Local currents in a two-dimensional topological insulator

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Two-dimensional topological insulator

- System exhibiting a quantum spin-Hall effect
- 2D bulk insulator with topologically protected edge states
- Spin is locked to the wave vector of the electron
- Conductance of the edge state is insensitive to disorder which does not break time reversal symmetry

Predicted (Bernevig, Hughes, and Zhang, 2006) and observed (König et al., 2007) in CdTe/HgTe/CdTe quantum well structures
Bernevig-Hughes-Zhang (BHZ) model

"Inverted" band structure

Square lattice with four basis states $\alpha$ on each site $i$:

$$\begin{align*}
|s, \uparrow\rangle, |s, \downarrow\rangle, |p_x + ip_y, \uparrow\rangle, |p_x - ip_y, \downarrow\rangle
\end{align*}$$

Hamiltonian:

$$H = \sum_{i,\sigma,\alpha} \epsilon_{\alpha} c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma} - \sum_{i,\sigma,\alpha} t_{a\sigma,\alpha\beta} c_{i+\alpha\sigma}^\dagger c_{i\beta\sigma}$$

$$t_{a\sigma} = \begin{pmatrix}
    t_{ss} & t_{sp} e^{i\sigma_\theta_a} \\
    t_{sp} e^{-i\sigma_\theta_a} & -t_{pp}
\end{pmatrix}$$

$\theta_a$ - angle of bond $a$ with $x$ axis

$\epsilon_s - \epsilon_p > 4(t_{ss} + t_{pp})$ - band insulator

$\epsilon_s - \epsilon_p < 4(t_{ss} + t_{pp})$ - topological insulator

Fu and Kane, PRB 76, 045302 (2007)
Tight-binding Green’s function technique

Dyson equation:

\[ G = G^0 + G^0 V G \]

Layer-dependent spectral density:

\[ A_n(E, k_x) = -\text{Im}[\text{Tr}G_{nn}(E, k_x)] \]

Layer-dependent DOS:

\[ \rho_n(E) = -\frac{1}{\pi} \text{Im}[\text{Tr}G_{nn}(E)] \]
Layer-dependent spectral density

- Energy dependent oscillatory decay of the edge state into the bulk
Oscillatory decay of DOS

- $E = 0$
- $E = 0.25$
- $E = 0.5$

Oscillatory decay of the edge state into the bulk
Complex band structure

For a given energy, there are three types of solutions:

- **Bloch state**: \( \varphi \sim e^{i k_y y} \) - oscillation
- **Evanescent state**: \( \varphi \sim e^{-\kappa y} \) - decay
- **Complex solution**: \( \varphi \sim e^{i k_y y} e^{-\kappa y} \) - oscillation and decay

DOS is superposition of two waves with opposite Re\((k_y)\):

\[
\rho(y) \propto e^{-2\kappa y} \cos^2 \left( k_y y + \phi \right)
\]
Oscillatory decay of DOS

Layer-dependent DOS using parameters extracted from the complex band structure

\[ \rho(y) \propto e^{-2\kappa y} \cos^2 \left( k_y y + \phi \right) \]
Electronic transport: model and methods

- Finite width strip within the BHZ tight-binding model
- Green’s function formalism
  \[ G(E) = \left[ E - H - \Sigma_L - \Sigma_R \right]^{-1} \]
- Landauer-Büttiker approach
Local conductance

Local current: \( I_{ij} = Tr(\rho J_{ij}) \)

where

\[
J_{ij} = \frac{e}{i\hbar} \left[ H_{ij} \langle i | j \rangle - H_{ji} \langle j | i \rangle \right]
\]

\[
\rho = \int \left[ f_L(E) A_L(E) + f_R(E) A_R(E) \right] dE
\]

\[
A_{L,R}(E) = iG(E) \left[ \Sigma_{L,R}(E) - \Sigma_{L,R}^\dagger(E) \right] G^\dagger(E)
\]

Within linear response

\[
\rho = \rho_0 + eV \int \left( -\frac{\partial f_0}{\partial E} \right) A_L(E) dE
\]

Local conductance (per spin):

\[
\Gamma_{ij} = \frac{I_{ij}}{V} = \frac{e^2}{\hbar} \text{Im} Tr \left[ A_{Lij}(E_F) H_{ij} - A_{Lji}(E_F) H_{ji} \right]
\]

Total conductance (per spin):

\[
\Gamma = \frac{e^2}{\hbar} T = Tr \left[ (\Sigma_L - \Sigma_L^\dagger) G(\Sigma_R^\dagger - \Sigma_R) G^\dagger \right]
\]
Local conductance for an isolated edge

- Oscillation in the local conductance
- Correlation between local conductance and local density of states
- Explained by the complex band structure
- $T = 1$, as expected
Effect of impurity

Perturbation due to impurity:

\[ V_{\text{imp}} = \begin{pmatrix} \Delta \varepsilon_s & 0 \\ 0 & \Delta \varepsilon_p \end{pmatrix} \]

Real space Green’s function:

\[ G_{mn} = G_{mn}^0 + G_{mi}^0 V_{ii} \left( 1 - G_{ii}^0 V_{ii} \right)^{-1} G_{in}^0 \]
Effect of impurity

- Strong effect on local current distribution
- No back-scattering: $T = 1$, as expected
Effect of impurity

Impurity $E_i = 1.25$

Impurity $E_i = -0.45$

- Intricate current distributions
- Current vortex due to impurity
Effect of vacancy

- Current vortex due to internal edge
- Chirality is determined by propagating mode spin state
- Counterclockwise current
Narrow width strip

- For a given spin, two propagating states on the two edges
- Coupling between the edge states
- Backscattering due to impurities
Oscillatory band gap

