TOPOLOGICAL INSULATORS

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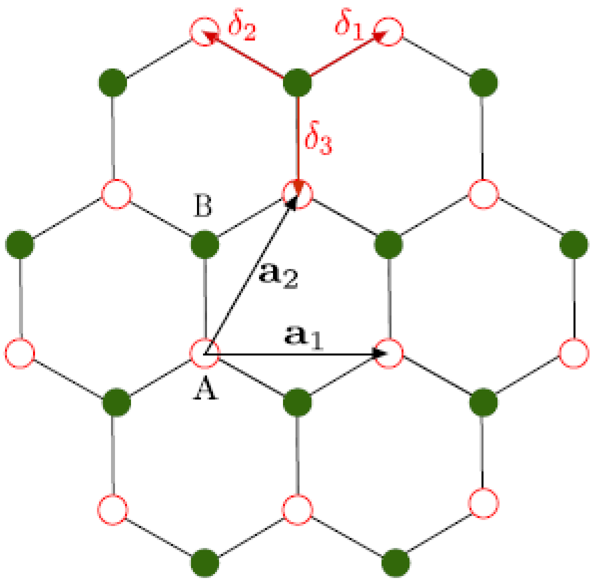
Graphene

- Graphene and Dirac Equation
- A honeycomb lattice of carbon atoms with two sublattices A and B



triangular Bravais lattice basis vectors:

$$\vec{a}_1 = \sqrt{3}a\vec{e}_x \qquad \vec{a}_2 = \frac{a}{2}\left(\sqrt{3}\vec{e}_x + 3\vec{e}_y\right)$$

$a = 0{,}142\,\mathrm{nm}$ is the length of the C-C bond.

The vectors connecting any A-site to its three B-site nearest neighbours;

$$\vec{\delta}_{1,2} = \frac{a}{2}\left(\pm\sqrt{3}\vec{e}_x + \vec{e}_y\right) \qquad \vec{\delta}_3 = -a\vec{e}_y$$

- The tight-binding Hamiltonian

$$H = t\sum_{\vec{r}_A}\sum_{\alpha=1}^{3} c_B^{\dagger}\left(\vec{r}_A + \vec{\delta}_\alpha\right)c_A\left(\vec{r}_A\right) + h.c.$$

where $t \cong -2.7\,\mathrm{eV}$ is the hopping amplitude between two adjacent carbon atoms.

- c_A destroys a fermion at site $\vec{r}_A$ and $c_B^{\dagger}$ creates a fermion at site $\vec{r}_A + \vec{\delta}_\alpha$

- By doing the Fourier transformation

$$c_a\left(\vec{r}_i\right) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}.\vec{r}_i} c_a\left(\vec{k}\right)$$

one obtains the Hamiltonian in the form

$$H = \sum_{\vec{k}} c_a^{\dagger}(\vec{k})[h(\vec{k})]_{ab}\, c_b(\vec{k})$$

- $h(\vec{k})$ is the Bloch Hamiltonian

$$h(\vec{k}) = d_1(\vec{k})\sigma_1 + d_2(\vec{k})\sigma_2$$

σ_i are Pauli matrices and

$$d_1(\vec{k}) = t\sum_{\alpha=1}^{3}\cos(\vec{k}.\,\vec{\delta}_\alpha) \qquad\qquad d_2(\vec{k}) = t\sum_{\alpha=1}^{3}\sin(\vec{k}.\,\vec{\delta}_\alpha)$$

hence, $d_1(\vec{k})$ is even and $d_2(\vec{k})$ is odd functions

$$d_1(-\vec{k}) = d_1(\vec{k}) \qquad\qquad d_2(-\vec{k}) = -d_2(\vec{k})$$

- Corresponding energy spectrum is given by the length of the vector $\vec{d} = (d_1, d_2)$

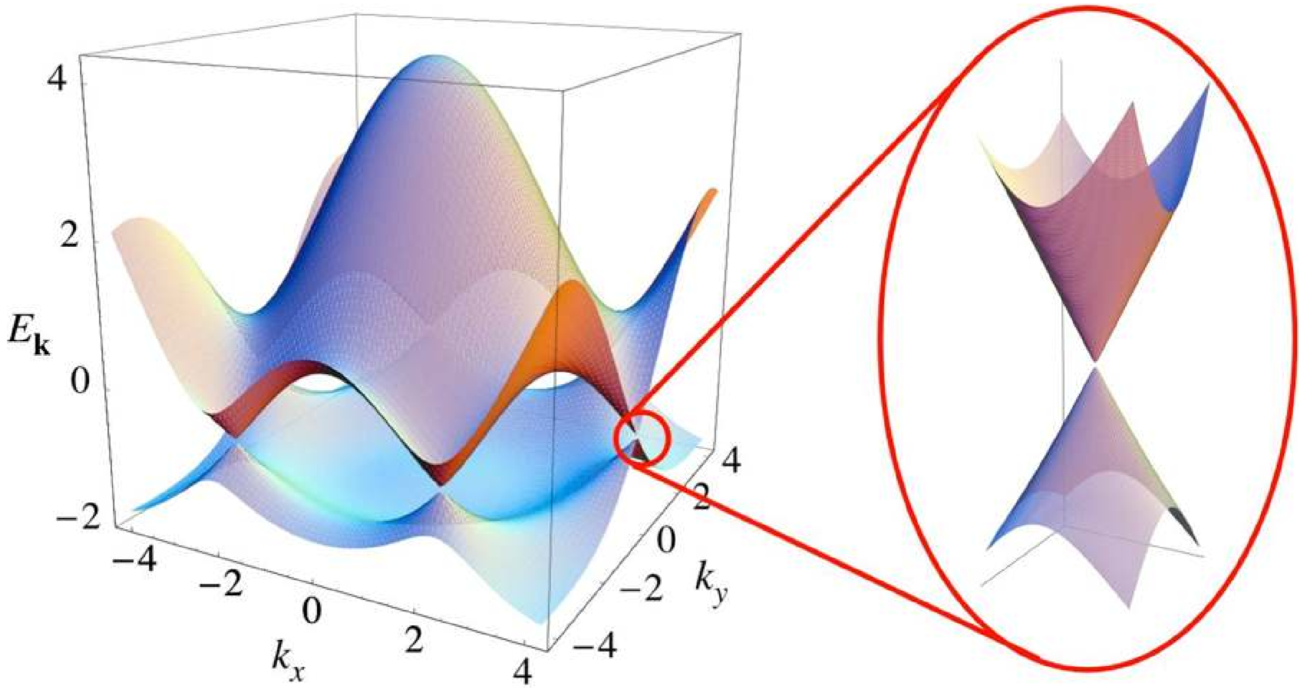
$$E(\vec{k}) = \pm\left|\vec{d}(\vec{k})\right| = \pm\sqrt{d_1(\vec{k})^2 + d_2(\vec{k})^2}$$

which describes a valence band (minus sign) and a conduction band (plus sign) that are symmetric w.r.t. $E = 0$

- The valence and conduction bands touch at isolated points of the BZ, which are obtained by solving the equation $\vec{d}(\vec{k}) = 0$

