Topologically protected states in 2D and 3D: spin-momentum and valley-momentum locking mechanism

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The General Scheme

The Berry phase and the Berry Connection

The Chern Number

Chern topological insulators (Haldane’s model)

$\mathbb{Z}_2$ topological insulators (Kane-Mele model)

3D topological topological insulators, different locking mechanisms, etc.
The Berry phase

The phase factor collected after the walk through the closed path in parameter space:

$$|\psi\rangle \rightarrow e^{i\gamma} |\psi\rangle$$

Adiabatic change of parameter:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H(\lambda(t)) |\psi\rangle$$

$$|\psi(t)\rangle = U(t) |n(\lambda(t))\rangle$$

$$H(\lambda) |n(\lambda)\rangle = 0$$

$$e^{-i \int dt E_0(t)/\hbar}$$

The final phase factor:

$$A_i(\lambda) = -i \langle n | \frac{\partial}{\partial \lambda_i} | n \rangle$$

$$e^{i\gamma} = \exp \left( -i \int_C A_i(\lambda) \, d\lambda^i \right)$$
The Berry connection

“Gauge invariance” due to phase factors in basis functions:

\[ |n'(\lambda)\rangle = e^{i\omega(\lambda)} |n(\lambda)\rangle \]

\[ A'_i = -i \langle n'| \frac{\partial}{\partial \lambda^i} |n'\rangle = A_i + \frac{\partial \omega}{\partial \lambda^i} \]

The Berry curvature (gauge invariant quantity):

\[ F_{ij}(\lambda) = \frac{\partial A_i}{\partial \lambda^j} - \frac{\partial A_j}{\partial \lambda^i} \]

\[ e^{i\gamma} = \exp \left( -i \oint_C A_i(\lambda) d\lambda^i \right) = \exp \left( -i \int_S F_{ij} dS^{ij} \right) \]
Example: spin in magnetic field

Example calculation of the Berry curvature for spin-1/2 in external magnetic field. Parameters = magnetic field components.

\[ H = -\vec{B} \cdot \vec{\sigma} \]

\[ H = -B \begin{pmatrix} \cos \theta - 1 & e^{-i\phi} \sin \theta \\ e^{+i\phi} \sin \theta & -\cos \theta - 1 \end{pmatrix} \]

\[ |\downarrow\rangle = \begin{pmatrix} e^{-i\phi} \sin \theta /2 \\ -\cos \theta /2 \end{pmatrix} \quad \text{and} \quad |\uparrow\rangle = \begin{pmatrix} e^{-i\phi} \cos \theta /2 \\ \sin \theta /2 \end{pmatrix} \]

Berry curvature computed for the filled (spin-down) band:

\[ \mathcal{F}_{ij}(\vec{B}) = -\epsilon_{ijk} \frac{B^k}{2|\vec{B}|^3} \]
The Chern number

Two variants of calculation should coincide

\[ e^{i\gamma} = \exp\left(-i \int_S \mathcal{F}_{ij} \, dS^{ij}\right) = \exp\left(\frac{i\Omega}{2}\right) \]

\[ \int \mathcal{F}_{ij} \, dS^{ij} = 2\pi C \]

The Chern number, C=0, +1, +2, ....
The Chern number in momentum space

Momentum components as parameters:

\[ H(k) = \vec{h}(k) \cdot \vec{\sigma} \]

\[ \text{d}F = \frac{1}{4} \epsilon^{ijk} h^{-3} h_i \, \text{d}h_j \wedge \text{d}h_k: \]

\[ \text{d}h_j \wedge \text{d}h_k = \frac{\partial h_j}{\partial k_a} \frac{\partial h_k}{\partial k_b} \, \text{d}k_a \wedge \text{d}k_b \]

\[ c_1 = \frac{1}{4\pi} \int_{\text{BZ}} \frac{\vec{h}}{||\vec{h}||^3} \cdot \left( \frac{\partial \vec{h}}{\partial k_x} \times \frac{\partial \vec{h}}{\partial k_y} \right) \, \text{d}k_x \wedge \text{d}k_y \]

