The Pauli Matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x^2 = 1, \sigma_y^2 = 1, \sigma_z^2 = 1$$

$$\sigma_y \sigma_z = -\sigma_z \sigma_y = i\sigma_x$$

$$\sigma_z \sigma_x = -\sigma_x \sigma_z = i\sigma_y$$

$$\sigma_x \sigma_y = -\sigma_x \sigma_y = i\sigma_z$$

Derive the spin transverse force

$$H = \frac{\mathbf{p}^2}{2m} + \lambda(\mathbf{p}_x\sigma_y - \mathbf{p}_y\sigma_x)$$

$$\mathbf{v} = \frac{1}{i\hbar}[\mathbf{r}, H]$$

$$m\frac{d\mathbf{v}}{dt}$$

Shen, PRL 95, 187203(2005)

The Dirac Equation in Topological Insulators & Superconductors

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A. Einstein, 1905

$$E = mc^2 \qquad m = \sqrt{m_0^2 + p^2 / c^2}$$

$$E^2 = m_0^2 c^4 + p^2 c^2$$

P. Dirac, 1928

$$H = cp \cdot \alpha + m_0 c^2 \beta$$

$$\alpha_i^2 = \beta^2 = 1$$

$$\alpha_i \beta = -\beta \alpha_i ; \alpha_i \alpha_j = -\alpha_j \alpha_i$$

In 1D:

α and β are any two Pauli matrices.

In 2D:

α and β are the three Pauli matrices.

In 3D:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Consequences:

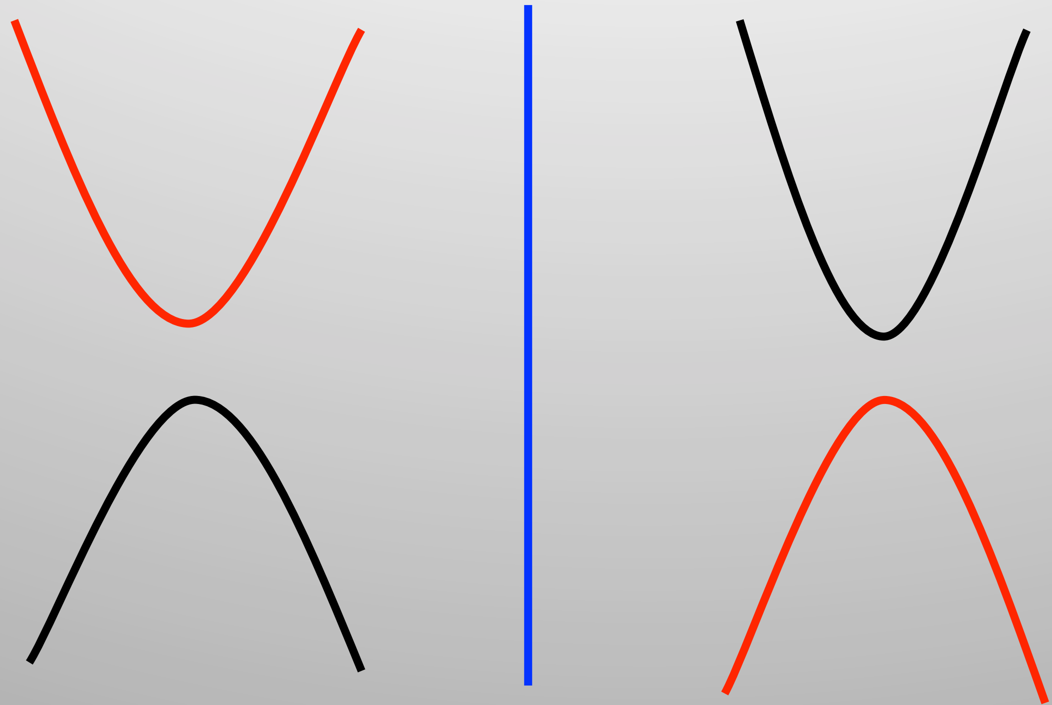
- Electron spin
- Positron: antiparticle
- Positive and negative energy
- ……

Based on the Pauli exclusion principle, Diarc proposed a many-body theory for electron.

Zero Energy Bound State: 1D example

Jackiw & Rebbi, PRD 13, 3398(76)

$+m_1$



$-m_2$

$$H = cp_x\sigma_x + m_1c^2\sigma_z \;|\; H = cp_x\sigma_x - m_2c^2\sigma_z$$

Zero-energy mode: $\Psi(x) = \sqrt{\frac{c}{\hbar}\frac{m_1m_2}{m_1+m_2}}\begin{pmatrix} i \\ 1 \end{pmatrix} e^{-m_i c|x|/\hbar}$

The stationary equation:

$$\begin{pmatrix} m(x)v^2 & -iv\hbar\partial_x \\ -iv\hbar\partial_x & -m(x)v^2 \end{pmatrix} \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = E \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix}.$$

For either $x < 0$ or $x > 0$, the equation is a second-order ordinary differential equation. We can solve the equation at $x < 0$ and $x > 0$ separately. The solution of the wave function should be continuous at $x = 0$. In order to have a solution of a bound state near the junction, we take the Dirichlet boundary condition that the wave function must vanish at $x = \pm\infty$. For $x > 0$, we set the trial wave function

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} e^{-\lambda_+ x} \quad \rightarrow \quad \det \begin{pmatrix} m_2v^2 - E & iv\hbar\lambda_+ \\ iv\hbar\lambda_+ & -m_2v^2 - E \end{pmatrix} = 0.$$

$$\lambda_+ = \pm\sqrt{m_2^2v^4 - E^2}/v\hbar$$

We choose a positive λ to satisfy the boundary condition. Similary, for x<0,

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = \begin{pmatrix} \varphi_1^- \\ \varphi_2^- \end{pmatrix} e^{+\lambda_- x}$$

Consider the continuity of the wave function at x=0: $\begin{pmatrix} \varphi_1^+ \\ \varphi_2^+ \end{pmatrix} = \begin{pmatrix} \varphi_1^- \\ \varphi_2^- \end{pmatrix}$

Zero energy solution!

