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)

↓

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:

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

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:

$$\mathcal{A}_i(\lambda) = -i\langle n|\frac{\partial}{\partial\lambda^i}|n\rangle$$

$$e^{i\gamma} = \exp\left(-i\oint_C \mathcal{A}_i(\lambda)\,d\lambda^i\right)$$

The Berry connection

"Gauge invariance" due to phase factors in basis functions :

$$|n'(\lambda)\rangle = e^{i\omega(\lambda)}\,|n(\lambda)\rangle$$

$$\mathcal{A}'_i = -i\langle n'|\frac{\partial}{\partial\lambda^i}|n'\rangle = \mathcal{A}_i + \frac{\partial\omega}{\partial\lambda^i}$$

The Berry curvature (gauge invariant quantity):

$$\mathcal{F}_{ij}(\lambda) = \frac{\partial\mathcal{A}_i}{\partial\lambda^j} - \frac{\partial\mathcal{A}_j}{\partial\lambda^i}$$

$$e^{i\gamma} = \exp\left(-i\oint_C \mathcal{A}_i(\lambda)\,d\lambda^i\right) = \exp\left(-i\int_S \mathcal{F}_{ij}\,dS^{ij}\right)$$

Example: spin in magnetic field

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

$$H = -\vec{B}\cdot\vec{\sigma}$$

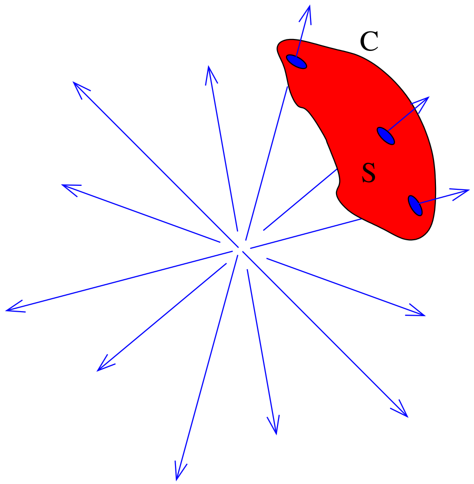
$$H = -B\begin{pmatrix} \cos\theta - 1 & e^{-i\phi}\sin\theta \\ e^{+i\phi}\sin\theta & -\cos\theta - 1 \end{pmatrix}$$

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

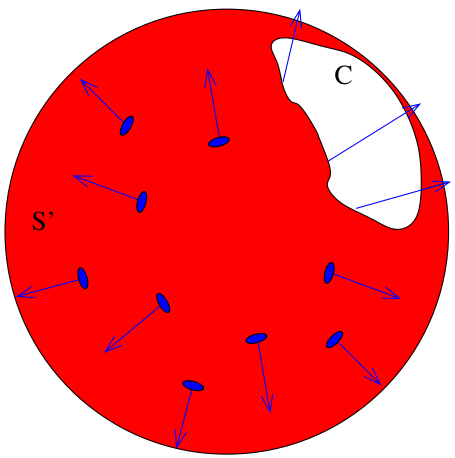
Berry curvature computed for the filled (spin-down) band:

$$\mathcal{F}_{ij}(\vec{B}) = -\epsilon_{ijk}\frac{B^k}{2|\vec{B}|^3}$$

The Chern number



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



$$e^{i\gamma'} = \exp\left(-i\int_{S'} \mathcal{F}_{ij}\, dS^{ij}\right) = \exp\left(\frac{-i(4\pi-\Omega)}{2}\right) = e^{i\gamma}$$

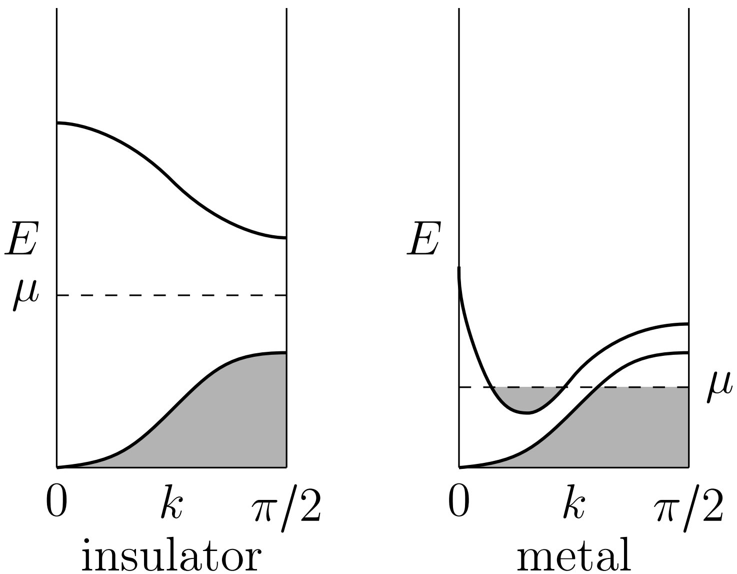
Two variants of calculation should coincide

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

The Chern number, C=0,+-1, +-2....

The Chern number in momentum space

Momentum components as parameters:



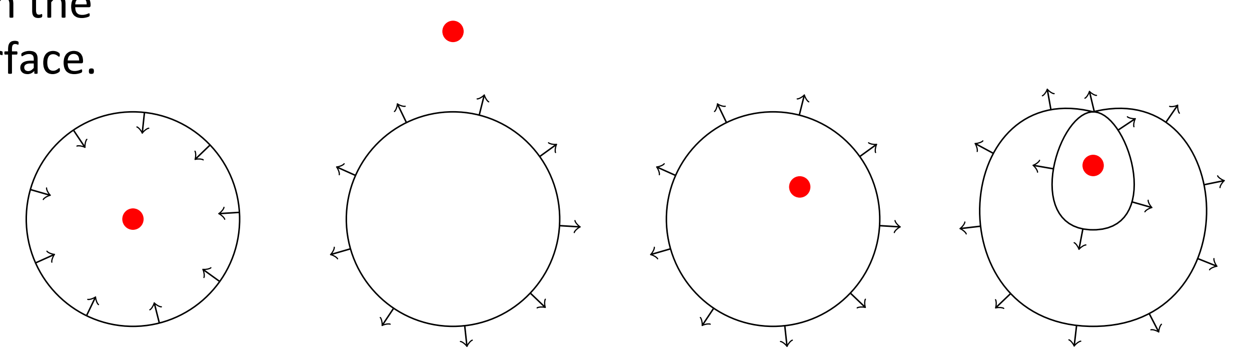
$$H(k) = \vec{h}(k) \cdot \vec{\sigma}$$

$$\mathrm{d}F = \frac{1}{4}\,\epsilon^{ijk}\,h^{-3}\,h_i\,\mathrm{d}h_j \wedge \mathrm{d}h_k$$

$$\mathrm{d}h_j \wedge \mathrm{d}h_k = \frac{\partial h_j}{\partial k_a}\,\frac{\partial h_k}{\partial k_b}\,\mathrm{d}k_a \wedge \mathrm{d}k_b$$