Geometrical interpretation: vector flow through the oriented surface.
Chern topological insulator (2D Haldane’s model)

The model is written on hexagonal lattice:

Hamiltonian for spinless fermions:

\[
\hat{H} = t \sum_{\langle i,j \rangle} |i \rangle \langle j| + t_2 \sum_{\langle i,j \rangle} |i \rangle \langle j| + M \left[ \sum_{i \in A} |i \rangle \langle i| - \sum_{j \in B} |j \rangle \langle j| \right]
\]

Peierls substitution:

\[
t_{ij} \rightarrow t_{ij} \exp \left( -i \frac{e}{\hbar} \int_{\Gamma_{ij}} \vec{A} \cdot d\vec{l} \right)
\]

\[
t \rightarrow t \quad \text{and} \quad t_2 \rightarrow t_2 e^{i\phi}
\]

Finally in momentum space:

\[
\mathcal{H}(k) = h^\mu(k) \sigma_\mu
\]

\[
\vec{h}(k + G_{mn}) = \vec{h}(k)
\]
Chern topological insulator (2D Haldane’s model)

Phase diagram:

\[ M/t_2 \]

\[ C_1 = 0 \]

\[ C_1 = -1 \]

\[ C_1 = +1 \]

Metal on the border between two distinct insulating phases
Edge states in the Chern topological insulator

Connection between mass gap and the Chern number

Calculation through the intersection number

\[ c_1 = \frac{1}{2} \sum_{k \in D} \text{sign} [h(k) \cdot n(k)] \quad n(k) - \text{normal vector to } \Sigma \]

We choose z-direction: \( h_x(k) = h_y(k) = 0 \) \( k \) at K-points

Masses:

\[ m = h_z(K) = M - 3\sqrt{3}t_2 \sin \phi \]
\[ m' = h_z(K') = M + 3\sqrt{3}t_2 \sin \phi \]

Chern number:

\[ c_1 = (\text{sign } m - \text{sign } m')/2 \]
Edge states in the Chern topological insulator

Linearized Hamiltonian near the K-point (mass should change the sign at the border):

\[ H_1 = -i \nabla \cdot \sigma_{2d} + m(y) \sigma_z = \begin{pmatrix} m(y) & -i \partial_x - \partial_y \\ -i \partial_x + \partial_y & -m(y) \end{pmatrix} \]

Single edge mode with linear dispersion:

\[ \psi_{q_x}(x, y) \propto e^{i q_x x} \exp \left[ - \int_0^y m(y') dy' \right] \begin{pmatrix} 1 \\ 1 \end{pmatrix} \]

\[ E(q_x) = E_F + \hbar v_F q_x. \]

Time-reversal invariance is broken
**Z₂ Topological insulator**

Appears in time-reversal invariant system with spin-orbital coupling

\[
\Theta = e^{-i\pi J_y/\hbar} \mathcal{K}
\]

\[
\Theta^2 = -1
\]

\[
H(-k) = \Theta H(k) \Theta^{-1}
\]

Kramers pairs:

\[
\Theta |u_1(k)\rangle = |u_2(-k)\rangle.
\]

Chern Number always vanishes: \( F_\alpha(k) = -F_\alpha(-k) \)

**Time-Reversal Invariant Momenta (TRIM):**

![Diagram of time-reversal invariant momenta](image)
**Z₂ Topological insulator**

Reduction to 1D integrals:

\[ 2\pi Z = -\int_0^{2\pi} \int_0^{2\pi} dk_x dk_y (\partial_x A_y - \partial_y A_x) \]

\[ = \int_0^{2\pi} dk_y \partial_y \left( \int_0^{2\pi} dk_x A_x (k_x, k_y) \right) \]

\[ = \int_0^{2\pi} d\theta(k_y). \]

\[ \theta(k_y) = \int_0^{2\pi} dk_x A_x \]

\[ F_\alpha(k) = -F_\alpha(-k) \]

guarantees the intersection at TRIM

**Z₂ insulator:**

New topological invariant:

\[ |Z| \text{ mod } 2 \]