$$E = 0$$

General solution: m(x) and E=0

$$\left[-iv\hbar\partial_x\sigma_x + m(x)v^2\sigma_z\right]\varphi(x) = 0.$$

Multiplying σ_x from the left-hand side, we have

$$\partial_x\varphi(x) = -\frac{m(x)v}{\hbar}\sigma_y\varphi(x).$$

Thus, the wave function should be the eigenstate of σ_y,

$$\sigma_y\varphi_\eta(x) = \eta\varphi_\eta(x)$$

with

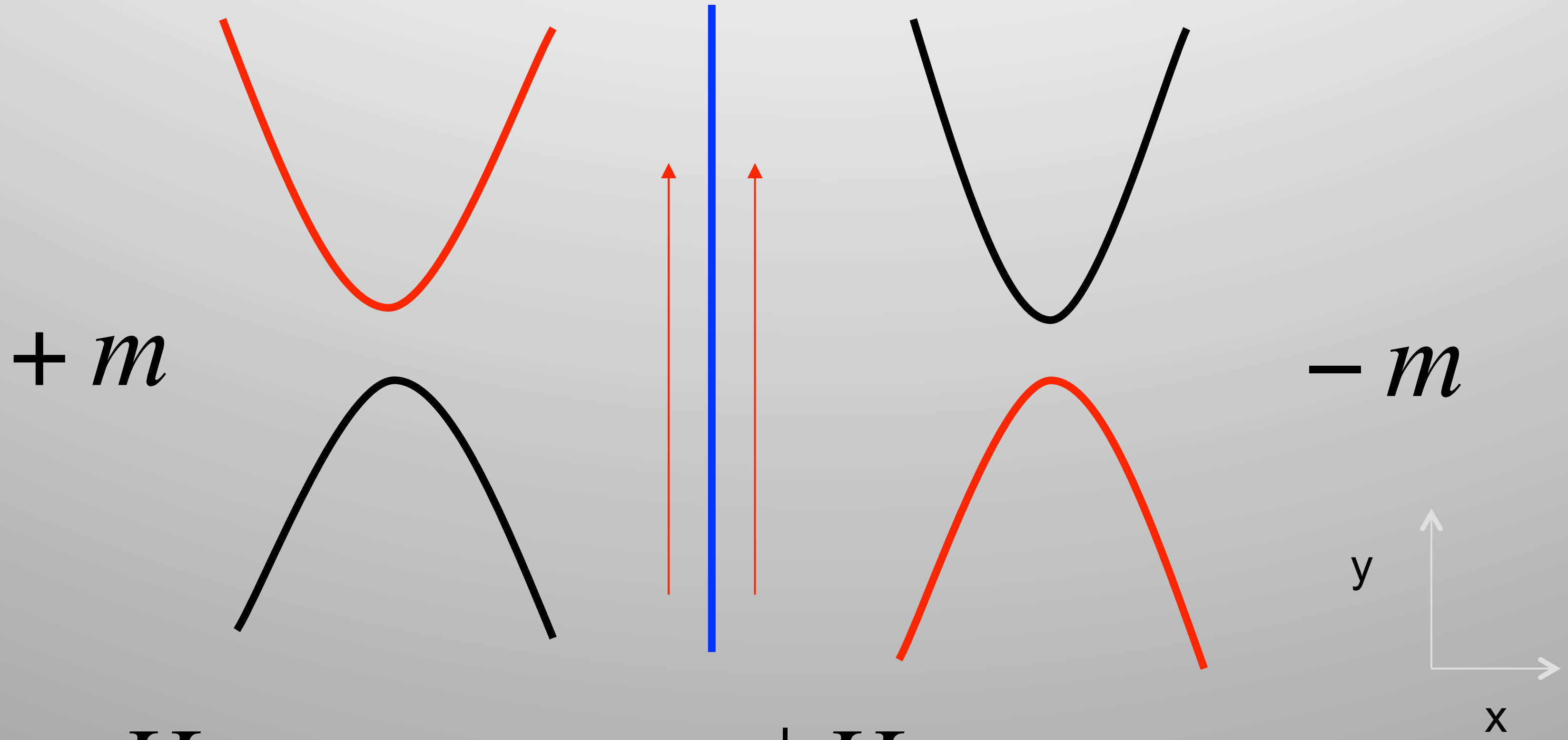
$$\varphi_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \end{pmatrix}\varphi(x).$$

The wave function has the form

$$\varphi_\eta(x) \propto \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \eta i \end{pmatrix}\exp\left[-\int^x \eta\frac{m(x')v}{\hbar}dx'\right].$$

The zero energy solution of the domain wall is robust against the distribution of the mass, but depends on the signs of m at the boundary far away from the domain wall. It is a solution of solition.

2D example: Chiral Bound State carrying 1 e^2/h conductance



$$H = p\cdot\sigma + m\sigma_z \mid H = p\cdot\sigma - m\sigma_z$$

Chiral mode:

$$\Psi(x,y) \propto \begin{pmatrix} i \\ 1 \end{pmatrix} e^{-(\lambda|x| + ik_y y)/\hbar}$$

Dispersion:

$$E = vp$$

Why Not Dirac Equation?

The Dirac equation is marginal: there is no difference in the equation between m_0 and $-m_0$.

$$H = cp \cdot \alpha + m_0 c^2 \beta$$

Symmetry:

$$m_0 \rightarrow -m_0$$

$$\beta \rightarrow -\beta$$

Modified Dirac Equation

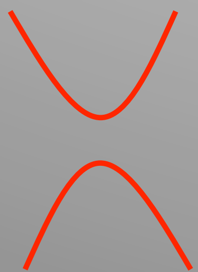
Shen, Shan and Lu, SPIN 1, 33 (2011)
arxiv: 1009.5502

$$H = vp\cdot\alpha + (mv^2 - Bp^2)\beta$$

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Under the time reversal,

$$p \to -p \qquad \alpha_i \to -\alpha_i \qquad \beta \to +\beta$$

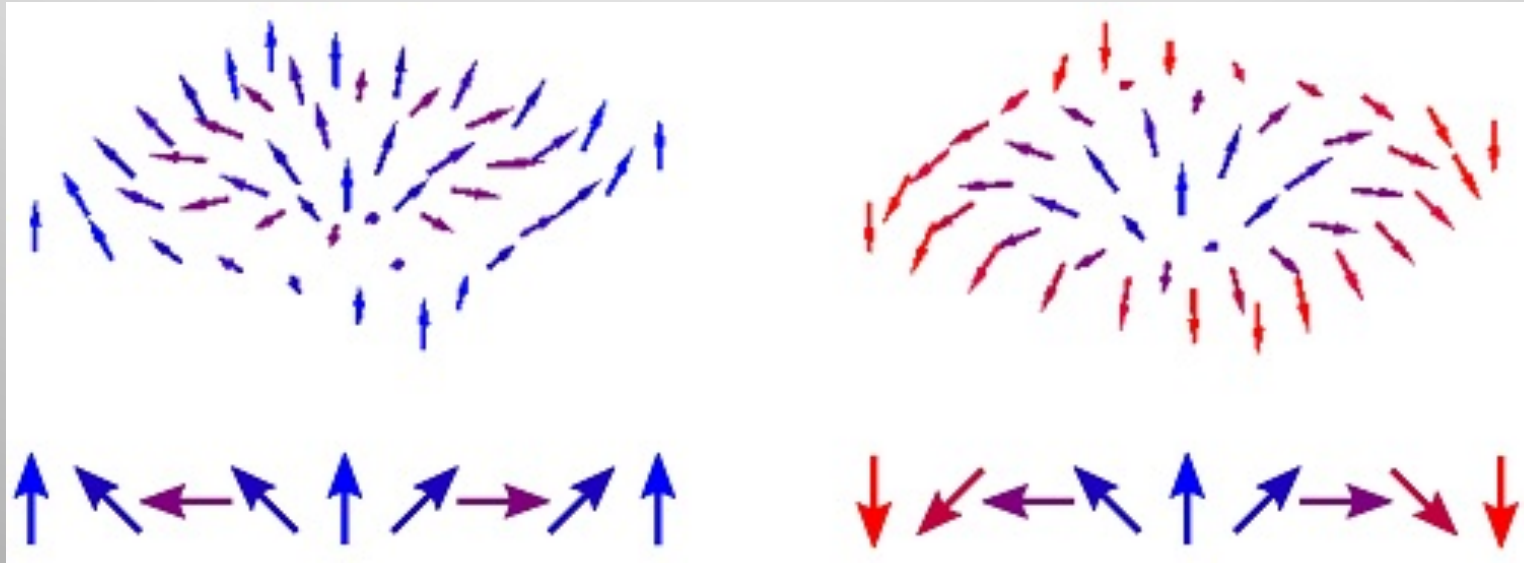


$$E_\pm = \pm\sqrt{p^2 v^2 + (mv^2 - Bp^2)^2}$$

$$J = L + \frac{\hbar}{2}\sigma$$

Spin Distribution in the momentum space

Lu et al, Phys. Rev. B 81, 115407 (2010)



$mB < 0$

Topologically trivial

$mB > 0$

Topologically non-trivial

$$H = vp \cdot \alpha + (mv^2 - Bp^2)\beta$$

Topological Invariant

The general solution:

$$\Psi_\nu = u_\nu(\mathbf{p}) \exp[i(\mathbf{p}\cdot\mathbf{r} - E_{p,\nu}t)/\hbar]$$

$$u_\nu(\mathbf{p}) = S u_\nu(\mathbf{p}=0)$$

$$S = \sqrt{\frac{\epsilon_p}{2E_{p,1}}}\begin{pmatrix} 1 & 0 & -\frac{p_z v}{\epsilon_p} & -\frac{p_- v}{\epsilon_p} \\ 0 & 1 & -\frac{p_+ v}{\epsilon_p} & \frac{p_z v}{\epsilon_p} \\ \frac{p_z v}{\epsilon_p} & \frac{p_- v}{\epsilon_p} & 1 & 0 \\ \frac{p_+ v}{\epsilon_p} & -\frac{p_z v}{\epsilon_p} & 0 & 1 \end{pmatrix}$$

The time reversal operator

$$\Theta \equiv -i\alpha_x\alpha_z\mathcal{K}$$

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

$$\{\langle u_\mu(\mathbf{p})|\,\Theta\,|u_\nu(\mathbf{p})\rangle\}$$

$$\begin{pmatrix} 0 & i\frac{mv^2-Bp^2}{E_{p,1}} & -i\frac{p_- v}{E_{p,1}} & i\frac{p_z v}{E_{p,1}} \\ -i\frac{mv^2-Bp^2}{E_{p,1}} & 0 & i\frac{p_z v}{E_{p,1}} & i\frac{p_+ v}{E_{p,1}} \\ i\frac{p_- v}{E_{p,1}} & -i\frac{p_z v}{E_{p,1}} & 0 & i\frac{mv^2-Bp^2}{E_{p,1}} \\ -i\frac{p_z v}{E_{p,1}} & -i\frac{p_+ v}{E_{p,1}} & -i\frac{mv^2-Bp^2}{E_{p,1}} & 0 \end{pmatrix}$$

The Pfaffian for two negative energy states:

$$P(\mathbf{p}) = i\frac{mv^2 - Bp^2}{\sqrt{(mv^2 - Bp^2)^2 + v^2p^2}}$$

According to Kane and Mele, an even or odd number of pairs of the zeros in Pfaffian defines the Z_2 invariant:

1 for mB>0 and 0 for mB<0.