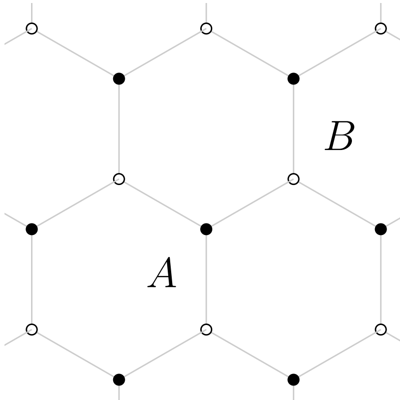
$$c_1 = \frac{1}{4\pi}\int_{\mathrm{BZ}} \frac{\vec{h}}{||h||^3} \cdot \left(\frac{\partial \vec{h}}{\partial k_x} \times \frac{\partial \vec{h}}{\partial k_y}\right)\,\mathrm{d}k_x \wedge \mathrm{d}k_y$$

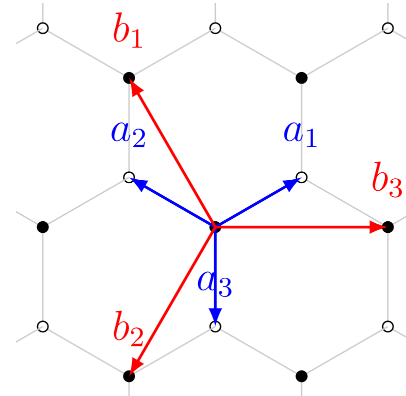
Geometrical interpretation: vector flow through the oriented surface.



Chern topological insulator (2D Haldane's model)

The model is written on hexagonal lattice:





Hamiltonian for spinless fermions:

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

Peierls substitution: $$t_{ij} \rightarrow t_{ij} \exp\left(-\mathrm{i}\frac{\mathrm{e}}{\hbar} \int_{\Gamma_{ij}} \vec{A} \cdot \mathrm{d}\vec{\ell} \right)$$

$$t \longrightarrow t \qquad \text{and} \qquad t_2 \longrightarrow t_2 \mathrm{e}^{\mathrm{i}\phi}$$

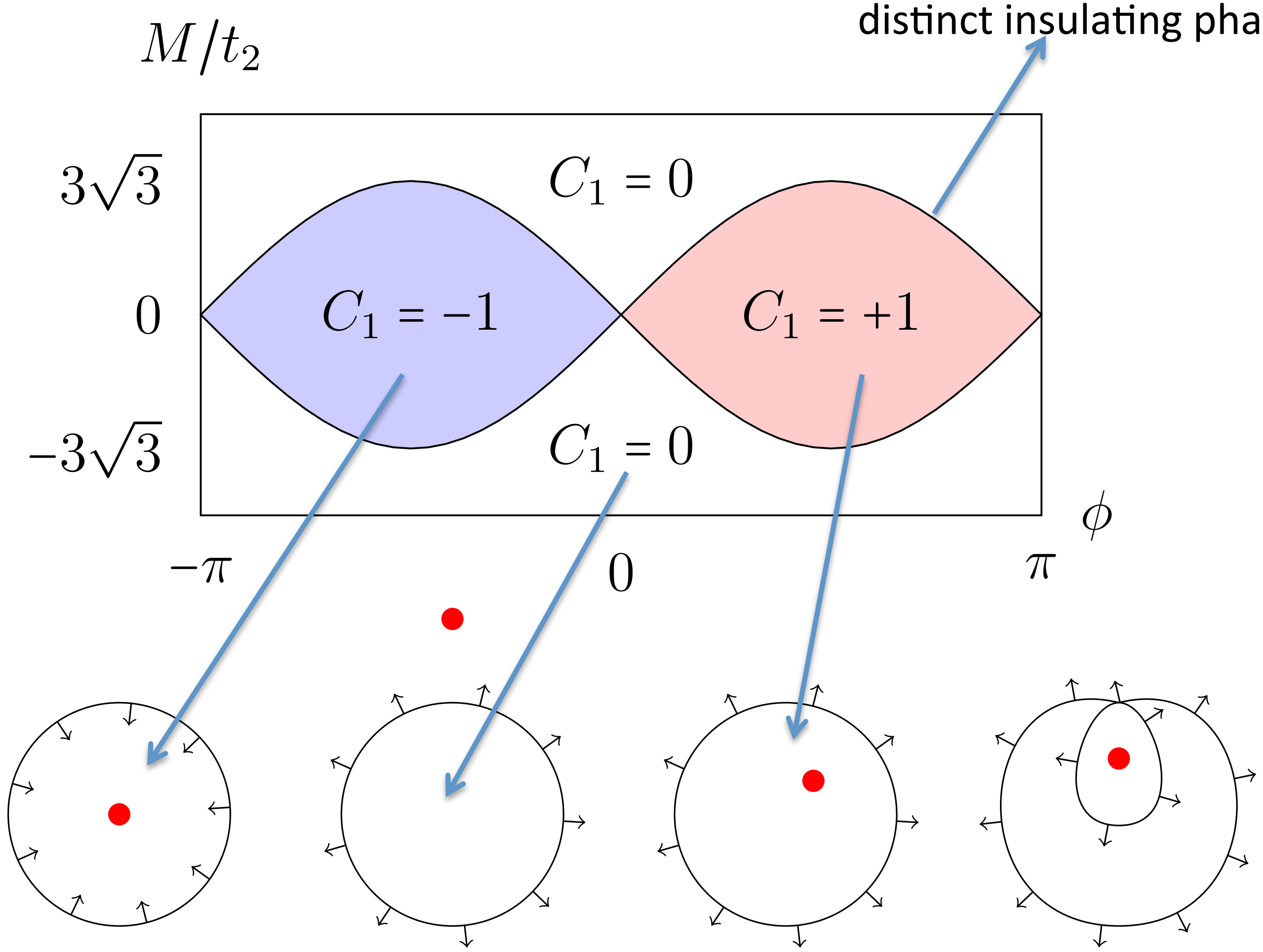
Finally in momentum space: $$\mathcal{H}(k) = h^{\mu}(k)\sigma_{\mu}$$

$$\vec{h}(k + G_{mn}) = \vec{h}(k)$$

Chern topological insulator (2D Haldane's model)