Can be computed from the eigenstates at TRIM
The Kane-Melev model

Hexagonal lattice:

\[ h_{\text{KM}} = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + i\lambda \sum_{\ll ij \gg} \sum_{\alpha\beta} \nu_{ij} c_{i\alpha}^\dagger \sigma_{\alpha\beta} c_{j\beta} \]

The basis

\[ (A \uparrow, A \downarrow, B \uparrow, B \downarrow) \]

\[ H(k) = d_0(k) 1 + \sum_{i=1}^{5} d_i(k) \Gamma_i \quad E_{\pm}(k) = d_0(k) \pm \sqrt{\sum_{i=1}^{5} d_i^2(k)} \]

\[ \Gamma_1 = \mathcal{P} = \sigma_x \otimes 1 \quad \Gamma_2 = \sigma_y \otimes 1 \quad \Gamma_3 = \sigma_z \otimes s_x \quad \Gamma_4 = \sigma_z \otimes s_y \quad \Gamma_5 = \sigma_z \otimes s_z \]

\[ \text{Z}_2 \text{ topological invariant: } \prod_{\lambda \in \Lambda} \text{sign } d_1(\lambda) \quad \text{All } d_i \text{ except } d_1 \text{ vanish at TRIM} \]
Edge states in Kane-Mele model: spin-momentum locking

Topological insulator, where only $d_1 (\lambda_0)$ is negative

Trivial insulator, where all $d_i$ are positive

Spin up

Spin down

Hamiltonian at the border:

$H_1(q) = q_x \Gamma_5 - q_y \Gamma_2 + m(y) \Gamma_1$

$H_1 = \begin{pmatrix} H_{\uparrow} & 0 \\ 0 & H_{\downarrow} \end{pmatrix}$

$H_{\uparrow} = \begin{pmatrix} -i \partial_x & m(y) + \partial_y \\ m(y) - \partial_y & i \partial_x \end{pmatrix}$

$H_{\downarrow} = \begin{pmatrix} +i \partial_x & m(y) + \partial_y \\ m(y) - \partial_y & i \partial_x \end{pmatrix}$

$\psi_{q_x,\uparrow}(x, y) \propto e^{-iq_x x} \exp \left[ - \int_0^y m(y') dy' \right] \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$\psi_{q_x,\downarrow}(x, y) \propto e^{+iq_x x} \exp \left[ - \int_0^y m(y') dy' \right] \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$
3D topological insulators

Weak topological insulators: $v_x, v_y, v_z$ – separate $Z_2$ topological invariants; each of them can be computed as corresponding 2D $Z_2$ invariant in $k_x=\pi, k_y=\pi, k_z=\pi$ planes correspondingly.

Strong topological insulators: new $Z_2$ invariant $v_0=0,1$. Here two planes should be taken into account: $k_x=0, \pi$ or $k_y=0, \pi$ or $k_z=0, \pi$. If usual $Z_2$ invariants are different in those planes, $v_0=1$ otherwise $v_0=0$. 
3D topological insulators

Cubic lattice: Bi₂Se₃.
Can be described by lattice Wilson fermions (with slightly unconventional parameters)

\[ \mathcal{H}_0(k) = \sum_j \sin k_j \cdot \alpha_j + m(k) \beta. \]

\[ m(k) = m_0 + r \sum_j (1 - \cos k_j). \]

\[ \alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \]

The system is topologically non-trivial (strong Z₂ TI) if:

\[ 0 > m_0 > -2r \]
\[ -4r > m_0 > -6r \]

Topological properties are defined by the sign of \( m(k) \) at TRIM

Can be modeled with lattice QCD algorithms without sign problem!
3D topological insulators

Diamond lattice:

\[ H_0 = \sum_{\langle i,j \rangle, \sigma} (t + \delta t_{ij}) c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{4i\lambda}{a^2} \sum_{\langle\langle i,j \rangle\rangle, \sigma\sigma'} c_{i\sigma}^{\dagger} \mathbf{s} \cdot (\mathbf{d}_{ij}^{1} \times \mathbf{d}_{ij}^{2}) c_{j\sigma'} \]