Physical Systems

- 1D: Conducting polymer, p-wave superconductors, …….
- 2D: Quantum spin Hall effect, quantized anomalous Hall effect, p-wave superconductor, A-phase in Helium 3 liquid,……
- 3D: Topological insulators, B phase in Helium 3 liquid, p-wave superconductor,…..

Boundary solutions

1. One dimension: the end states of zero energy
2. Two dimensions: a chiral edge state or a pair of helical edge states
3. Three dimensions: a single Dirac cone of the surface state

One Dimension

$$H = vp_x \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + (mv^2 - Bp_x^2) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} mv^2 - Bp_x^2 & 0 & 0 & vp_x \\ 0 & mv^2 - Bp_x^2 & vp_x & 0 \\ 0 & vp_x & -mv^2 + Bp_x^2 & 0 \\ vp_x & 0 & 0 & -mv^2 + Bp_x^2 \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} mv^2 - Bp_x^2 & vp_x & 0 & 0 \\ vp_x & -mv^2 + Bp_x^2 & 0 & 0 \\ 0 & 0 & mv^2 - Bp_x^2 & vp_x \\ 0 & 0 & vp_x & -mv^2 + Bp_x^2 \end{pmatrix}$$

$$vp_x \sigma_x + (mv^2 - Bp_x^2)\sigma_z$$

$$\begin{pmatrix} mv^2 - Bp_x^2 & vp_x \\ vp_x & -mv^2 + Bp_x^2 \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = E \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

Find Bound State Solution!

$$\begin{pmatrix} mv^2 - Bp_x^2 & vp_x \\ vp_x & -mv^2 + Bp_x^2 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = E\begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

We take $\hbar$=1

$$p_x \rightarrow -i\hbar\partial_x \qquad \varphi,\chi \rightarrow e^{-\lambda x}$$

The Dirichlet Conditions

$$\left.\begin{pmatrix} \varphi \\ \chi \end{pmatrix}\right|_{x=+\infty} = \left.\begin{pmatrix} \varphi \\ \chi \end{pmatrix}\right|_{x=0} = 0$$

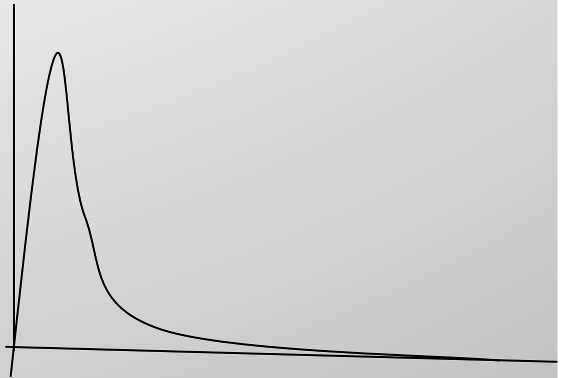
$$\det\begin{pmatrix} mv^2 + B\lambda^2 - E & vi\lambda \\ vi\lambda & -mv^2 - B\lambda^2 - E \end{pmatrix} = 0$$

$$E^2 - (mv^2 + B\lambda^2)^2 + v^2\lambda^2 = 0$$

Four roots: $\pm\lambda_+, \pm\lambda_-$

One Dimension: Zero Energy Solution

Zero mode solution $E = 0 \quad (L >> \lambda)$



$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = C \begin{pmatrix} \mathrm{sgn}(B) \\ i \end{pmatrix} (e^{-\lambda_+ x} - e^{-\lambda_- x})$$

Near x=0

$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = C \begin{pmatrix} \mathrm{sgn}(B) \\ i \end{pmatrix} (e^{-\lambda_+ (L-x)} - e^{-\lambda_- (L-x)})$$

Near x=L

Existing condition: $MB > 0$

$$\lambda_\pm = \frac{1}{2} \frac{|v|}{|B|} \left(1 \pm \sqrt{1 - 4mB}\right)$$

For a small gap: $\lambda_+^{-1} = \frac{\hbar B}{v} \qquad \lambda_-^{-1} = \frac{\hbar}{mv}$

Two Dimensions: Edge States

$$H = vp_x \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + vp_y \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} + (mv^2 - Bp^2) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} mv^2 - Bp^2 & 0 & 0 & vp_x - ivp_y \\ 0 & mv^2 - Bp^2 & vp_x + ivp_y & 0 \\ 0 & vp_x - ivp_y & -mv^2 + Bp^2 & 0 \\ vp_x + ivp_y & 0 & 0 & -mv^2 + Bp^2 \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} mv^2 - Bp^2 & vp_x - ivp_y & 0 & 0 \\ vp_x + ivp_y & -mv^2 + Bp^2 & 0 & 0 \\ 0 & 0 & mv^2 - Bp^2 & vp_x + ivp_y \\ 0 & 0 & vp_x - ivp_y & -mv^2 + Bp^2 \end{pmatrix}$$

Boundary Condition: the wave function vanishes at the boundary, $x = 0$ and p_y is a good a quantum number

Notice: the sign difference

$$\left[\begin{pmatrix} mv^2 - Bp_x^2 & vp_x \\ vp_x & -mv^2 + Bp_x^2 \end{pmatrix} + \begin{pmatrix} -Bp_y^2 & -ivp_y \\ +ivp_y & +Bp_y^2 \end{pmatrix}\right]\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = E\begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

$$p_x \longrightarrow -i\hbar\partial_x \qquad p_y \longrightarrow \hbar k_y$$

$$H_{2D} = H_{1D}(x) + V(\hbar k_y)$$

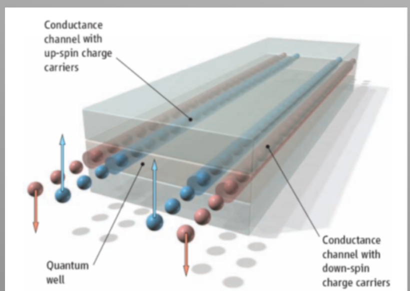
When $k_y = 0$, the equation is reduced to the equation for 1D and zero mode solution.

$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = C\begin{pmatrix} \mathrm{sgn}(B) \\ i \end{pmatrix}(e^{-\lambda_+ x} - e^{-\lambda_- x})$$

When $k_y \neq 0$, the dispersion becomes

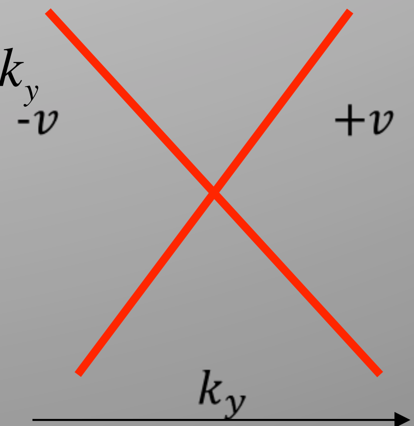
$$E_+(k_y) = \int dx(\varphi^*, \chi^*)\begin{pmatrix} -Bk_y^2 & -iv\hbar k_y \\ +iv\hbar k_y & Bk_y^2 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \mathrm{sgn}(B)v\hbar k_y$$

$$E_-(k_y) = \int dx(\varphi^*, \chi^*)\begin{pmatrix} -Bk_y^2 & +iv\hbar k_y \\ -iv\hbar k_y & Bk_y^2 \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = -\mathrm{sgn}(B)v\hbar k_y$$