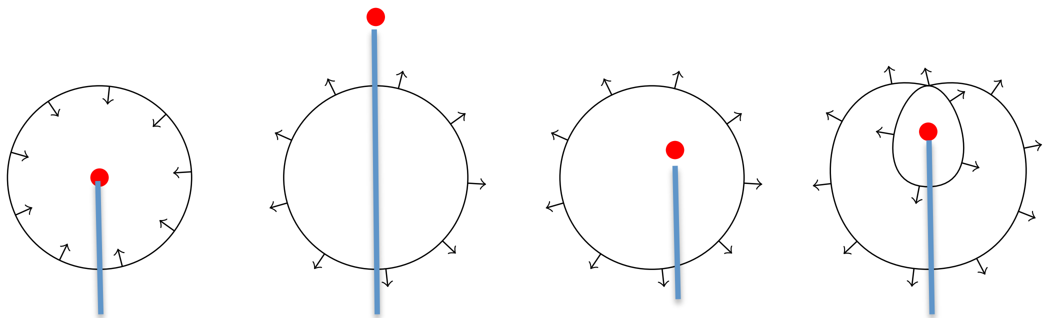
Phase diagram:

Metal on the border between two distinct insulating phases



Edge states in the Chern topological insulator

Connection between mass gap and the Chern number



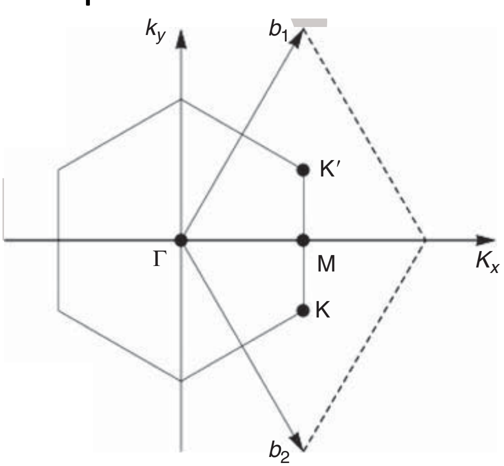
Calculation through the intersection number

$$c_1 = \frac{1}{2} \sum_{k \in D} \mathrm{sign}\,[h(k) \cdot n(k)]$$

$n(k)$ -normal vector to Σ

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:

$$c_1 = (\mathrm{sign}\, m - \mathrm{sign}\, m')/2$$

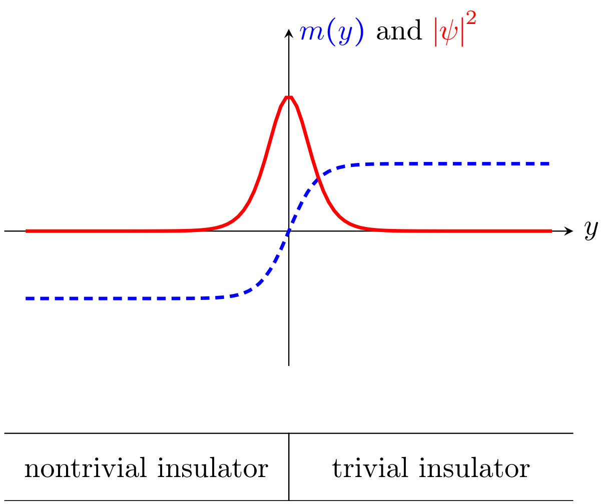
Edge states in the Chern topological insulator

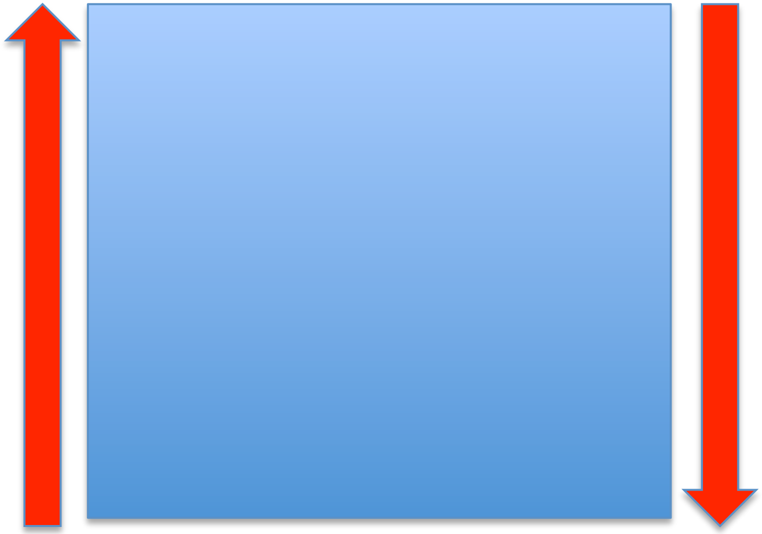
Linearized Hamiltonian near the K-point (mass should change the sign at the border):

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

Single edge mode with linear dispersion:

$$\psi_{q_x}(x,y) \propto \mathrm{e}^{\mathrm{i}q_x x} \exp\left[-\int_0^y m(y')\,\mathrm{d}y'\right] \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad E(q_x) = E_\mathrm{F} + \hbar v_\mathrm{F} q_x$$