Nearest-neighbor hoppings are modified in one direction
Engineering the topological state

\[ H = H_g + H_a + H_c, \]

\[ H_g = H_t - \delta \mu \sum_{j=1}^{6} c_{r,j}^\dagger c_{r,j}, \]

\[ H_a = \sum_{m=0, \pm 1} \epsilon_m d_m^\dagger d_m + \Lambda_{so}(d_1^\dagger s^z d_1 - d_{-1}^\dagger s^z d_{-1}) \]
\[ + \sqrt{2} \Lambda'_{so}(d_0^\dagger s^- d_{-1} + d_0^\dagger s^+ d_1 + \text{H.c.}), \]

\[ H_c = - \sum_{m=0, \pm 1} (t_m C_m^\dagger d_m + \text{H.c.}), \]

In the first approximation can be modeled through local Kane-Mele SOC terms

Induces spin-orbit coupling

PRX, 1, 021001
Clusterization of adatoms destroy the topological state in a sense that the currents are concentrated not at the edges of the sample, but at the edge of the “islands” [PRL 113, 246603].

FIG. 3 (color online). Spin-resolved spectral current distribution for $r = 0.5 \mathrm{~nm}$ and $E = -33.5 \mathrm{meV}$ (a),(b); $r = 1.5 \mathrm{~nm}$ and $E = 21.5 \mathrm{meV}$ (c),(d); and $r = 2 \mathrm{~nm}$ and $E = -33.5 \mathrm{meV}$ (e),(f). The corresponding energies and conductance are indicated by black dots in Fig. 2. The insets in panels (c)–(f) illustrate the local average current distribution in the regions indicated by the squares.
Valley-momentum locking (1)

Hopping distribution

Hamiltonian:

\[ H = - \sum_{r} \sum_{\ell=1}^{3} t_{r,\ell} a_{r}^\dagger b_{r+s_{\ell}} + H.\text{c.} \]

\[ t_{r,\ell}/t_{0} = 1 + 2 \text{Re} \left[ \Delta e^{i(pK_{+}+qK_{-})\cdot s_{\ell} + iG\cdot r} \right] \]

\[ G \equiv K_{+} - K_{-} = \frac{4}{9} \pi \sqrt{3}(1, 0) \]

Low energy effective theory in the vicinity of superlattice K-points:

\[ \mathcal{H} = v_{\sigma} (p \cdot \sigma) \otimes \tau_{0} + v_{\tau} \sigma_{0} \otimes (p \cdot \tau) \]

\( \tau \) acts in valley space and plays the role of spin.

arXiv:1708.08348
Valley-momentum locking (2)

Hoppings distribution

Effective Wannier functions within the supercell

Different valleys correspond now to different orbital momentum within the supercell
Stability of TIs with respect to interaction effects

Kane-Mele-Hubbard model:

\[
h_{\text{KM}} = -t \sum_{\langle ij \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} + i \lambda \sum_{\ll ij \gg} \sum_{\alpha \beta} \nu_{ij} c_{i \alpha}^\dagger \sigma_{\alpha \beta} c_{j \beta}
\]

\[
H_I = U \sum_i n_i^\uparrow n_i^\downarrow
\]

(a)

Competition between AFM and topological mass terms.
arXiv:1206.3103

Antiferromagnetic mass term: the same sign at different K points.
Topological mass term: different signs at K-points
Stability of TIs with respect to disorder

Magnetic impurities can cause spin-flip process and introduce the possibility for backscattering.

However, in the presence of interaction, spontaneous magnetization appears in the vicinity of resonant scatterers:

Example calculation for graphene [PRL 114, 246801]

FIG. 2: Distribution of average spin. Color scale corresponds to \( \langle S_z \rangle \) at the site in the zero bare mass limit.
Stability of TIs with respect to disorder

The same effect also exists for TIs [arXiv:0910.4604]