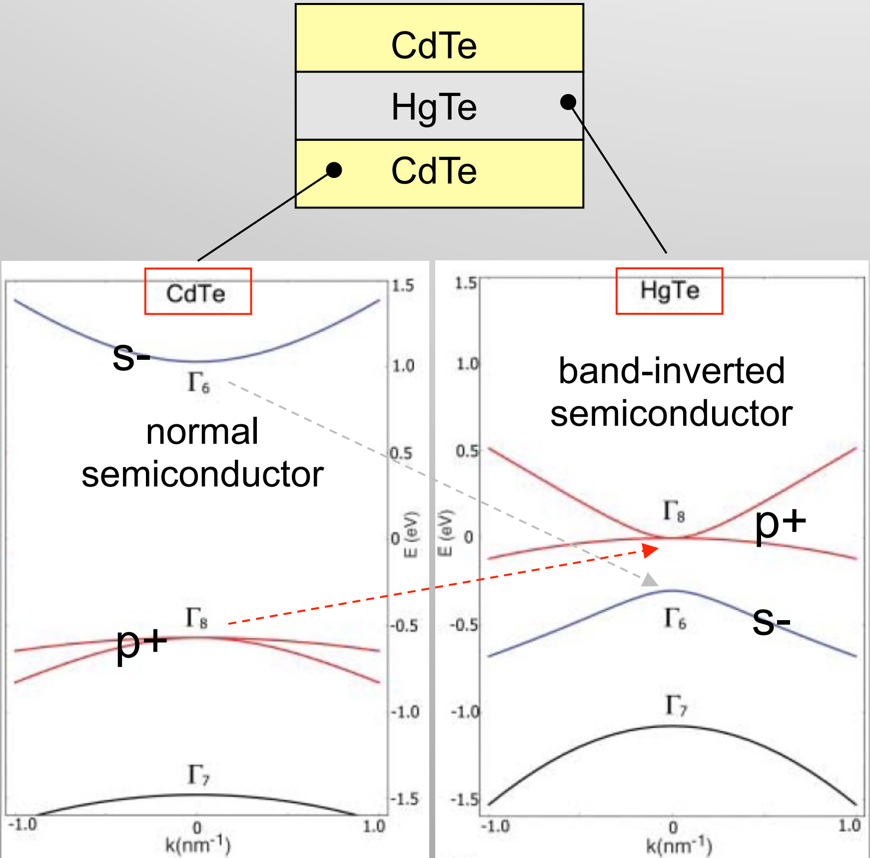
Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.

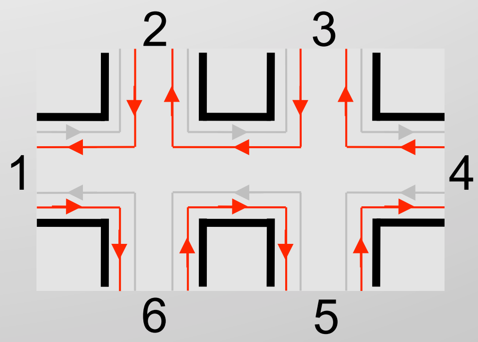
Solutions for helical edge states!
Quantum Spin Hall Effect!



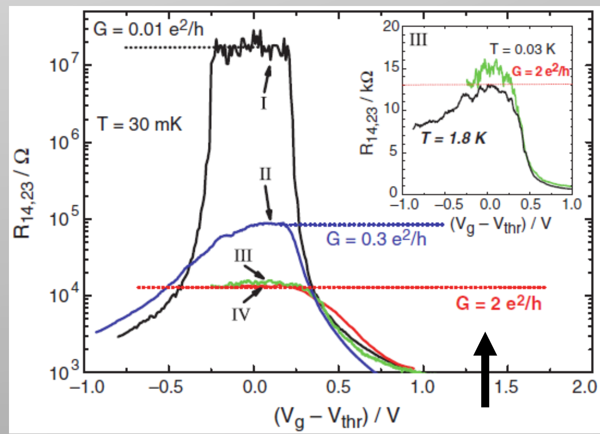
Quantum Spin Hall Effect

First 2D topological insulator (Quantum Spin Hall Effect): HgTe/CdTe quantum well





helical edge states



quantized transport due to the helical edge states

Theoretical predicted: Bernevig, Hughes,and Zhang, Science 314 1757 (2006)
Experimental confirmed: Konig et al, Science 318, 766 (2007); Roth et al, Science 325, 294 (2009);
Topical review: Konig et al, J. Phys. Soc. Jpn. 77, 031007 (2008)

Three dimension and surface states

$$H = vp_x\begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + vp_y\begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} + vp_z\begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} + (mv^2 - Bp^2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$H_0 = vp_x\begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + (mv^2 - Bp_x^2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$V(p_x, p_y) = vp_y\begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} + vp_y\begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} - (Bp_y^2 + Bp_z^2)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Two zero energy solutions for H_0

$$\Psi_1 = \begin{pmatrix} \varphi \\ 0 \\ 0 \\ \chi \end{pmatrix} \qquad \Psi_2 = \begin{pmatrix} 0 \\ \varphi \\ \chi \\ 0 \end{pmatrix}$$

The effective model for the surface states

$$H_{eff} = \begin{pmatrix} \langle\Psi_1|V|\Psi_1\rangle & \langle\Psi_1|V|\Psi_2\rangle \\ \langle\Psi_2|V|\Psi_1\rangle & \langle\Psi_2|V|\Psi_2\rangle \end{pmatrix}$$

$$H_{eff} = \mathrm{sgn}(B)v(p \times \sigma)_x$$

The Dirac Cone

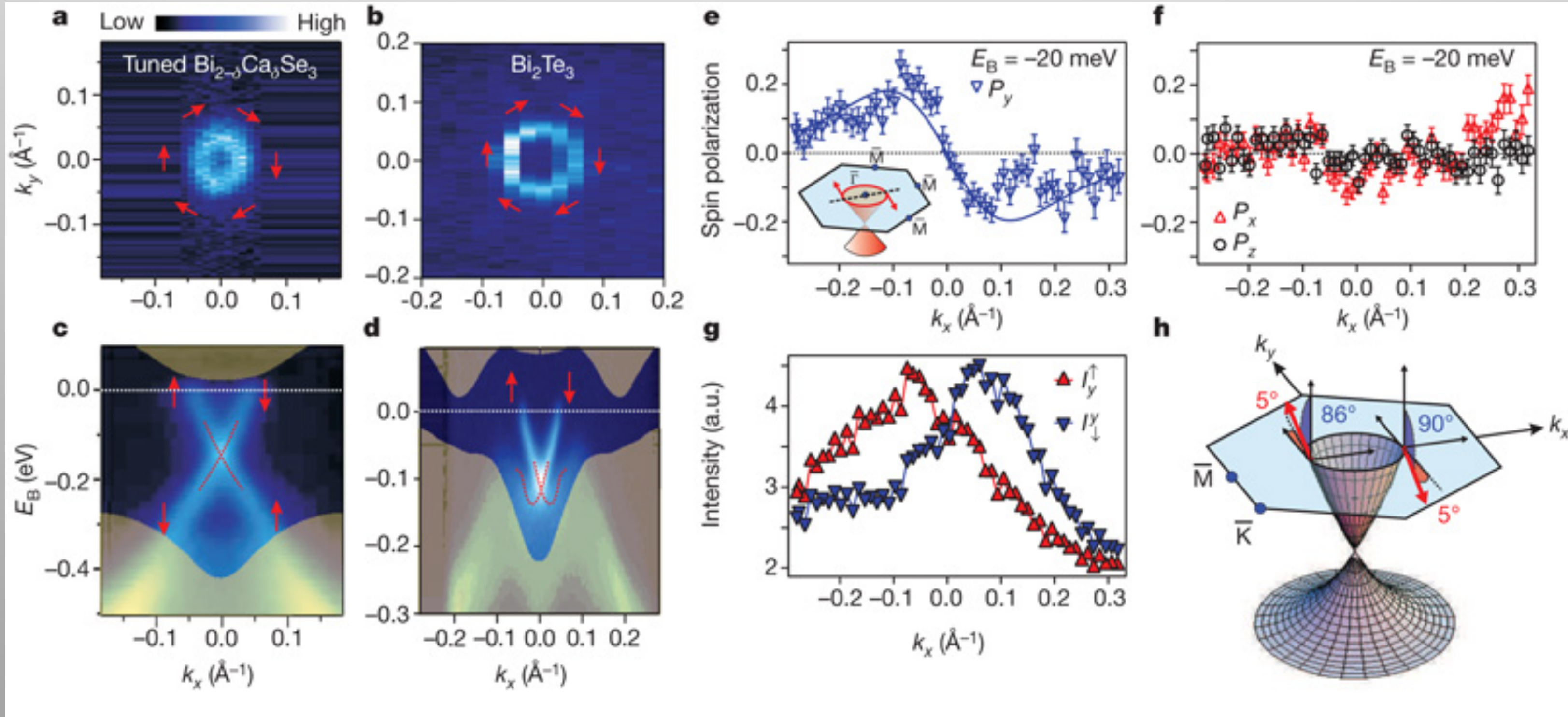
$$(\mathbf{p} \times \sigma)_x = p_y \sigma_z - p_z \sigma_y$$