- There are only two inequivalent such points called Dirac points located at

$$\vec{k} = \pm\vec{K} = \pm\frac{4\pi}{3\sqrt{3}a}\vec{e}_x$$



- We consider the low-energy theory near the Dirac points.
- The momenta close to the zero-energy points are ($|\vec{q}|a << 1$)

$$\vec{k} = \pm\vec{K} + \vec{q}$$

- By expanding to first-order in momenta, the Hamiltonian describing the low energy excitations near $\vec{k} = \pm\vec{K}$ is found as

$$H^{(\pm\vec{K})} = v_F \sum_{\vec{k}} \begin{pmatrix} c^{\dagger}_{A\pm\vec{K}}(\vec{q}) & c^{\dagger}_{B\pm\vec{K}}(\vec{q}) \end{pmatrix} \begin{pmatrix} 0 & \pm q_x - iq_y \\ \pm q_x + iq_y & 0 \end{pmatrix} \begin{pmatrix} c_{A\pm\vec{K}}(\vec{q}) \\ c_{B\pm\vec{K}}(\vec{q}) \end{pmatrix}$$

where $v_F = -\frac{3at}{2} \cong 10^6 m/s \cong c/300$ is the Fermi velocity and

$$c_{A\pm\vec{K}} = c_A(\pm\vec{K} + \vec{q}) \qquad \vec{q} = q_x\vec{e}_x + q_y\vec{e}_y$$

- Using the convenient spinor representation

$$c_\alpha^\dagger(\vec{q}) = \left(c_{A\,K}^\dagger \quad c_{B\,K}^\dagger \quad c_{A\,-K}^\dagger \quad c_{B\,-K}^\dagger\right)$$

the Hamiltonian can be written in the Bloch form

$$H = \sum_{\vec{q}} \sum_{\alpha,\beta=1}^{4} c_\alpha^\dagger(\vec{q}) \left[v_F \left(q_x \sigma_1 \tau_3 + q_y \sigma_2 \right) \right]_{\alpha\beta} c_\beta(\vec{q})$$

which has exactly the form of the the Dirac Hamiltonian describing the spin-1/2 relativistic particles with zero mass.
(τ_3 is the Pauli matrix acts on K,-K points)

- Corresponding dispersion relation is linear in momentum

$$E(\vec{q}) = v_F |\vec{q}|$$

which is typical for a relativistic massless particle, with the velocity of light replaced by the Fermi velocity.

• Symmetries and Mass Terms in Graphene

- Dirac points are robust as long as some fundamental symmetries are obeyed.
- These fundamental symmetries are
  - Time-reversal (TR) symmetry T
  - Inversion symmetry P

- Inversion operator

$$P:(x,y)\rightarrow(-x,-y)$$

If $[H,P]=0$, then the Hamiltonian has inversion symmetry.

- Effect of P on Pauli matrices and Bloch Hamiltonian

$$P:(\sigma_1,\sigma_2,\sigma_3)\rightarrow(\sigma_1,-\sigma_2,-\sigma_3)$$

$$Ph(\vec{k})P^{-1}=h(-\vec{k})$$

- Inversion is represented by $P=\sigma_1$ and the graphene Bloch Hamiltonian is invariant under inversion ($d_1(\vec{k})$ even, $d_2(\vec{k})$ odd)

$$Ph(\vec{k})P^{-1}=\sigma_1\left(d_1(\vec{k})\sigma_1+d_2(\vec{k})\sigma_2\right)\sigma_1=h(-\vec{k})$$

- TR operation

$$T : t \rightarrow -t$$

If $[H, T] = 0$, then the Hamiltonian has TR symmetry.

- Effect of T on Pauli matrices and Bloch Hamiltonian

$$T : (\sigma_1, \sigma_2, \sigma_3) \rightarrow (\sigma_1, -\sigma_2, \sigma_3)$$

$$T h(\vec{k}) T^{-1} = h(-\vec{k})$$

- TR operation is represented by $T = \sigma_0 K$ and the graphene Bloch Hamiltonian is invariant under TR

($\sigma_0 = I$ and K is complex conjugation)

$$\begin{aligned} T h(\vec{k}) T^{-1} &= \sigma_0 \left(d_1^*(\vec{k}) \sigma_1 - d_2^*(\vec{k}) \sigma_2 \right) \sigma_0 \\ &= d_1(-\vec{k}) \sigma_1 + d_2(-\vec{k}) \sigma_2 \\ &= h(-\vec{k}) \end{aligned}$$

- By breaking one of these symmetries or adding spin degrees of freedom, one can add a mass term and open a gap.
- A mass term anticommutes with the Hamiltonian, hence it enters as a σ_3 term with possible different coefficient functions $d_3(\vec{k})$.

- For example, a generic two-band model for spinless fermions on a bipartite lattice can be written as

$$\begin{aligned} h(k) &= \varepsilon_0(k)\sigma_0 + d_1(k)\sigma_1 + d_2(k)\sigma_2 + d_3(k)\sigma_3 \\ &= \varepsilon_0(k)\sigma_0 + \vec{d}(k).\vec{\sigma} \end{aligned}$$

- When the spin is included, there are 16 possible different mass terms, some breaks and some respects the symmetries.
- However, we consider 3 types of mass terms.

  (Semenov, Haldane and Kane-Mele masses)

- *i) Semenov mass*
- The simplest choice of a mass term is

$$d_3(k) = M_S$$

- It enters to the Hamiltonian as a staggered on-site potential term that breaks inversion and respects TR

$$H_1 = \sum_i M_{S_i} c_i^\dagger c_i$$

($i = A, B$ and $M_{S_A} = -M_{S_B}$)

- The mass term is independent of k and has same sign at K and K'= - K points.
- Dispersion relation becomes

$$E^2 = v_F^2 p^2 + M_S^2$$

- *ii) Haldane mass*
- Another possibility is adding a phase to the second-neighbour hopping term in the Hamiltonian.
- This is done by magnetic fluxes ϕ and breaks TR symmetry,

$$H_2 = t_2 \sum_{i=1}^{3} \left(\sum_{r_A} c_A^\dagger(r_A) c_A(r_A + b_i) e^{i\phi} + \sum_{r_B} c_B^\dagger(r_B) c_B(r_B + b_i) e^{-i\phi} \right) + h.c.$$

- This gives a mass term in Dirac Hamiltonian at K and K' points

$$d_3(k \cong \pm K) = \mp 3\sqrt{3} t_2 \sin\phi$$

- Sign of the mass term at K and K' is different.
- Dispersion relation becomes

$$E^2 = v_F^2 p^2 + 27 t_2^2 \sin^2 \phi$$

- *iii) Kane-Mele mass*
- By adding spin degrees of freedom, one can write a mass term that respects inversion and TR symmetries.
- This corresponds to the intrinsic spin-orbit coupling term,

$$H_3 = i\lambda_{SO} \sum_{<<i,j>>} \nu_{ij} c^{\dagger}_{i\alpha} (s_3)_{\alpha\beta} c_{j\beta}$$

where $\nu_{ij} = \pm 1$ and s_3 is the physical spin of the electrons ($s_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$).

- This gives a mass term

$$d_3(\pm K) = \pm 3\sqrt{3}\lambda_{SO} s_3$$

- Hence, different signs at K and K' points.
- Dispersion relation is

$$E^2 = v_F^2 p^2 + 27\lambda_{SO}^2$$

- Different signs of the mass term at K and K' points will give the topological insulator property of the system.

What is a Topological Insulator?

- A topological insulator (TI) is an insulator (gapped) in the bulk and has also gapless states at the edge or surface.