- Energy gap due to coupling between the edge states
- Oscillatory behavior as a function of strip width
Oscillatory band gap

Edge states:

\[ \psi_1(x, y) \propto e^{-\kappa y} \left( e^{ik_y} + re^{-ik_y} \right) e^{ik_x x} \]

\[ \psi_2(x, y) \propto e^{-\kappa(L-y)} \left( e^{ik(L-y)} + re^{-ik(L-y)} \right) e^{-ik_x x} \]

Energy gap:

\[ E_g \propto \left| \langle \psi_1 | \psi_2 \rangle \right| = e^{-\kappa L} \left| \cos(kL) + \frac{\alpha}{L} \sin(kL) \right|, \quad \alpha = \frac{1+r^2}{4rk} \]
Oscillatory band gap

Excellent agreement
Complex band structure of Bi$_2$Se$_3$

- Real component of the wave vector in the bulk gap region

In collaboration with J. Velev (UPR)

- Real component of the wave vector in the bulk gap region

Diagram showing band structure with real bands (blue) and complex bands (red). The bulk gap is highlighted with a green circle.
Oscillatory band gap in Bi$_2$Se$_3$

Nearly perfect agreement with the complex band structure parameters
Friedel oscillations: density of states

- No Friedel oscillations for an isolated edge
- For a finite strip, LDOS oscillates away from the impurity with no decay
- Oscillation period depends on the Fermi energy
**Friedel oscillations: model**

**Model Hamiltonian:**

\[
H(k) = \begin{pmatrix}
\hbar v k & \Delta \\
\Delta & -\hbar v k
\end{pmatrix}
\]

**Green’s function:**

\[
G_0(x-x', E) = \frac{-i}{2\hbar^2 v^2 k} e^{ik|x-x'|} \begin{pmatrix}
E + \hbar v k \text{sgn}(x-x') & \Delta \\
\Delta & E - \hbar v k \text{sgn}(x-x')
\end{pmatrix}
\]

**Dyson equation within Born approximation:**

\[
G(x,x', E) \approx G_0(x,x', E) + \int_{-\infty}^{\infty} G_0(x-x'', E)V(x'')G_0(x''-x', E)dx''
\]

where \( V(x) = \lambda \delta(x) \) is a local perturbation due to impurity

**Resulting perturbation in LDOS:**

\[
\Delta \rho(x) = -\frac{1}{\pi} \text{Im Tr}[G - G_0] = \frac{\lambda \Delta^2}{\pi \hbar^4 v^4} \frac{\sin(2k_F|x|)}{k_F^2}
\]
Friedel oscillations: local conductance

- Periodically repeated vortices in spin-resolved current distribution
- No Friedel oscillations in net local conductance
Resonant channel: full back-scattering due to bound state created by impurity
Resonant scattering: antiresonance

Energy dependent transmission

- Full suppression of net current
- Destructive interference of the incoming and reflected waves

Antiresonances
Antiresonance

- Two bound states (electron-like and hole-like)
- Antiresonances in transmission at the bound state energies
- Decreasing antiresonance width with increasing strip width L
Antiresonance: model

Scattering problem: \( \psi(x) = \phi_k(x) + \int_{-\infty}^{\infty} G(x, x')V(x')\psi(x')\,dx' \)

\[ G_{TI} = \frac{-i}{\hbar v} \begin{pmatrix} e^{ik(x-x')} \theta(x-x') & 0 \\ 0 & e^{ik(x'-x)} \theta(x'-x) \end{pmatrix} \]

\[ G_{\text{imp}} = \frac{\chi(x)\chi^*(x')}{E-E_i + i\eta} \]

Transmission: \( T(E) = \frac{(E-E_i)^2}{(E-E_i)^2 + \gamma^2} \)

- Antiresonance in transmission characterized by width \( \gamma = \frac{\lambda^2|\chi(0)|^2}{\hbar v} \)
Antiresonance: local conductance

- Perfect back scattering due to antiresonance
- No net local currents
- Total transmission is zero
Effect of magnetic impurity

Magnetic impurity Hamiltonian:

\[ H_{\text{ex}} = -\frac{\Delta}{2} \hat{m} \cdot \vec{\sigma} \]

\[ \hat{m} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \]

- Breaks time reversal symmetry
- Expected back-scattering due to mixing of spin channels
- Effect depends on the impurity magnetic moment angle

Effect on transport spin polarization:

\[ SP = \frac{|G_{\uparrow} - G_{\downarrow}|}{G_{\uparrow} + G_{\downarrow}} \]
Backscattering seen in spin-down channel
Magnetic impurity: local conductance

- **Spin up**
- **Spin down**
- **Total**

- $SP = 0.93$

- Nearly perfect backscattering
Antiresonance in transmission due to magnetic impurity at the critical angle of the magnetic moment

Magnetic impurity: angular dependence
Magnetic impurity: local conductance

\[ \theta = 0 \quad \theta = \theta_0 = 54^\circ \quad \theta = 90^\circ \]

- \( SP = 0 \)
- \( SP = 0.98 \)
- \( SP = 0.33 \)

- Current vertex at the antiresonance conditions
The BHZ model for a 2D topological insulator implemented within the tight-binding Green’s function technique reveals:

- Oscillatory decay of the local conductance away from the TI edge
- Intricate current distributions and formation of current vertices of different chirality around impurities
- Oscillatory behavior of the edge-state energy gap as a function of 2D TI width
- Impurity-driven Friedel oscillations in electron density and spin-dependent local conductance for sufficiently narrow TI strips
- Resonant back scattering and antiresonances in transmission for finite-size impurity system
- Back scattering produced by magnetic impurity and resonant-type transmission as a function of magnetic moment angle