$$(\mathbf{p} \times \sigma)_z = p_x \sigma_y - p_y \sigma_x$$

$$p_x \boldsymbol{\sigma}_x + p_y \boldsymbol{\sigma}_y$$

Detection of spin-momentum locking of spin-helical Dirac electrons in Bi_2Se_3 and Bi_2Te_3 using spin-resolved ARPES

D Hsieh *et al. Nature* **460**, 1101-1105 (2009)



From continuous to lattice model

Mapping the continuous model into a hyper-cubic lattice model:

$$k_i \to \frac{1}{a}\sin k_i a$$

$$k_i^2 \to \frac{4}{a^2}\sin^2\frac{k_i a}{2} = \frac{2}{a^2}\left(1-\cos k_i a\right)$$

The lattice model with the periodic boundary condition:

$$H(k) = \frac{\hbar v}{a}\sum_i \sin k_i a + \left(mv^2 - B\frac{4\hbar^2}{a^2}\sum_i \sin^2\frac{k_i a}{2}\right)\beta$$

Performing the Fourier transformation, one obtains a lattice model in the real space.
As the the mapping is only valid in the long wavelength limit, the two models are not exactly Identical.

Fourier Transformation

$$c_{i.\sigma} = \frac{1}{\sqrt{Na}} \sum_{k_n} e^{ik_n R_i} c_{k_n,\sigma}, \tag{3.2a}$$

$$c^\dagger_{i.\sigma} = \frac{1}{\sqrt{Na}} \sum_{k_n} e^{-ik_n R_i} c^\dagger_{k_n,\sigma}, \tag{3.2b}$$

and the periodic boundary condition gives $e^{ik_n R_i} = e^{ik_n(R_i+Na)}$ and $k_n = 2n\pi/Na$ ($n = 0, 1, \ldots, N-1$). In this way, the Hamiltonian can be diagonalized

Modified Dirac Model on a Hypercubic Lattice

$$H = \sum_{i,n,m} \Delta c_{i,n}^{\dagger} \beta_{nm} c_{i,m} - t \sum_{\langle i,j \rangle,} c_{j,n}^{\dagger} \beta_{nm} c_{i,m}$$

$$+ i t' \sum_{i,a,n,m} \left[c_{i+a,n}^{\dagger} (\alpha_a)_{nm} c_{i,m} - c_{i,n}^{\dagger} (\alpha_a)_{nm} c_{i+a,m} \right].$$

$$t' = \frac{\hbar v}{2a} = v/2,\ \Delta - 2dt = mv^2,\ t = -B\hbar^2/a^2 = -B.$$

Denote $(c_{i,1}^{\dagger}, c_{i,2}^{\dagger}, \ldots, c_{i,D}^{\dagger})$ by $c_i^{\dagger}$. In this way, the equation can be written in a compact form

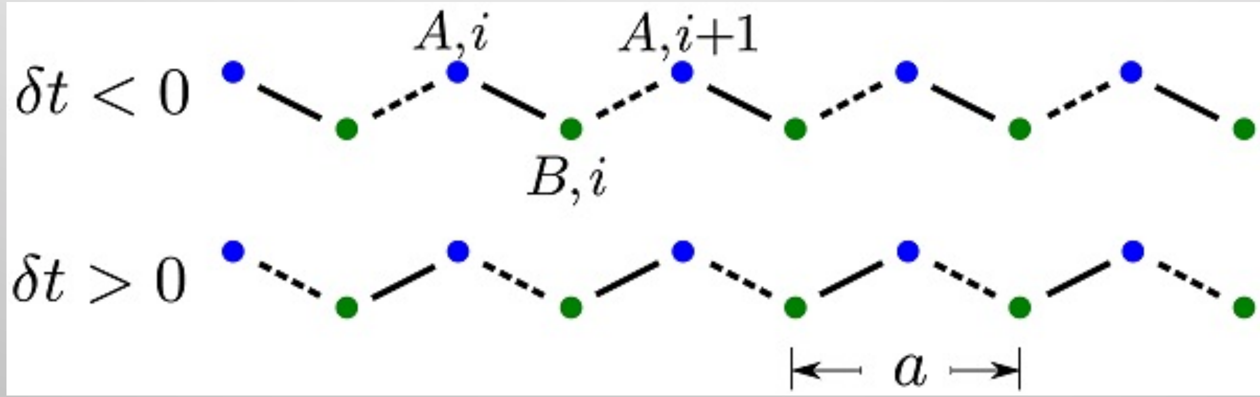
$$H = \sum_{i} \Delta c_i^{\dagger} \beta c_i - t \sum_{\langle i,j \rangle,} c_j^{\dagger} \beta c_i + i t' \sum_{i,a} \left[c_{i+a}^{\dagger} \alpha_a c_i - c_i^{\dagger} \alpha_a c_{i+a} \right]. \qquad (3.10)$$

Find an edge or surface state solution

- Make use of of the Fourier transformation to reduce the issue to a one-dimensional problem.
- Consider a strip or a finite thick film

Several Physical Systems

Su-Schrieffer-Heeger Model



$$H = \sum_{n=1}^{N} (t + \delta t) c_{A,n}^{+} c_{B,n} + \sum_{n=1}^{N-1} (t - \delta t) c_{A,n}^{+} c_{B,n+1} + h.c.$$

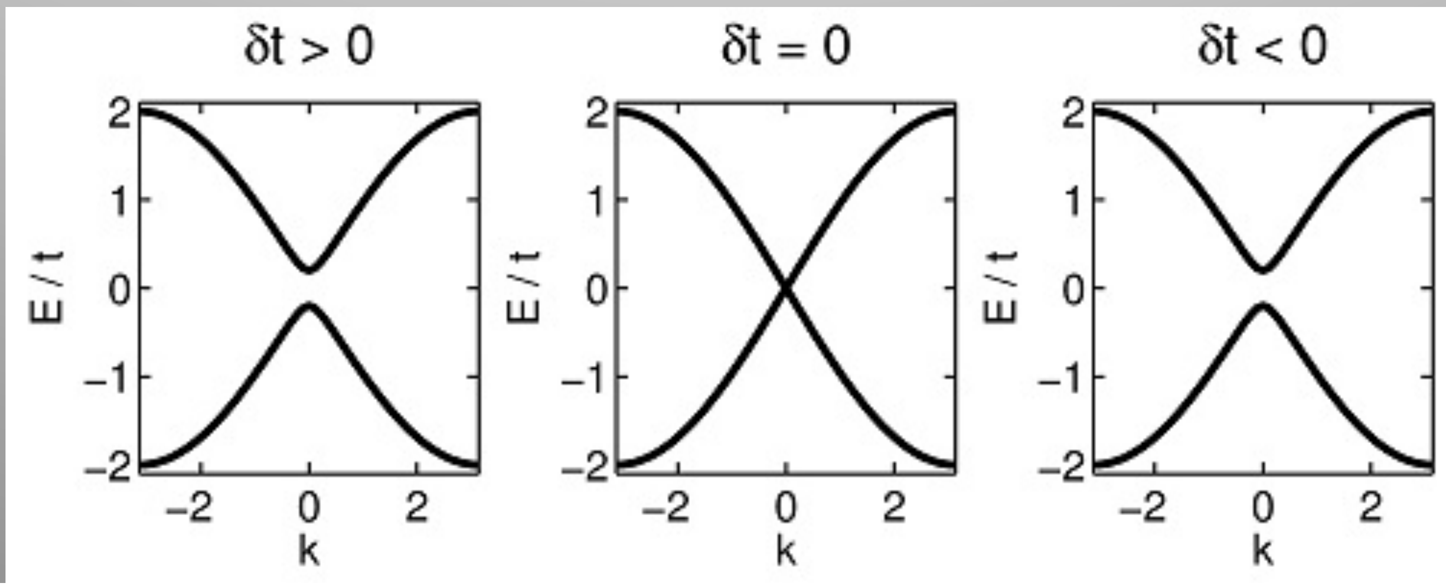
Gap Closing and Re-Opening

Fourier transformation: $a_k = \frac{1}{\sqrt{N}} \sum \exp[-ik \cdot R_n] c_{A,n}; b_k = \frac{1}{\sqrt{N}} \sum \exp[-ik \cdot R_n] c_{B,n}$