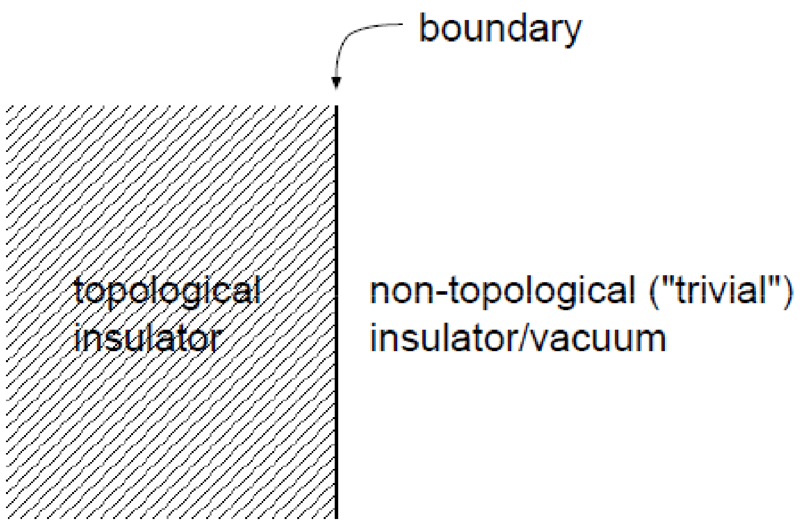
- Topological insulators are characterized by topological orders. Different topological orders define different classes of TIs.

- A TI Hamiltonian must be a gapped Hamiltonian. A TI Hamiltonian in one topological class cannot be deformed continuously to a Hamiltonian in another topological class.

  (deformation means changing Hamiltonian parameters without closing the gap)

- To convert one topological class Hamiltonian to another one, there must be a gapless state between two classes. Hence, the insulating phase must disappear. These are the edge states.

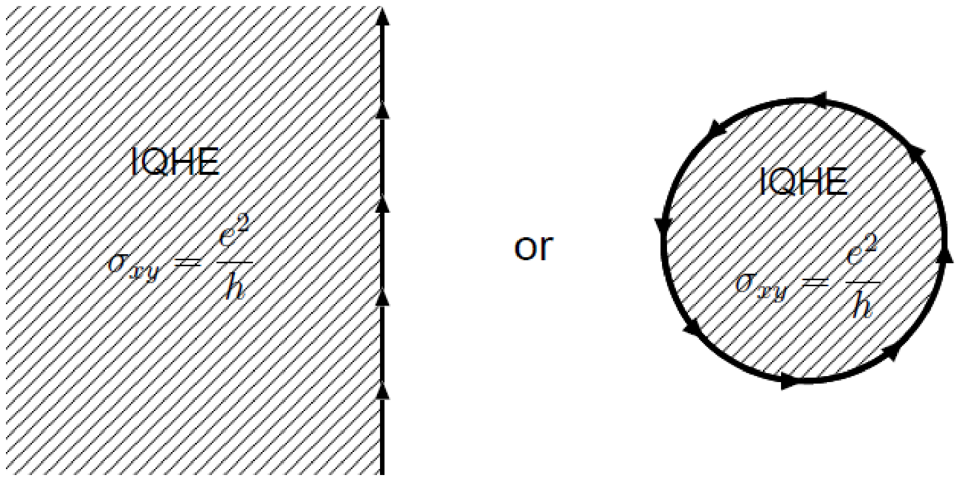
- For example, a topological insulator which has an interface with an ordinary insulator (or vacuum) has a gapless boundary, although insulating at the bulk.



- The gapless boundary degrees of freedom are robust to perturbations, as long as these perturbations do not close the bulk gap and preserve the symmetries of the system.

- There are mainly two types of topological insulators;
  - $\mathbb{Z}$ Insulators (Chern Insulators)
  - $\mathbb{Z}_2$ Insulators

- An example for the first type is the Integer Quantum Hall Effect (IQHE).
- In this case, an applied magnetic field to a d=2 dimensional electron system results a gapless edge state which corresponds to a charge current at the edge.



- The applied magnetic field breaks TR symmetry.

- The quantized Hall conductivity σ_{xy} at the edge can take integer multiples of e^2/h .

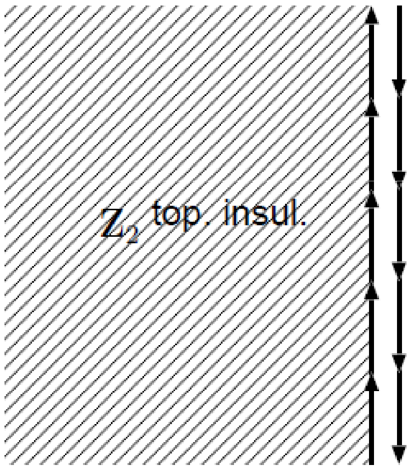
- This edge state possesses a chirality inherited from the applied magnetic field and propagates only in one direction.

- IQHE can be generalized to cases without an applied magnetic field bu a TR breaking term in the Hamiltonian.

- These are called Chern insulators.

- The set of different topological classes is $\mathbb{Z}$. (corresponds to the number of edge states)

- Second type of topological insulators is Quantum Spin Hall Effect or $\mathbb{Z}_2$ Insulators.
- In this case, TR symmetry is conserved and the edge states propagate in two opposite directions (with opposite spin) as pairs.



- Hence, there is no net charge current at the edge, however there is non-zero spin current.

- There are only two different topological classes in this case, hence the name $\mathbb{Z}_2$.

- If there are even number of pairs at the edge, we have a trivial insulator.
- If there are odd number of pairs at the edge, we have a topological insulator.

- The topological class of a topological insulator Hamiltonian is determined by the topological invariants.
- That is Chern number for Chern insulators and $\mathbb{Z}_2$ invariant for $\mathbb{Z}_2$ insulators.

Chern Insulators

- Different topological classes of a Chern insulator are characterized by a topological invariant called Chern number.
- It is defined from the eigenstates of the Hamiltonian.

Bloch States, Berry Connection and Curvature

- Eigenstates of the Bloch Hamiltonian are called Bloch states

$$h(k)\left|u_n(k)\right\rangle = E_n(k)\left|u_n(k)\right\rangle$$

- Eigenvalues $E_n(k)$ are periodic in momentum and all distinct eigenvalues are located in the first BZ.

- Eigenstates $|u_n(k)\rangle$ are equivalent up to a phase.
- Let us consider a loop (closed curve) C in the BZ.

  Along such a loop the eigenstates acquire a phase

$$|u_n(k)\rangle \rightarrow e^{i\gamma_n}|u_n(k)\rangle$$

where $\gamma_n = \oint_C dk\ A_n(k)$ is the Berry phase.

- The Berry connection is defined in terms of the eigenstates as

$$A_n(k) = i\langle u_n(k)|\nabla_k|u_n(k)\rangle$$

- The Berry curvature is

$$F_n(k) = \nabla_k \times A_n(k)$$
$$= \nabla_k \times \langle u_n(k)|i\nabla_k|u_n(k)\rangle$$

• Chern Number

- Chern number is defined as the integral of the Berry curvature over the BZ

$$C_1 = \frac{1}{2\pi}\int_{BZ} dk\ F(k)$$

(this is defined in 2D and called the first Chern number, there are generalizations to higher dimensions and $F(k) = \sum_n F_n(k)$)

- Chern number is a topological invariant and it takes only integer values.

- For the IQHE the quantization of Hall conductivity is expressed by the Chern number

$$\sigma_H = C_1 \frac{e^2}{h}$$

- Hence, the Chern number gives the number of chiral edge states for Chern insulators (and IQHE).
- Its sign determines the direction of the edge current.