Time-reversal invariance is broken

Z_2 Topological insulator

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

$$\Theta = e^{-i\pi J_y/\hbar}\,\mathcal{K}$$

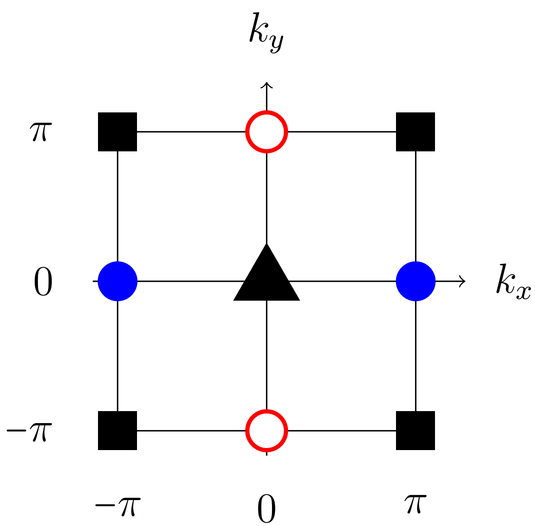
$$\Theta^2 = -\mathbb{1}$$

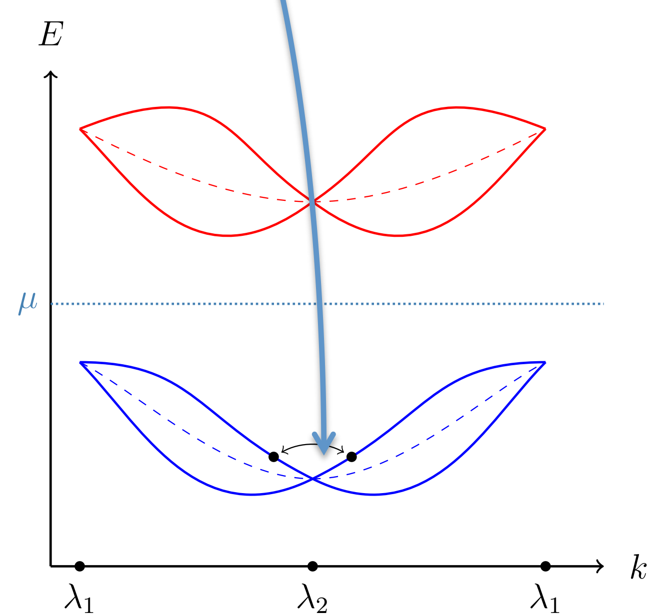
$$H(-k) = \Theta H(k) \Theta^{-1}$$

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):

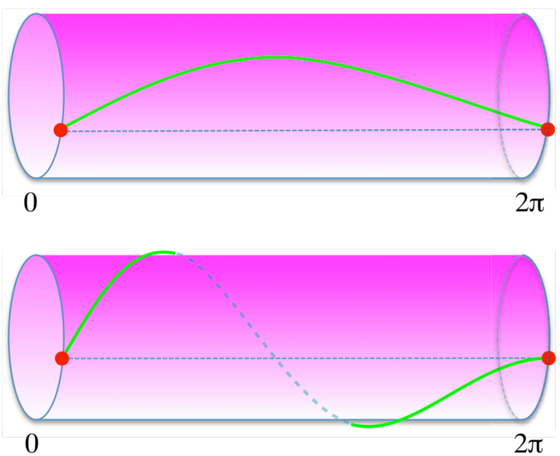




Z_2 Topological insulator

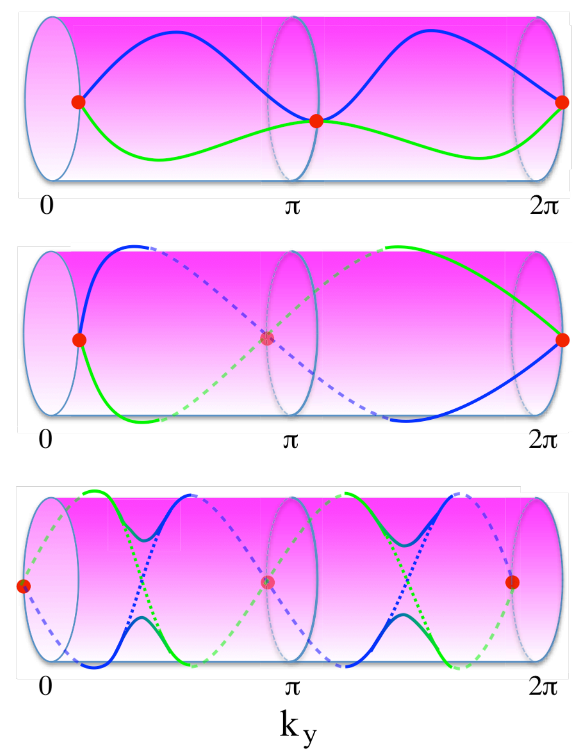
Reduction to 1D integrals:

$$2\pi Z = -\int_0^{2\pi}\int_0^{2\pi} dk_x dk_y (\partial_x A_y - \partial_y A_x)$$
$$= \int_0^{2\pi} dk_y \partial_y \left(\int_0^{2\pi} dk_x A_x(k_x, k_y)\right)$$
$$= \int_0^{2\pi} d\theta(k_y).$$



Chern insulator

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



$$F_\alpha(k) = -F_\alpha(-k)$$

guarantees the intersection at TRIM

Z_2 insulator:

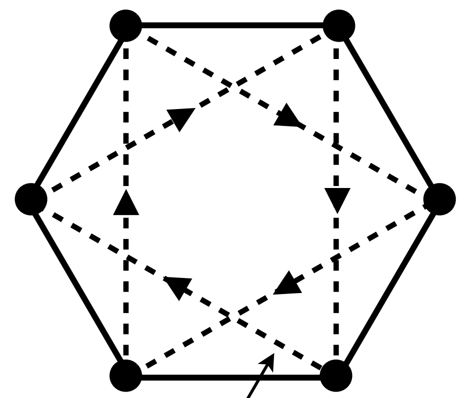
New topological invariant:

$$|Z| \bmod 2$$

Can be computed from the eigenstates at TRIM

The Kane-Mele model

Hexagonal lattice:



Spin-Orbital coupling

$$h_{\mathrm{KM}} = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + i\lambda \sum_{\ll ij \gg} \sum_{\alpha\beta} \nu_{ij} c^\dagger_{i\alpha} \sigma^z_{\alpha\beta} c_{j\beta}$$