$$H = \sum_k (a_k^+, b_k^+) \begin{pmatrix} 0 & (t+\delta t) + (t-\delta t)e^{-ik} \\ (t+\delta t) + (t-\delta t)e^{+ik} & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$$H(k) = \left[(t+\delta t) + (t-\delta t)\cos k\right]\sigma_x + (t-\delta t)\sin k \sigma_y$$

$$E_\pm = \pm\sqrt{[(t+\delta t) + (t-\delta t)\cos k]^2 + (t-\delta t)^2 \sin^2 k}$$



From SSH to Dirac equation

$$H(k) = \left[(t+\delta t) + (t-\delta t)\cos k\right]\sigma_x + (t-\delta t)\sin k\sigma_y$$

Taking the replacement $k \rightarrow k+\pi$

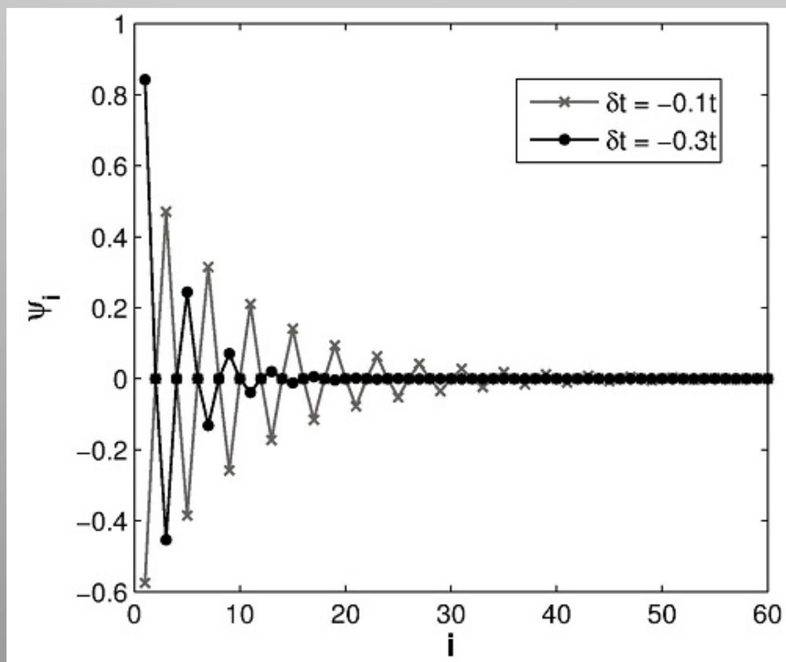
$$H(k) = -(t-\delta t)\sin k\sigma_y + \left[2\delta t + 2(t-\delta t)\sin^2\frac{k}{2}\right]\sigma_x$$

For a small k, using $\sin x \approx x$

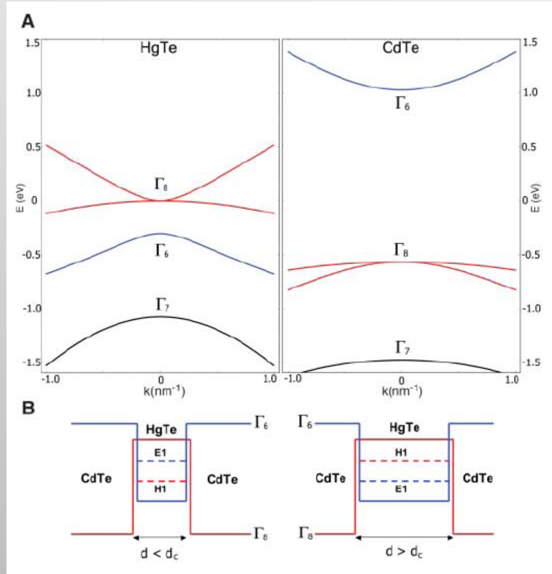
$$H(k) = -(t-\delta t)k\sigma_y + \left[2\delta t + \frac{1}{2}(t-\delta t)k^2\right]\sigma_x$$

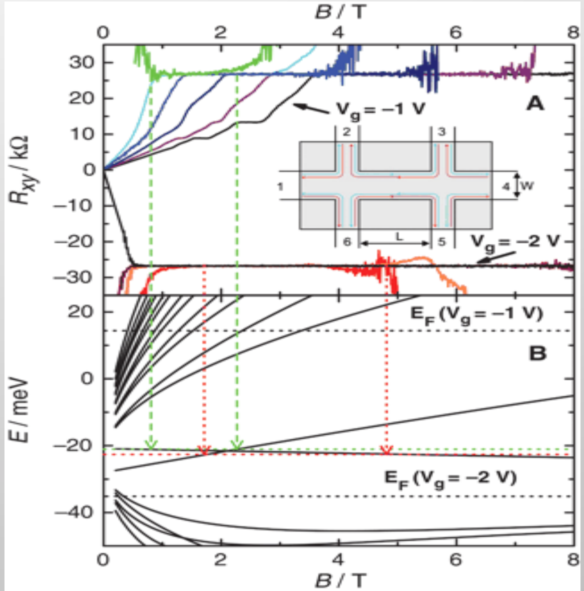
Numerical Calculation

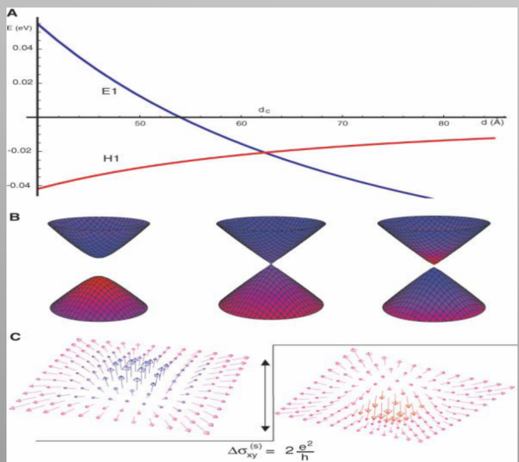
$$H = \begin{pmatrix} 0 & t+\delta t & 0 & 0 & 0 & 0 & 0 \\ t+\delta t & 0 & t-\delta t & 0 & 0 & 0 & 0 \\ 0 & t-\delta t & 0 & t+\delta t & 0 & 0 & 0 \\ 0 & 0 & t+\delta t & 0 & t-\delta t & 0 & 0 \\ 0 & 0 & 0 & t-\delta t & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 & t+\delta t \\ 0 & 0 & 0 & 0 & 0 & t+\delta t & 0 \end{pmatrix}$$