- In 2D, for the systems with Bloch Hamiltonian

$$h(k) = \vec{d}(k).\vec{\sigma}$$

one can write the Chern number as follows

$$C_1 = \frac{1}{4\pi}\int_{BZ} d^2k \left(\frac{\partial \hat{d}(k)}{\partial k_x} \times \frac{\partial \hat{d}(k)}{\partial k_y} \right) . \, \hat{d}(k)$$

where

$$\hat{d}(k) = \frac{\vec{d}(k)}{\left|\vec{d}(k)\right|} \qquad \text{and} \qquad \left|\vec{d}(k)\right| = \sqrt{d_1^2(k) + d_2^2(k) + d_3^2(k)}$$

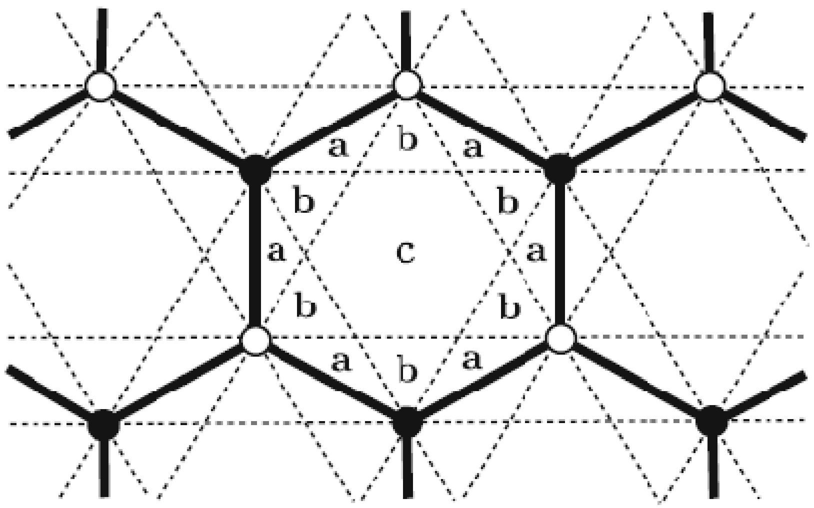
- For massive Dirac Hamiltonians, explicit calculation of the Chern number gives the result that it depends only on the mass term $d_3(k)$.
- For massive graphene Hamiltonians, the sign of the mass term at K and K' points determine the value of the Chern number;

$$C_1 = \frac{1}{2}\left[\mathrm{sgn}\left(d_3(k)\ \mathrm{at}\ K\right) - \mathrm{sgn}\left(d_3(k)\ \mathrm{at}\ K'\right)\right]$$

- Hence, the mass terms that have different signs at K and K' points result a non-zero Chern number and a non-trivial topological insulator phase.
- If the sign of the mass terms at K and K' points are same, then the Chern number is zero and we have an ordinary trivial insulator phase.

- Haldane Model

- Spinless fermion model for the IQHE without Landau levels.
- QHE may result from the broken TR symmetry without any net magnetic flux through the unit cell of a periodic 2D lattice.
- We have a graphene honeycomb lattice and a periodic magnetic flux density normal to the plane with the full symmetry of the lattice and with the zero total flux through the unit cell.



The flux ϕ_a in the region a and the flux ϕ_b in the region b have the relation $\phi_a = -\phi_b$. and the flux ϕ_c in the region c is $\phi_c = 0$.

Hence, the total flux in the unit cell is zero. (Haldane, PRL 61, 2015 (1988))

- Haldane model Hamiltonian is

$$H = M\sum_i \varepsilon_i c_i^\dagger c_i + t_1 \sum_{<i,j>} c_i^\dagger c_j + t_2 \sum_{<<i,j>>} e^{-i\nu_{ij}\phi} c_i^\dagger c_j$$

- The first term is inversion-symmetry breaking term with $\varepsilon_i = \pm 1$ that is on-site energies $+M$ for $i = A$ and $-M$ for $i = B$.

- Second term is the nearest-neighbour hopping term.

- Third term is the second-nearest-neighbour hopping term with a phase and $\phi = \frac{2\pi}{\phi_0}(2\phi_a + \phi_b)$

$\phi_0 = h/c$ and $\nu_{ij} = \pm 1$ gives the different phases for different hopping terms.

- After doing Fourier transformation, one obtains the two-band Bloch Hamiltonian as follows;

$$h(k) = d_i(k) \, . \, \sigma_i$$

where

$$d_0(k) = \varepsilon(k) = 2t_2 \cos\phi \sum_i \cos(\vec{k} \, . \, \vec{b}_i)$$

$$d_1(k) = t_1 \sum_i \cos(\vec{k} \, . \, \vec{a}_i)$$

$$d_2(k) = t_1 \sum_i \sin(\vec{k} \, . \, \vec{a}_i)$$

$$d_3(k) = M - 2t_2 \sin\phi \sum_i \sin(\vec{k} \, . \, \vec{b}_i)$$

here $\vec{a}_i$ are Bravais lattice basis vectors and

$$\vec{b}_1 = \vec{a}_2 - \vec{a}_3 \quad , \quad \vec{b}_2 = \vec{a}_3 - \vec{a}_1 \quad , \quad \vec{b}_3 = \vec{a}_1 - \vec{a}_2$$

- By considering low energy limit at K and K' points, we obtain the Bloch Hamiltonians;

$$h(K+k) = -3t_2\cos\phi + \frac{3}{2}at_1\left(-k_x\sigma_1 - k_y\sigma_2\right) + \left(M + 3\sqrt{3}t_2\sin\phi\right)\sigma_3$$

$$h(K'+k) = -3t_2\cos\phi + \frac{3}{2}at_1\left(k_x\sigma_1 - k_y\sigma_2\right) + \left(M - 3\sqrt{3}t_2\sin\phi\right)\sigma_3$$

- Hence, we have the mass terms at K and K' points

$$d_3(K) = M + 3\sqrt{3}t_2\sin\phi \qquad d_3(K') = M - 3\sqrt{3}t_2\sin\phi$$

- Consequently, we can find the Chern number as follows

$$C_1 = \frac{1}{2}\left[\mathrm{sgn}\left(M + 3\sqrt{3}t_2\sin\phi\right) - \mathrm{sgn}\left(M - 3\sqrt{3}t_2\sin\phi\right)\right]$$

- We consider three cases;

- i) $M = 3\sqrt{3}t_2 \sin\phi$ or $M = -3\sqrt{3}t_2 \sin\phi$
- In this case, the Hamiltonian is gapless at K' and gapped at K

  or gapless at K and gapped at K'

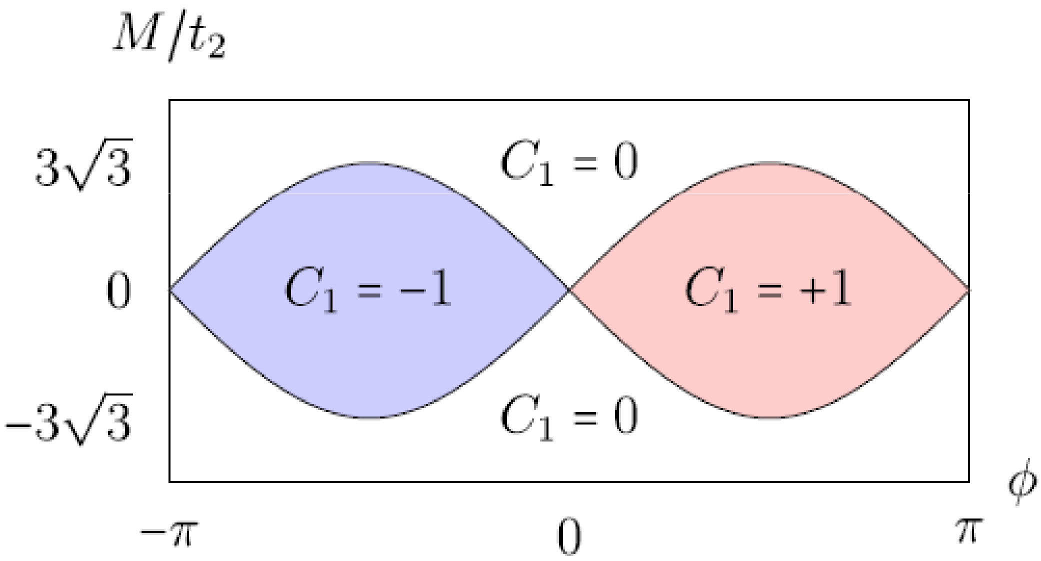
- ii) for $M > 3\sqrt{3}t_2 \sin\phi$
- In this case, Chern number is zero.