The basis

$(A \uparrow, A \downarrow, B \uparrow, B \downarrow)$

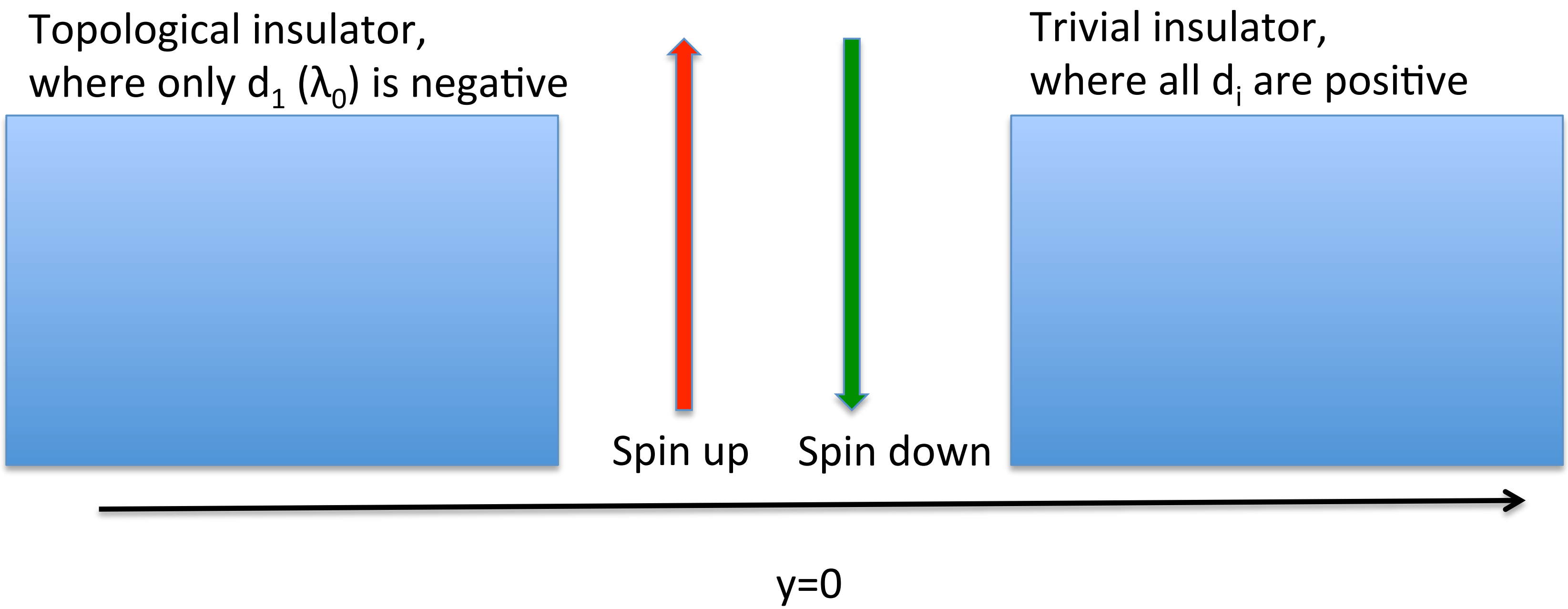
$$H(k) = d_0(k)\,\mathbb{1} + \sum_{i=1}^{5} d_i(k)\,\Gamma_i \qquad E_\pm(k) = d_0(k) \pm \sqrt{\sum_{i=1}^{5} d_i^2(k)}$$

$\Gamma_1 = \mathcal{P} = \sigma_x \otimes \mathbb{1}$ $\Gamma_2 = \sigma_y \otimes \mathbb{1}$ $\Gamma_3 = \sigma_z \otimes s_x$ $\Gamma_4 = \sigma_z \otimes s_y$ $\Gamma_5 = \sigma_z \otimes s_z$

Z_2 topological invariant: $\prod_{\lambda \in \Lambda} \mathrm{sign}\; d_1(\lambda)$

All d_i except d_1 vanish at TRIM

Edge states in Kane-Mele model: spin-momentum locking



Hamiltonian at the border: $H_1(q) = q_x\Gamma_5 - q_y\Gamma_2 + m(y)\Gamma_1$

$$H_1 = \begin{pmatrix} H_\uparrow & 0 \\ 0 & H_\downarrow \end{pmatrix} \qquad H_\uparrow = \begin{pmatrix} -\mathrm{i}\partial_x & m(y)+\partial_y \\ m(y)-\partial_y & \mathrm{i}\partial_x \end{pmatrix} \qquad H_\downarrow = \begin{pmatrix} +\mathrm{i}\partial_x & m(y)+\partial_y \\ m(y)-\partial_y & \mathrm{i}\partial_x \end{pmatrix}$$

$$\psi_{q_x,\uparrow}(x,y) \propto \mathrm{e}^{-\mathrm{i}q_x x} \exp\left[-\int_0^y m(y')\,\mathrm{d}y'\right] \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad \psi_{q_x,\downarrow}(x,y) \propto \mathrm{e}^{+\mathrm{i}q_x x} \exp\left[-\int_0^y m(y')\,\mathrm{d}y'\right] \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

3D topological insulators

Weak topological insulators: ν_x, ν_y, ν_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 $\nu_0 = 0,1$.
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, $\nu_0 = 1$ otherwise $\nu_0 = 0$.

3D topological insulators

Cubic lattice: Bi_2Se_3.
Can be described by lattice Wilson fermions (with slightly unconventional parameters)

$$\mathcal{H}_0(\boldsymbol{k}) = \sum_j \sin k_j \cdot \alpha_j + m(\boldsymbol{k})\beta$$

$$m(\boldsymbol{k}) = m_0 + r\sum_j (1 - \cos k_j)$$

$$\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \qquad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The system is topologically non-trivial (strong Z_2 TI) if:

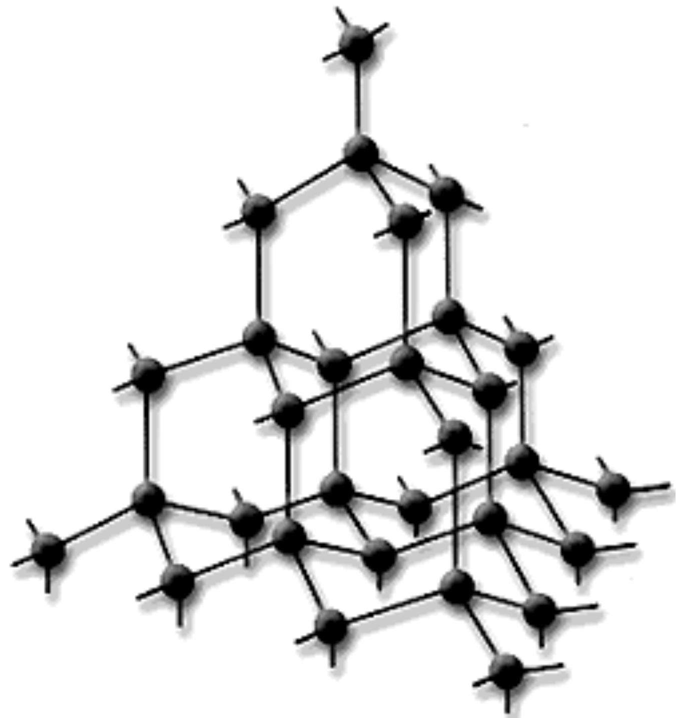
$$0 > m_0 > -2r$$
$$-4r > m_0 > -6r$$

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:



Spin-orbital coupling

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

Nearest-neighbor hoppings are modified in one direction

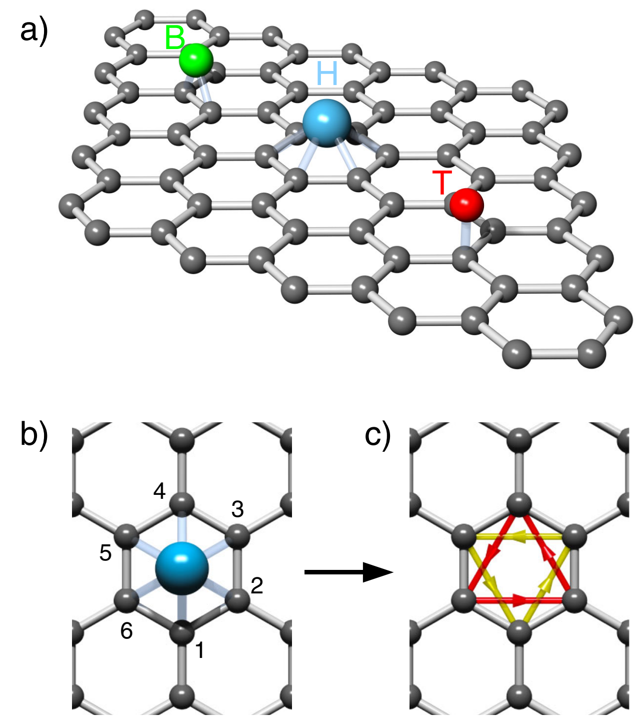
Engineering the topological state

$$H = H_g + H_a + H_c,$$

$$H_g = H_t - \delta\mu \sum_{j=1}^{6} c_{\mathbf{r}_j}^{\dagger} c_{\mathbf{r}_j},$$

$$H_a = \sum_{m=0,\pm1} \epsilon_{|m|} d_m^{\dagger} d_m + \Lambda_{\rm so}(d_1^{\dagger} s^z d_1 - d_{-1}^{\dagger} s^z d_{-1}) + \sqrt{2}\Lambda'_{\rm so}(d_0^{\dagger} s^- d_{-1} + d_0^{\dagger} s^+ d_1 + \text{H.c.}),$$

$$H_c = -\sum_{m=0,\pm1} (t_{|m|} C_m^{\dagger} d_m + \text{H.c.}),$$



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

Induces spin-orbit coupling

PRX, 1, 021001

Engineering the topological state: clusterization of adatoms

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].

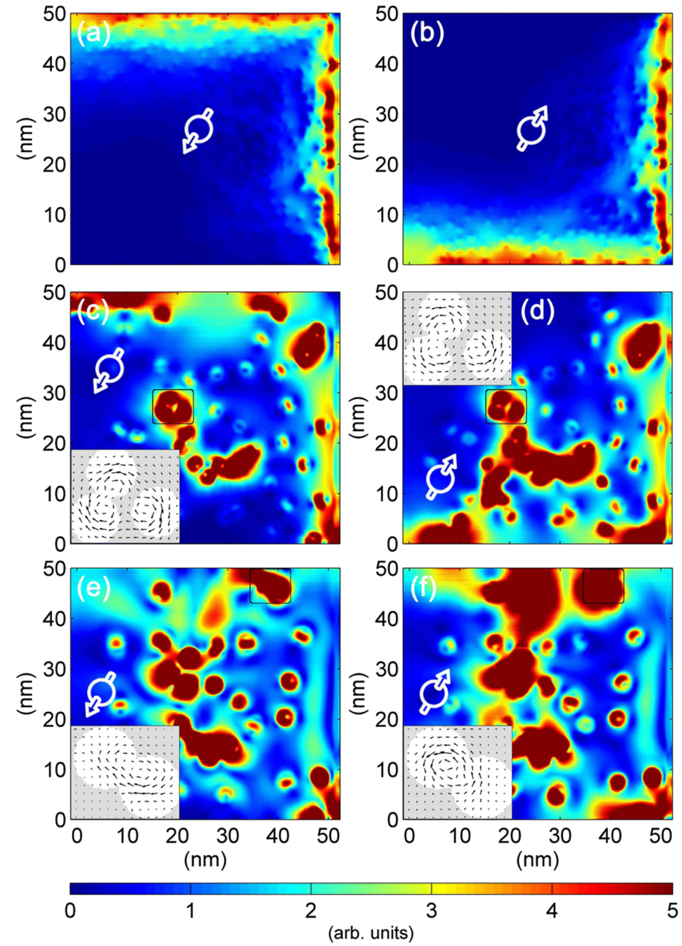
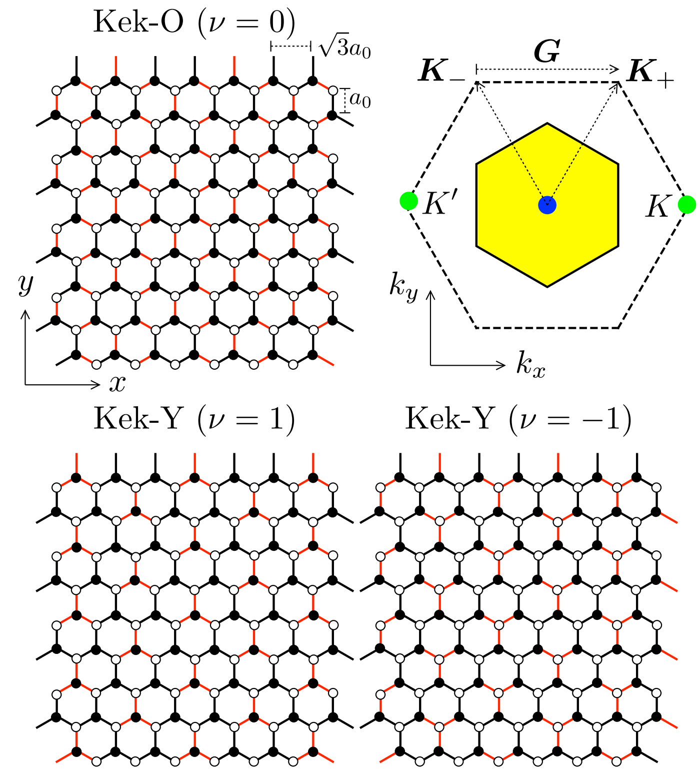