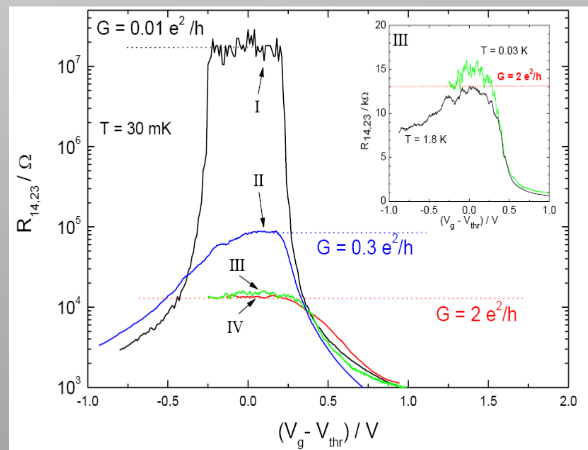


QSHE in HgTe/CdTe Quantum Well





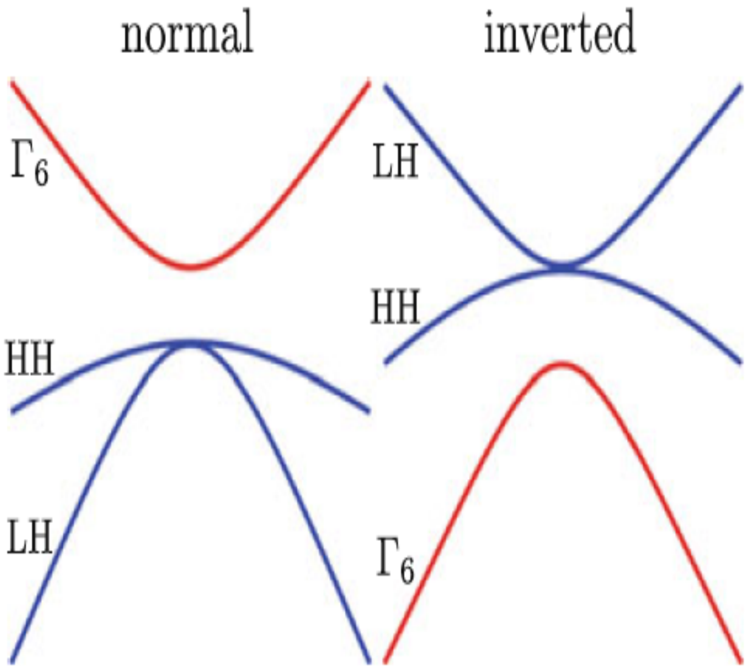




Bernevig et al, Science 314, 1757 (2006)

Konig et al, Science 318, 766 (2007)

Bernevig-Hughes-Zhang Model



$$u_1(\mathbf{r}) = \left|\Gamma_6, +\frac{1}{2}\right\rangle_c = S\uparrow,$$

$$u_2(\mathbf{r}) = \left|\Gamma_6, -\frac{1}{2}\right\rangle_c = S\downarrow,$$

$$u_3(\mathbf{r}) = \left|\Gamma_8, +\frac{3}{2}\right\rangle_v = \frac{1}{\sqrt{2}}(X + iY)\uparrow,$$

$$u_4(\mathbf{r}) = \left|\Gamma_8, +\frac{1}{2}\right\rangle_v = \frac{1}{\sqrt{6}}\left[(X + iY)\downarrow - 2Z\uparrow\right],$$

$$u_5(\mathbf{r}) = \left|\Gamma_8, -\frac{1}{2}\right\rangle_v = -\frac{1}{\sqrt{6}}\left[(X - iY)\uparrow + 2Z\downarrow\right],$$

$$u_6(\mathbf{r}) = \left|\Gamma_8, -\frac{3}{2}\right\rangle_v = -\frac{1}{\sqrt{2}}(X - iY)\downarrow.$$

6 X 6 Kane Model

$$H = \begin{pmatrix} T & 0 & -\frac{1}{\sqrt{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{6}}Pk_- & 0 \\ 0 & T & 0 & -\frac{1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{2}}Pk_- \\ -\frac{1}{\sqrt{2}}Pk_- & 0 & U+V & -S_- & R & 0 \\ \sqrt{\frac{2}{3}}Pk_z & -\frac{1}{\sqrt{6}}Pk_- & -S_-^\dagger & U-V & 0 & R \\ \frac{1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & R^\dagger & 0 & U-V & S_+^\dagger \\ 0 & \frac{1}{\sqrt{2}}Pk_+ & 0 & R^\dagger & S_+ & U+V \end{pmatrix}$$

$$k_\parallel^2 = k_x^2 + k_y^2, k_\pm = k_x \pm i k_y,$$

$$T = E_c(z) + \frac{\hbar^2}{2m_0}\left[(2F+1)k_\parallel^2 + k_z(2F+1)k_z\right]$$

$$U = E_v(z) - \frac{\hbar^2}{2m_0}\left(\gamma_1 k_\parallel^2 + k_z\gamma_1 k_z\right),$$

$$V = -\frac{\hbar^2}{2m_0}\left(\gamma_2 k_\parallel^2 - 2k_z\gamma_2 k_z\right),$$

$$R = -\frac{\hbar^2}{2m_0}\frac{\sqrt{3}}{2}\left[(\gamma_3 - \gamma_2)k_+^2 - (\gamma_3 + \gamma_2)k_-^2\right],$$

$$S_\pm = -\frac{\hbar^2}{2m_0}\sqrt{3}k_\pm(\gamma_3 k_z + k_z\gamma_3).$$

Outline to derive an effective model

- Quantum well structure: CdTe/HgTe/CdTe
- Find the bound states at $k_x=k_y=0$
- Using the solutions of the bound states of $k_x=k_y=0$ as thebasis

For $k_x = k_y = 0$,

$$H(k_\parallel = 0) = \begin{pmatrix} T & 0 & 0 & \sqrt{\frac{2}{3}}Pk_z & 0 & 0 \\ 0 & T & 0 & 0 & \sqrt{\frac{2}{3}}Pk_z & 0 \\ 0 & 0 & U+V & 0 & 0 & 0 \\ \sqrt{\frac{2}{3}}Pk_z & 0 & 0 & U-V & 0 & 0 \\ 0 & \sqrt{\frac{2}{3}}Pk_z & 0 & 0 & U-V & 0 \\ 0 & 0 & 0 & 0 & 0 & U+V \end{pmatrix}$$

On the subsector of $\{u_1, u_4\}$ for $j_z = \frac{1}{2}$

$$H_{\text{eff}} = \begin{pmatrix} T & \sqrt{\frac{2}{3}}Pk_z \\ \sqrt{\frac{2}{3}}Pk_z & U-V \end{pmatrix},$$

on the base $\{u_3\}$ of $j_z = \frac{3}{2}$

$$H_{eff} = U + V$$

φ_1 φ_2

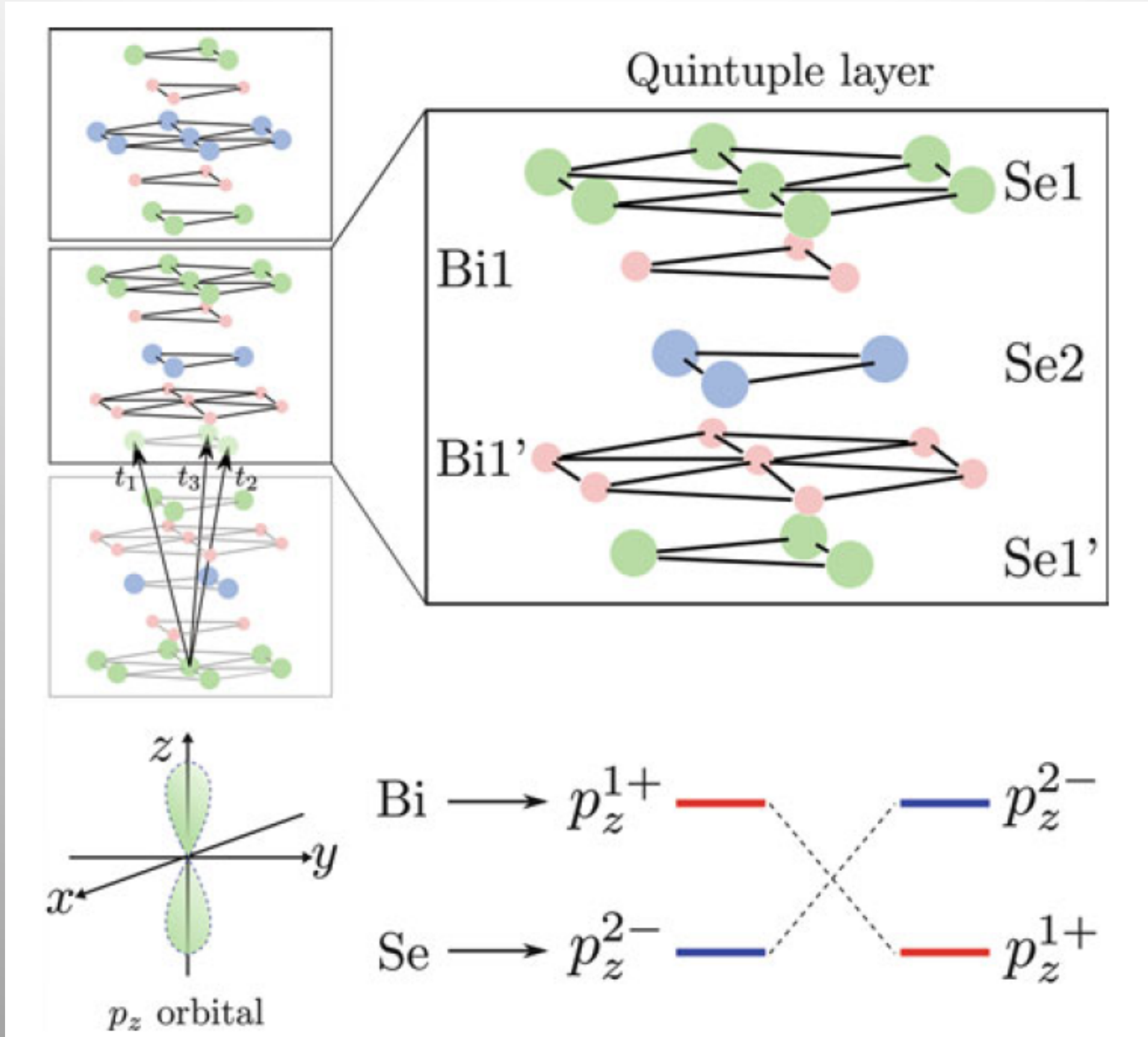
a solution for quantum well φ_2. Using these two states, one can have an effective Hamiltonian near the point of $k \neq 0$,