  So, we have a trivial insulator.

- iii) for $M < 3\sqrt{3}t_2 \sin\phi$
- In this case, Chern number is +1 for $\phi > 0$ and -1 for $\phi < 0$

  So, we have the topological insulator phase.

- By deforming the Hamiltonian parameters, we obtain different topological phases and between them there is a gapless transition point.
- The phases of the Haldane model and Chern numbers are given as the following diagram;



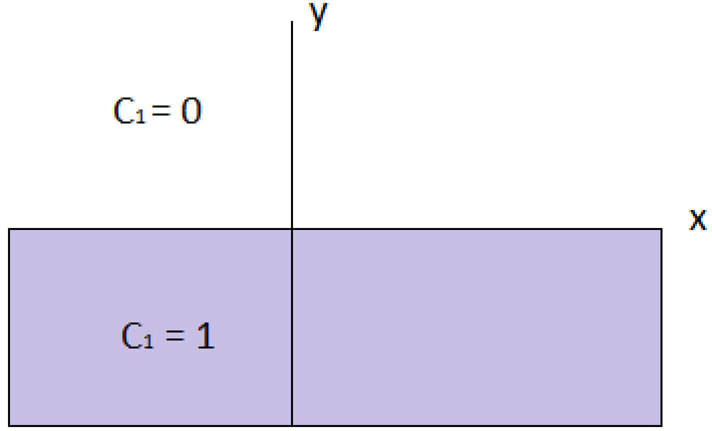
- For $\phi = 0$ (no magnetic fluxes), Haldane model reduces to an ordinary insulator and there are no topological phases ($C_1 = 0$).

• Chiral Edge States

- TIs are characterized by their gapless edge states.

  For Chern insulators, there are chiral edge states (edge states that go in one direction).
- Since the Chern number is a topological quantity, it cannot change simply through a continuous transformation, but only at a phase transition associated with a gap closing.

- Let us consider an interface at $y=0$ between a non-trivial insulator with $C_1 = 1$ for $y<0$ and a trivial insulator with $C_1 = 0$ for $y>0$



- Consider the mass terms of the Haldane model

$$m = d_3(K) = M + 3\sqrt{3}t_2 \sin\phi$$

$$m' = d_3(K') = M - 3\sqrt{3}t_2 \sin\phi$$

- Necessarily, one of the mass terms changes sign at the interface:

  $m'(y<0)<0$ and $m'(y>0)>0$, whereas the other one has constant sign $m>0$.

- This is because of the Chern number

$$C_1 = \frac{1}{2}\left(\mathrm{sgn}(m) - \mathrm{sgn}(m')\right)$$

- Then, it is natural to set $m(0)=0$, which implies that the gap closes at the interface.

- As the mass m depends on the position, by doing a unitary transformation the Bloch Hamiltonian for the Haldane model at K' point leads to the eigenvalue equation;

$$\begin{pmatrix} -i\partial_x & \partial_y + m'(y) \\ -\partial_y + m'(y) & i\partial_x \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

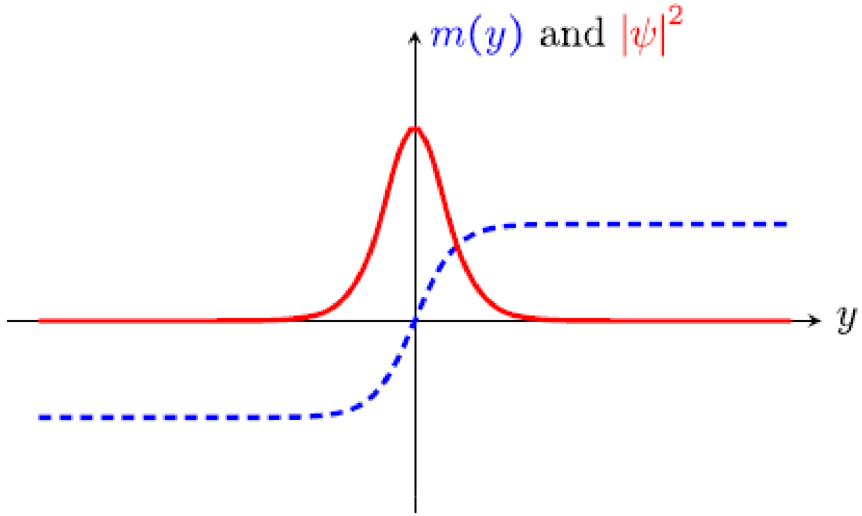
- For our choice of $m'(y)$, there is only one normalizable solution;

$$\Psi_{k_x}(x,y) \propto e^{ik_x x} \exp\left(-\int_0^y m'(y')dy' \right)\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

for the energy

$$E(k_x) = \hbar v_F k_x$$

- This solution is localized transverse to the interface where m' changes sign;



- The edge state crosses the Fermi energy at $k_x = 0$, with a positive group velocity v_F and thus corresponds to a 'chiral right moving' edge state.

- When considering a transition from an insulator with $C_1 = -1$ to the $C_1 = 0$, the eigenvalue becomes $E(k_x) = -\hbar v_F k_x$ and it has a negative group velocity and 'chiral left moving' edge state.

$\mathbb{Z}_2$ Insulators

- $\mathbb{Z}_2$ insulators are characterized by TR symmetry and spin-orbit interaction play a prominent role.
- Different topological classes are defined by $\mathbb{Z}_2$ invariants which take only two values.

• TR Symmetry, Kramers' Pairs, TRIM Points

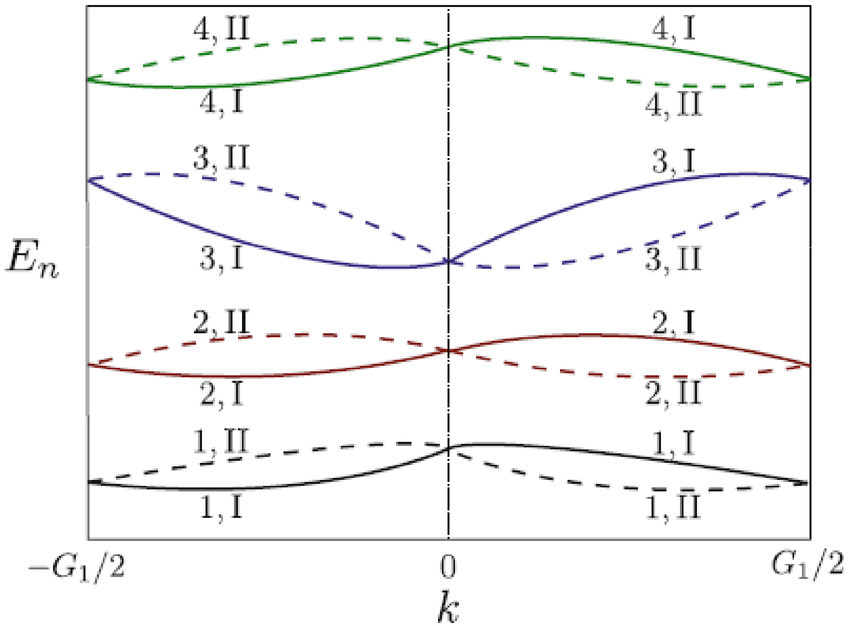
- For spin 1/2 particles TR operation has the property $T^2 = 1$.
- Over the BZ of the system, the TR operation relates the Bloch states at k with the Bloch states at -k.
- Bloch Hamiltonian at k and -k satisfy

$$h(-k) = Th(k)T^{-1}$$

- TR implies the existence of Kramers' pairs of eigenstates:

  Any eigenstate of $h(k)$ at k is an eigenstate of $h(-k)$ at -k with the same energy.