FIG. 3 (color online). Spin-resolved spectral current distribution for $r = 0.5$ nm and $E = -33.5$ meV (a),(b); $r = 1.5$ nm and $E = 21.5$ meV (c),(d); and $r = 2$ nm and $E = -33.5$ meV (e),(f). The corresponding energies and conductance are indicated by black dots in Fig. 2. The insets in panels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

Valley-momentum locking (1)

Hopping distribution



Hamiltonian:

$$H = -\sum_{\boldsymbol{r}} \sum_{\ell=1}^{3} t_{\boldsymbol{r},\ell}\, a_{\boldsymbol{r}}^{\dagger} b_{\boldsymbol{r}+\boldsymbol{s}_\ell} + \text{H.c.}$$

$$t_{\boldsymbol{r},\ell}/t_0 = 1 + 2\,\text{Re}\left[\Delta e^{i(p\boldsymbol{K}_+ + q\boldsymbol{K}_-)\cdot \boldsymbol{s}_\ell + i\boldsymbol{G}\cdot\boldsymbol{r}}\right]$$

$$\boldsymbol{G} \equiv \boldsymbol{K}_+ - \boldsymbol{K}_- = \tfrac{4}{9}\pi\sqrt{3}(1,0)$$

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

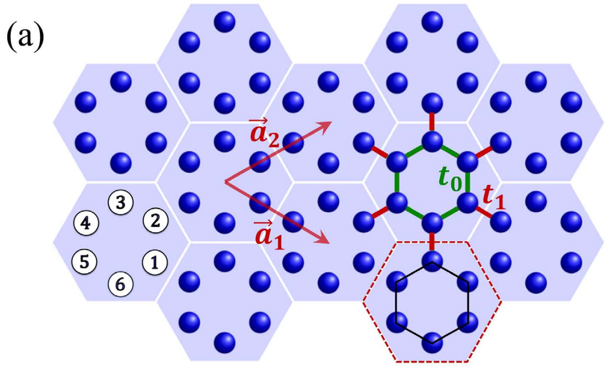
$$\mathcal{H} = v_\sigma\,(\boldsymbol{p}\cdot\boldsymbol{\sigma}) \otimes \tau_0 + v_\tau\,\sigma_0 \otimes (\boldsymbol{p}\cdot\boldsymbol{\tau})$$

τ acts in valley space and plays the role of spin.

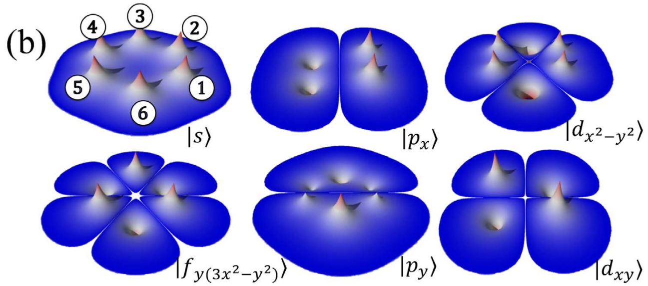
arXiv:1708.08348

Valley-momentum locking (2)

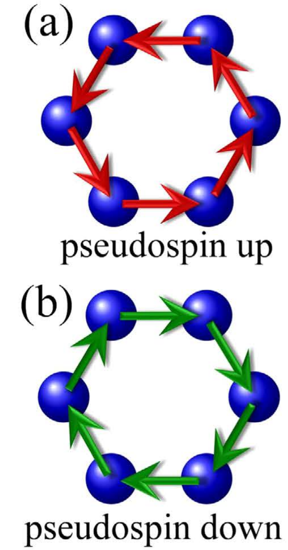
Scientific Reports, 6, 24347



Hoppings distribution



Effective Wannier functions within the supercell



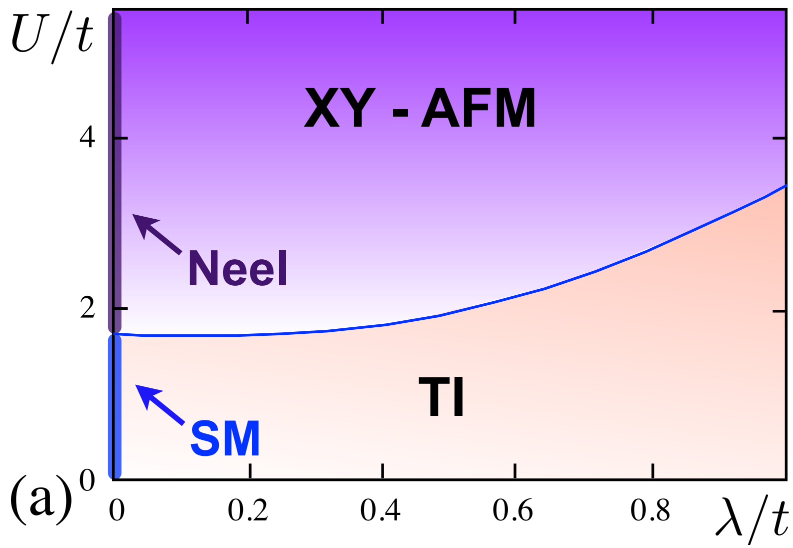
Different valleys correspond now to different orbital momentum within the supercell

Stability of TIs with respect to interaction effects

Kane-Mele-Hubbard model:

$$h_{\mathrm{KM}} = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + i\lambda \sum_{\langle\langle ij \rangle\rangle} \sum_{\alpha\beta} \nu_{ij} c^{\dagger}_{i\alpha} \sigma^{z}_{\alpha\beta} c_{j\beta}$$

