt{\tan\theta} \end{cases} \\
& \begin{cases} r = r(\xi,\theta) = \xi\sin\theta + a + R\sqrt{\cot\theta}\\ \eta(\theta) = \sqrt{|\partial_{\theta}r_{0}|^{2}} = \frac{R}{2}\frac{1}{\sqrt{\sin^{3}\theta\cos^{3}\theta}} \end{cases} \quad \begin{cases} e_{\xi} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\\ e_{\theta} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)\\ e_{\phi} = (-\sin\phi, \cos\phi, 0) \end{cases}
\end{aligned}$$

Derivation of the surface effective Hamiltonian

The zero-energy (degenerate)
basis eigenstates:
$$|\pm\rangle = \frac{1}{\sqrt{c(\theta)}} \begin{pmatrix} e^{-\kappa_1\xi} - e^{-\kappa_2\xi} \end{pmatrix} |\pm\rangle\rangle \qquad |+\rangle\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{bmatrix} \otimes \begin{bmatrix} 1 \\ i \end{bmatrix}$$
$$|-\rangle\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \sin(\theta/2) \\ -e^{i\phi}\cos(\theta/2) \end{bmatrix} \otimes \begin{bmatrix} 1 \\ -i \end{bmatrix}$$

The surface effective Hamiltonian:

 $|\pm\rangle =$

$$H_{\text{surf}} = \begin{bmatrix} \langle +|H_{\parallel}|+\rangle & \langle -|H_{\parallel}|+\rangle \\ \langle +|H_{\parallel}|-\rangle & \langle -|H_{\parallel}|-\rangle \end{bmatrix} = \begin{bmatrix} 0 & D_{-} \\ D_{+} & 0 \end{bmatrix}$$

where $D_{\pm} = \pm A_{\theta}\partial_{\theta} \pm \frac{\partial_{\theta}A_{\theta}}{2} + A_{\phi}\left(-i\partial_{\phi} + \frac{1}{2}\right)$

The velocities are renormalized by the curvature

$$\begin{cases}
A_{\theta} = \frac{\langle r \rangle}{\langle r(\eta - \xi) \rangle} \left(A + \frac{\left\langle \frac{r}{\eta - \xi} \right\rangle}{\langle r \rangle} m_2 \right) \equiv \frac{\langle r \rangle}{\langle r(\eta - \xi) \rangle} \tilde{A}_{\theta} \\
A_{\phi} = \frac{\langle \eta - \xi \rangle}{\langle r(\eta - \xi) \rangle} \left(A - \frac{\left\langle \frac{\eta - \xi}{r} \right\rangle \sin \theta}{\langle \eta - \xi \rangle} m_2 \right)
\end{cases}$$

Invasive vs. noninvasive surface state

Conclusions

(After a long period of slavery to the bulk) the surface state is now freed.

The introvert surface state sometimes wants to show off:
 e.g., on cylindrical and spherical surfaces. spin Berry phase
 role of the system's geometry: slab vs. cylinder, sphere
 flat vs. curved surfaces

• The "gaplessness" is not immune to finite-site size corrections associated with the spin connection.

Such a finite-size correction does not decay exponentially.

 \bullet The noninvasiveness of the surface state is protected by the Berry phase π

• (Reclassified as a *noninvasive metallic state*) the surface state is shown to be, by itself, topologically protected.

Other perspectives

So far, we have considered only "strong" topological insulators. = isotropic

Latest tendency of the field:

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headed for seek of the diversity?
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<u>A possible direction:</u> exploring the nature of weak topological insulators (WTI)

- Specific features associated with the anisotropic character

- WTI is actually not that weak !

In WTI, topological non-triviality is not weak but only hidden.

KI, Okamoto, Yoshimura, Takane & Ohtsuki, Phys. Rev. B **86**, 245436 (2012)

> KI, Takane & Tanaka, Phys. Rev. B **84**, 035443 (2011)

Ringel, Kraus & Stern, Phys. Rev. B **86**, 045112 (2012).

Stability of WTI against disorder: the global phase diagram

Kobayashi, Ohtsuki & KI, arXiv:1210.4656, PRL in press.

Experiments on finite-size effects

1) Slab (this film) geometry

Zhang et al., Nature. Phys. (2010)

2) Prism (nanowire) geometry