- So, all eigenstates can be labelled by pairs;



We denote I, II as Kramers' pairs index and $n = 1, \ldots, N$ as non-Kramers' pairs index.

Kramers pairs eigenstates are orthogonal to each other.

- TR transforms eigenstates at k of bands I into eigenstates at -k of bands II and vice versa, but only up to a phase factor,

$$\left|u_n^I(-k)\right\rangle = e^{i\chi_{k,n}} T \left|u_n^{II}(k)\right\rangle$$

- Some points of the BZ are invariant under TR operation. These points are called TR invariant momentum (TRIM) or high symmetry points.

- These are fixed points of T and play and important role in TR invariant systems.

- At TRIM points Kramers' pairs are degenerate. (Since Kramers' pairs are orthogonal and possess the same energy, the spectrum is necessarily always degenerate at TRIM points.)

- Kramers' pairs and TRIM points can be used in defining topological invariants for TR invariant systems, and these invariants define the topological class of the system.

- # Kane-Mele Model

- The Haldane model of a Chern insulator shows that a non-trivial insulator with a non-zero Chern number can exist when TR symmetry is broken.

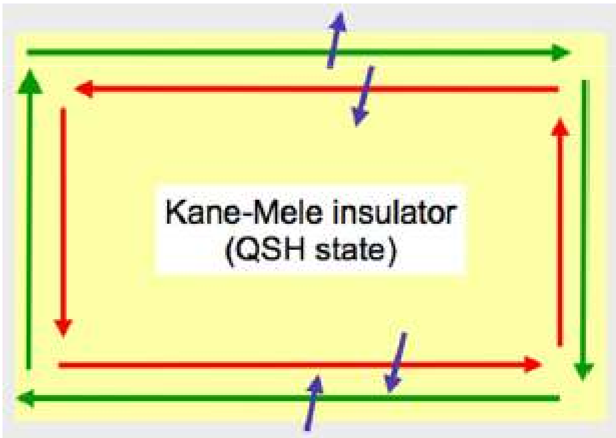
- Kane and Mele generalized the Haldane model to the graphene lattice model of electrons with spin 1/2.
  (Kane and Mele, PRL 95, 146802 (2005))

- They introduced the spin-orbit coupling between electron spin and momentum to replace the periodic magnetic flux and predicted a new quantum phenomenon; the quantum spin Hall effect (QSHE).

- Unlike the QHE in which the magnetic field breaks TR symmetry, the spin-orbit coupling preserves TR symmetry.

- In a system with TR symmetry, electrons with spin-up in the edge channel flow in one direction ($C_1 = 1$),
  while electrons with spin-down flow in the opposite direction ($C_1 = -1$)
  the net charge current in two edge channels is zero;

$$I_c = I_\uparrow + I_\downarrow = 0$$



- Instead, a pure spin current circulates around the boundary of the system;

$$I_s = \frac{\hbar}{2e}\left(I_\uparrow - I_\downarrow\right)$$

- The Kane-Mele model for the QSHE is a graphene model with the TR invariant spin-orbit coupling;

$$H = t\sum_{<i,j>} c_i^{\dagger} c_j + i\lambda_{SO} \sum_{<<i,j>>} v_{ij} c_i^{\dagger} s_z c_j + i\lambda_R \sum_{<i,j>} c_i^{\dagger} (\vec{s} \times \vec{d}_{ij})_z c_j + \lambda_v \sum_i \varepsilon_i c_i^{\dagger} c_i$$

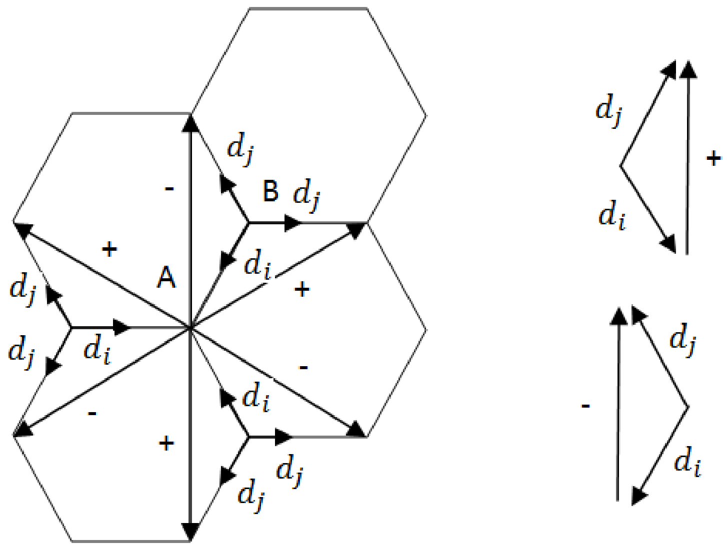
- The first term is the nearest neighbour hopping term on a graphene lattice, where $c_i^{\dagger} = (c_{i\uparrow}^{\dagger}, c_{i\downarrow}^{\dagger})$, $i = A, B$

- The second term is an intrinsic spin-orbit interaction, which involves spin-dependent second neighbour hopping.

Here $v_{ij} = \frac{2}{\sqrt{3}} (\vec{d}_i \times \vec{d}_j)_z = \pm 1$

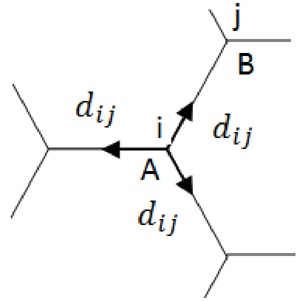
where d_i and d_j are two unit vectors along the two bonds the electron traverses going from site j to i.

The Pauli matrices s_i describe the electron spin.



- The third term is the nearest neighbour Rashba spin-orbit coupling term.

  Here $\vec{d}_{ij}$ is the distance between nearest neighbour sites;



  This term corresponds to the application of an electric field in the plane.

- The last term is the inversion symmetry breaking term (symmetry breaking w.r.t. $A \leftrightarrow B$)

  $\varepsilon_i = \pm 1$ depending on whether i is the A or B site (on-site energy term).

- We can obtain the Bloch Hamiltonian of the Kane-Mele model as

$$h(k) = \sum_{a=1}^{5} d_a(k)\Gamma_a + \sum_{a<b=1}^{5} d_{ab}(k)\Gamma_{ab}$$

- This is written in the basis of Γ_a and Γ_{ab} which are the generators of the Clifford algebra

$$\{\Gamma_a, \Gamma_b\} = 2\delta_{ab} \qquad a,b = 1,2,3,4,5$$

and $\Gamma_{ab} = \frac{1}{2i}[\Gamma_a, \Gamma_b]$

- The representation for basis matrices for the Kane-Mele model is as follows

$$\Gamma_{1,2,3,4,5} = (\sigma_1 \otimes I, \sigma_3 \otimes I, \sigma_2 \otimes s_1, \sigma_2 \otimes s_2, \sigma_2 \otimes s_3)$$

σ_i represents sublattice and s_i represents spin.