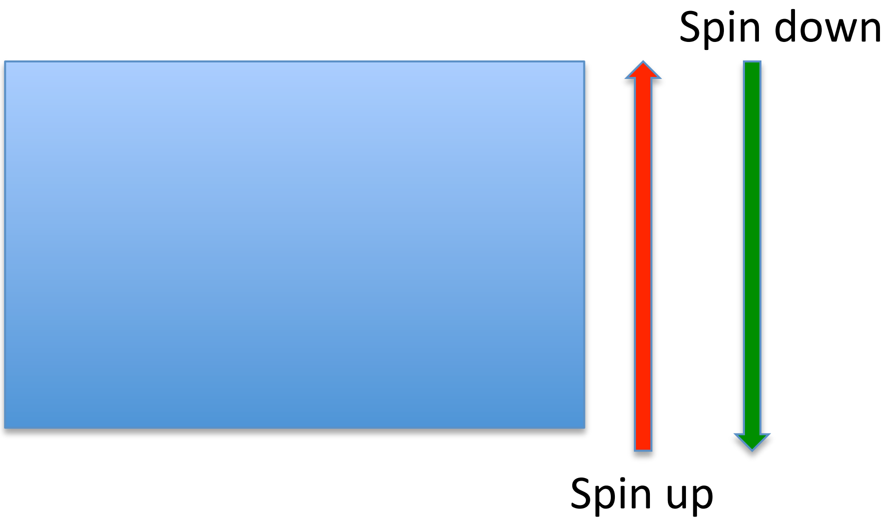
$$H_I = U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Competition between AFM and topological mass terms.
arXiv:1206.3103

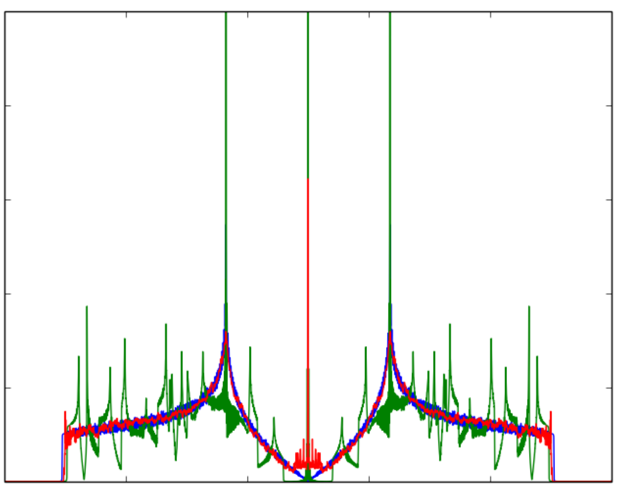
Antiferromagnetic mass term: the same sign at different K points.
Topological mass term: different signs at K-points

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:



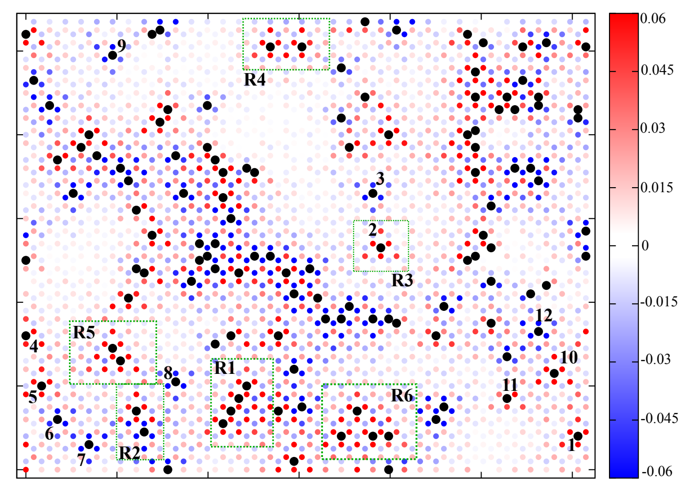
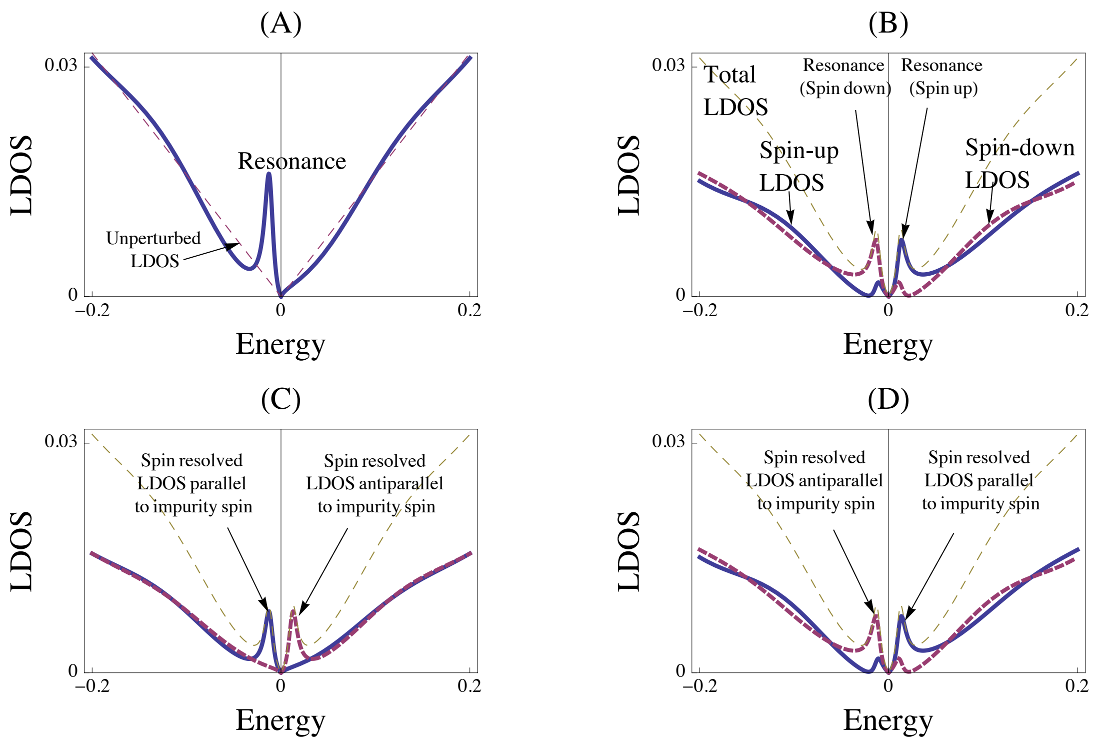


FIG. 2: Distibution of average spin. Color scale corresponds to $\langle S_z \rangle$ at the site in the zero bare mass limit.

Example calculation for graphene [PRL 114, 246801]

Stability of TIs with respect to disorder



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