- The functions in the Bloch Hamiltonian are found as

$d_1 = t\left(1 + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right)$	$d_{12} = -2t\cos\frac{k_x}{2}\sin\frac{\sqrt{3}k_y}{2}$
$d_2 = \lambda_v$	$d_{15} = \lambda_{SO}\left(2\sin k_x - 4\sin\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right)$
$d_3 = \lambda_R\left(1 - \cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right)$	$d_{23} = -\lambda_R\cos\frac{k_x}{2}\sin\frac{\sqrt{3}k_y}{2}$
$d_4 = -\sqrt{3}\lambda_R\sin\frac{k_x}{2}\sin\frac{\sqrt{3}k_y}{2}$	$d_{24} = \sqrt{3}\lambda_R\sin\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}$

- For the special case $\lambda_R = 0$, the Hamiltonian split into two independent parts; spin up and spin down copies of Haldane model.

- By taking the low-energy limit, we have the Bloch Hamiltonians at K and K' points as

$$h(K) = \lambda_v \sigma_3 \otimes I + 3\sqrt{3}\lambda_{SO}\sigma_3 \otimes s_3$$

$$h(K') = \lambda_v \sigma_3 \otimes I - 3\sqrt{3}\lambda_{SO}\sigma_3 \otimes s_3$$

here $\sigma_3 \otimes I = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}$ and $\sigma_3 \otimes s_3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}$

- Hence, Bloch Hamiltonians are diagonal in s matrices and they can split into up and down Hamiltonians.
- The mass terms are written as

$d_{3\uparrow}(K) = \left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right)$	$d_{3\downarrow}(K) = \left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right)$
$d_{3\uparrow}(K') = \left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right)$	$d_{3\downarrow}(K') = \left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right)$

- Chern numbers
- *i) in the case of* $\lambda_v > 3\sqrt{3}\lambda_{SO}$

$$C_{1\uparrow} = \frac{1}{2}\left[\mathrm{sgn}\left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right) - \mathrm{sgn}\left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right)\right] = 0$$

$$C_{1\downarrow} = \frac{1}{2}\left[\mathrm{sgn}\left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right) - \mathrm{sgn}\left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right)\right] = 0$$

total Chern number $C_{1\uparrow} + C_{1\downarrow} = 0$ and there is no spin current, since $C_{1\uparrow} - C_{1\downarrow} = 0$

- *ii) in the case of* $\lambda_v < 3\sqrt{3}\lambda_{SO}$

$$C_{1\uparrow} = \frac{1}{2}\left[\mathrm{sgn}\left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right) - \mathrm{sgn}\left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right)\right] = 1$$

$$C_{1\downarrow} = \frac{1}{2}\left[\mathrm{sgn}\left(\lambda_v - 3\sqrt{3}\lambda_{SO}\right) - \mathrm{sgn}\left(\lambda_v + 3\sqrt{3}\lambda_{SO}\right)\right] = -1$$

total Chern number $C_{1\uparrow} + C_{1\downarrow} = 0$, but there must be spin currents because of $C_{1\uparrow} - C_{1\downarrow} \neq 0$

- *iii) for* $\lambda_v = 3\sqrt{3}\lambda_{SO}$
  - Spin up Hamiltonian is gapless at K' , but gapped at K
  - Spin down Hamiltonian is gapless at K , but gapped at K'

  So, total Hamiltonian is gapless both at K and K'

- Hence, there is a gapless state between two different topological phases.
- The transition point is $\lambda_v = 3\sqrt{3}\lambda_{SO}$ between two different topological phases (cases (i) and (ii)).

- For $\lambda_R \neq 0$, spin up and spin down will mix together and we cannot separate the whole system into two independent parts.
- So, the Chern number is not useful, and we need $\mathbb{Z}_2$ invariant to describe these phases.

• Helical Edge States

- At the boundary between a Kane-Mele topological insulator and a trivial insulator, helical gapless edge states occur:

  the spin and the direction of these states are tight together.

- Let us consider the Hamiltonian

$$h(k) = d_1(k)\Gamma_1 + d_2(k)\Gamma_2 + d_5(k)\Gamma_5$$

- In d=2 there are four TRIM points $\lambda_i \quad (i = 0,\ldots,3)$
- The mass term of the model is determined by $d_1(\lambda_0)$ and it has different signs for trivial and non-trivial insulators.

- We have an interface at y=0 between
  - A trivial insulator for y>0 where $d_1(\lambda_0) > 0$ and
  - A topological insulator for y<0 where $d_1(\lambda_0) < 0$

- By defining $m(y) = d_1(\lambda_0)(y)$

  we have $m(y>0)>0$ and $m(y<0)<0$
- The Hamiltonian has two edge states solutions

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

  - One is spin up right moving state
  - The other is spin down left moving state
- They constitute a Kramers pairs of edge states.

- If there are even number of pairs of edge states, we have a trivial insulator
- If there are odd number of pairs of edge states, we have a topological insulator.

- $\mathbb{Z}_2$ Invariants

- $\mathbb{Z}_2$ invariants are topological invariants that characterizes the topological classes of $\mathbb{Z}_2$ insulators.
- We have a TR symmetric Bloch Hamiltonian $h(k)$ and its eigenstates $|u_i(k)\rangle$. Because of TR symmetry $T|u_i(k)\rangle$ are also eigenstates.

- Let us define the sewing matrix

$$w_{ij}(k) = \langle u_i(-k)|T|u_j(k)\rangle$$

At TRIM points this matrix is antisymmetric.

- For an antisymmetric matrix A, Pfaffian can be defined by

$$(\text{Pf } A)^2 = \det A$$

- Hence, the Pfaffian of the sewing matrix at TRIM points Λ_k

$$\text{Pf }\left(w_{ij}(\Lambda_k)\right) = \text{Pf }\left(\langle u_i(\Lambda_k)|T|u_j(\Lambda_k)\rangle\right)$$

- The $\mathbb{Z}_2$ invariant is defined as

$$(-1)^{\nu} = \prod_{\lambda \in \Lambda_k} \frac{\mathrm{Pf}\left(w(\lambda)\right)}{\sqrt{\det w(\lambda)}}$$

- At all TRIM points the quantity $\mathrm{Pf}/\sqrt{\det}$ has the value ± 1.
- The product of ± 1 values gives $+1$ or -1 which corresponds to $\nu = 0$ or $\nu = 1$.

- For $\nu = 0$, topologically trivial class
- For $\nu = 1$, topologically non-trivial class

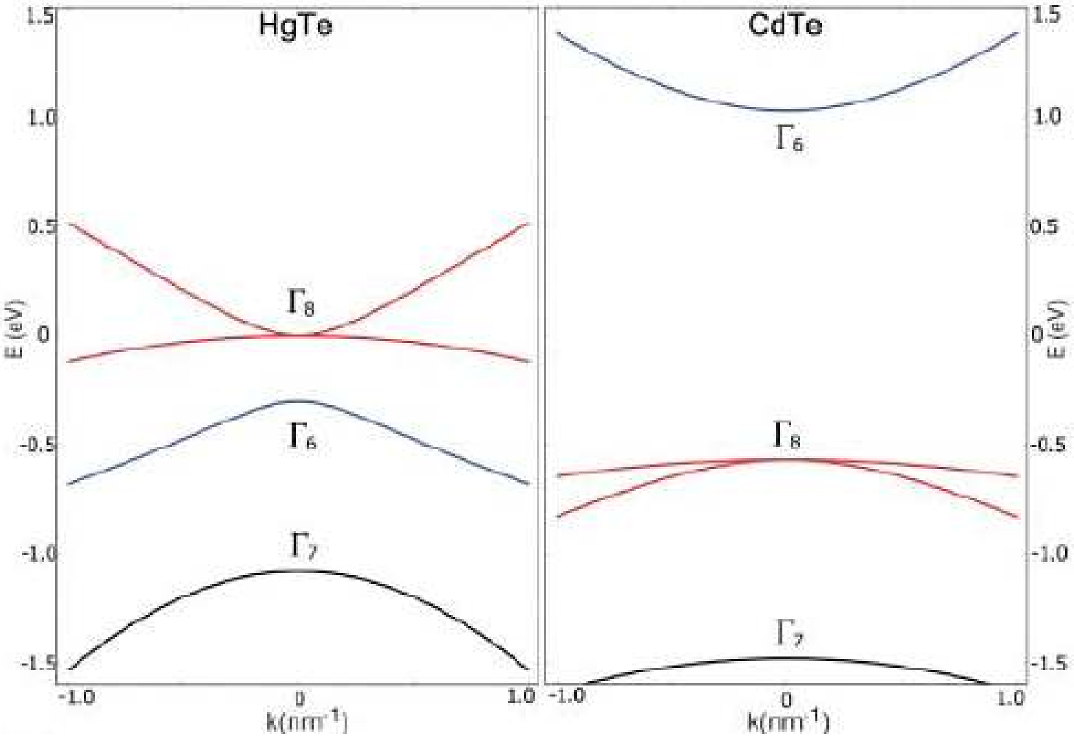
- The eigenstates $|u_i(k)\rangle$ of the Bloch Hamiltonian $h(k)$ at TRIM points Λ_k determine the topological property of the system.

- Since there are only two topological classes, they are called $\mathbb{Z}_2$ insulators. ($\mathbb{Z}_2$ is the group of two elements)

• Experimental Realizations: BHZ Model

- SO interaction for graphene is extremely small, so the $\mathbb{Z}_2$ insulator property is experimentally hard to achieve.
- However, effective model of HgTe/CdTe quantum wells gives an experimental realization.

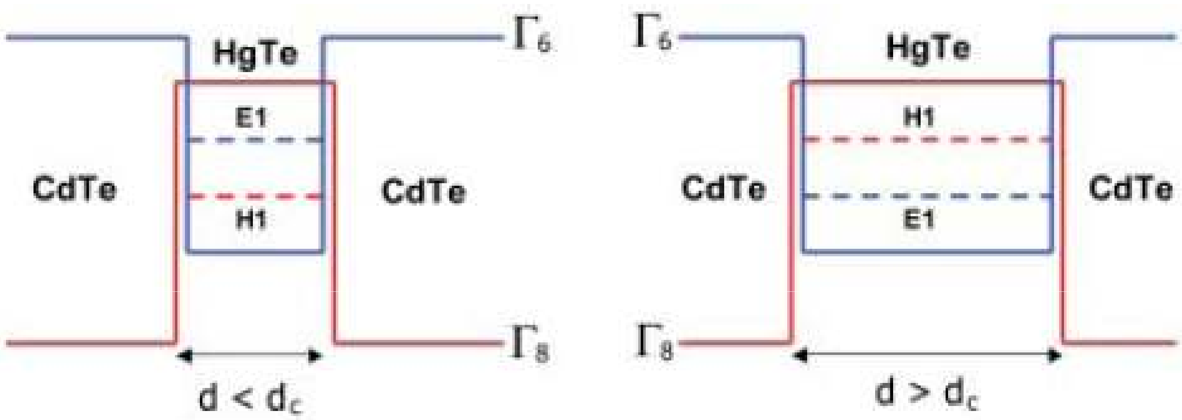
- Band structure of HgTe and CdTe near the Γ point



CdTe has a normal semi-conductor band progression which is Γ_6 s-type band lying above the Γ_8 p-type band.

HgTe has an inverted band progression, where s-type Γ_6 band lies below the p-type Γ_8 band.

- In a CdTe/HgTe/CdTe quantum well, $\Gamma_6 - \Gamma_8$ six bands combine to form an effective four-band model.



- E1 and H1 are linear combinations of $\Gamma_6 - \Gamma_8$ bands.
- If the thickness of the quantum well d is smaller than a critical thickness $d < d_c$ than $E1 > H1$ and if $d > d_c$ then $H1 > E1$.

- Effective Hamiltonian of the quantum well is written as

$$H_{eff}(k_x,k_y)=\begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}$$

where $h(k)=\varepsilon(k)I+d_i(k)\sigma_i$.

- The system has TR symmetry, we can split the spin up-down parts.

- Components of the spin up part are

$$\varepsilon(k)=C-Dk^2 \quad , \quad d_1(k)=Ak_x$$

$$d_2(k)=Ak_y \quad , \quad d_3(k)=M-Bk^2$$

- Hence we have

$$h(k)=C-Dk^2+A\left(k_x\sigma_x+k_y\sigma_y\right)+\left(M-Bk^2\right)\sigma_z$$

where A, B, C, D and M are material parameters and dependent on the thickness d of the quantum well.

- The signs of the A, B, C and D parameters does not change with d
- However, the sign of M changes at the critical thickness d_c . Because M is related to the difference between E1 and H1 bands.
- Hence, we have a sign changing mass term.

- The Chern numbers for spin up and down cases are found as

$$C_{1\uparrow} = \begin{cases} \pm 1 \;, & MB > 0 \;, \; d > d_c \\ 0 \;, & MB < 0 \;, \; d < d_c \end{cases}$$

$$C_{1\downarrow} = \begin{cases} \mp 1 \;, & MB > 0 \;, \; d > d_c \\ 0 \;, & MB < 0 \;, \; d < d_c \end{cases}$$

- So, we have a topological phase for QW thickness $d > d_c$.
- For $d < d_c$ we have ordinary insulating phase.

- For $d > d_c$ we have

$$C_{1\uparrow} + C_{1\downarrow} = 0 \quad \text{and} \quad C_{1\uparrow} - C_{1\downarrow} \neq 0$$

- Hence, there is spin current at the edge and there are helical edge states.
- So, this model is a $\mathbb{Z}_2$ topological insulator.

- This model is the first experimentally realized topological insulator. (Bernevig, Hughes and Zhang, Science 314, 1757 (2006)) (Molenkamp et al, Science 318, 766 (2007))

Summary

- Sign changing mass terms are responsable for the topological insulator property.
- Topological insulators are bulk insulating and edge conducting systems.
- To deform a Hamiltonian from one topological class to another, one must pass from a gapless metallic phase. (These are the edge states)
- There are two types of topological insulators: Chern insulators and $\mathbb{Z}_2$ insulators.
- Chern insulators are TR breaking systems and are characterized by integer topological invariants; Chern numbers. They have chiral edge states.
  Example: Haldane model.
- $\mathbb{Z}_2$ insulators are TR invariant systems and are characterized by two-valued topological invariants; $\mathbb{Z}_2$ invariants. They have helical edge states.
  Example: Kane-Mele model.
- There are experimentally realized materials that have topological insulator property.

… and what else?

- 3D topological insulators
- Classification and periodic table of TI
- Bundle theory and K-theory point of view to TI
- Topological field theory of TI
- Topological superconductors

References

- Books
- **Topological Insulators: Dirac Equation in Condensed Matters**, S.-Q. Shen, 2012
- **Topological Insulators and Topological Superconductors**, B. A. Bernevig and T. L. Hughes, 2013
- **Contemporary Concepts of Condensed Matter Science: Topological Insulators**, Eds. M. Franz and L. Molenkamp, 2014
- Reviews
- **Colloquium: Topological Insulators**, M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010)
- **Topological insulators and superconductors**, X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011)
- **Introduction to Dirac materials and topological insulators**, J. Cayssol, Comp. Rend. Phys. 14, 760 (2013)
- **An introduction to topological insulators**, M. Fruchart and D. Carpentier, Comp. Rend. Phys. 14, 779 (2013)