$$h(k) = (\langle\varphi_1| \, , \langle\varphi_2|) H(k) \begin{pmatrix} |\varphi_1\rangle \\ |\varphi_2\rangle \end{pmatrix}. \tag{6.66}$$

(u_2, u_5, u_6) gives other two states. In this way, Bernevig, Hughes, and Zhang derived an effective model for a quantum well of HgTe/CdTe [12],

$$H_{\mathrm{BHZ}} = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix} \tag{6.67}$$

where $h(k) = \epsilon(k) + A(k_x\sigma_x + k_y\sigma_y) + (M - Bk^2)\sigma_z$.



Crystal Structure of Bi_2Se_3

The three-dimensional Dirac equation can be applied to describe a large family of three-dimensional topological insulators. Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 have been confirmed to be topological insulators with a single Dirac cone of surface states. For example, in Bi_2Te_3, the electrons near the Fermi surfaces, mainly come from the p orbitals of Bi and Te atoms. According to the point group symmetry of the crystal lattice, p_z orbital splits from $p_{x,y}$ orbitals. Near the Fermi surface the energy levels turn out to be the p_z orbital, $|P1_z^+, \uparrow\rangle$, $|P1_z^+, \downarrow\rangle$, $|P2_z^-, \uparrow\rangle$, and $|P2_z^-, \downarrow\rangle$, where $\pm$ stand for the parity of the corresponding states and $\uparrow, \downarrow$ for the electron spin. Four low-lying states at the Γ point can be used a basis to construct the low-energy effective Hamiltonian [11]. In the basis of ($|P1_z^+, \uparrow\rangle$, $|P1_z^+, \downarrow\rangle$, $|P2_z^-, \uparrow\rangle$, $|P2_z^-, \downarrow\rangle$), we keep the terms up to the quadratic order in p and obtain

$$H = \epsilon(p) + \sum_{i=x,y,z} v_i p_i \alpha_i + \left(M - \sum_{i=x,y,z} B_i p_i^2 \right) \beta \tag{7.1}$$

P-wave pairing superconductor

In Bardeen-Copper-Schrieffer theory for superconductivity, the effective Hamiltonian has the form

$$H_{eff} = \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_k^+ c_k + \sum_k \frac{1}{2} \left(\Delta_k^* c_{-k} c_k + \Delta_k c_k^+ c_{-k}^+ \right)$$

$$H_{eff} = \frac{1}{2} \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_k^+ c_k + \frac{1}{2} \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_{-k}^+ c_{-k} + \sum_k \frac{1}{2} \left(\Delta_k^* c_{-k} c_k + \Delta_k c_k^+ c_{-k}^+ \right)$$

From the anti-commutation relation $c_{-k}^+ c_{-k} = 1 - c_{-k} c_{-k}^+$

$$H_{eff} = \frac{1}{2} \sum_k (c_k^+, \quad c_{-k}) \begin{pmatrix} \frac{\hbar^2 k^2}{2m} - \mu & \Delta_k \\ \Delta_k^* & -\frac{\hbar^2 k^2}{2m} + \mu \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^+ \end{pmatrix}$$

$$\varepsilon_k = \pm \frac{1}{2} \sqrt{\left| \Delta_k \right|^2 + \left(\frac{\hbar^2 k^2}{2m} - \mu \right)^2}$$

Bogoliubov-de Gennes Equation

The BCS wave function:

$$\left|BCS\right\rangle = \prod_{k'}\left(u_k + v_k c_k^+ c_{-k}^+\right)\left|0\right\rangle$$

with $\left|u_k\right|^2 + \left|v_k\right|^2 = 1$

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} - \mu & -\Delta_k^* \\ -\Delta_k & -\frac{\hbar^2 k^2}{2m} + \mu \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \varepsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

$$i\hbar\partial_t \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 k^2}{2m} - \mu & -\Delta_k^* \\ -\Delta_k & -\frac{\hbar^2 k^2}{2m} + \mu \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

p-wave superconductor & Dirac Equation

For a p-wave pairing superconductor,

$$\sum_k \Delta_k c_k^+ c_{-k}^+ = \sum_{-k} \Delta_{-k} c_{-k}^+ c_k^+ = -\sum_{-k} \Delta_{-k} c_k^+ c_{-k}^+$$

$$\Delta_k = -\Delta_{-k}$$

1D: $\Delta_k = \Delta_0 k$

$$K_{eff} = -\Delta_0 k \sigma_x + \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \sigma_z$$

2D (p+ip)-wave: $\Delta_k = \Delta_0 (k_x + i k_y)$

$$K_{eff} = -\Delta_0 \left(k_x \sigma_x + k_y \sigma_y \right) + \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \sigma_z$$

Bogoliubov Transformation

$$\gamma_k^+ = u_k c_k^+ + v_k c_{-k};$$

$$\gamma_k = u_k^* c_k + v_k^* c_{-k}^+$$

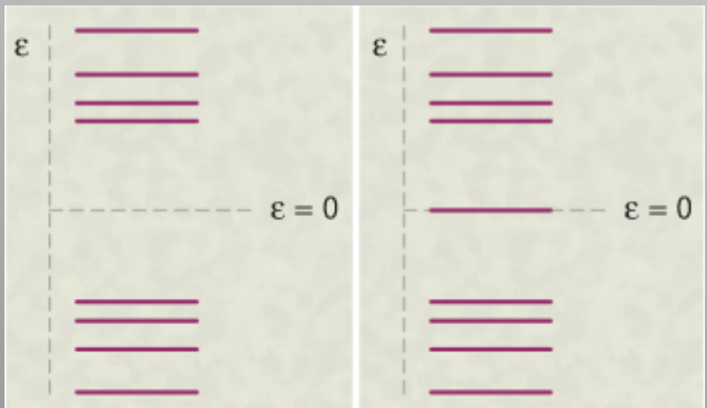
Majorana Fermions

$$\gamma_k^+ = \gamma_{-k}, u_k = v_{-k}^*$$

One-dimensional end state solution & Majorana fermions

$$K_{eff} = \Delta_0 i\partial_x \sigma_x - \left(\frac{\hbar^2}{2m}\partial_x^2 + \mu \right)\sigma_z$$

There is one solution near x=0 and one near x=L for mμ>0. The two solutions are degenerated. Due to the particle –hole symmetry, there is only one state, in which one half is located at x=0 and the other half is located at x=L.



$$\Delta = \langle \psi_0^+ | H | \psi_0^- \rangle, \langle \psi_0^\pm | H | \psi_0^\pm \rangle = 0$$

$$E_\pm = \pm|\Delta|$$

$$\psi_\pm = \frac{1}{\sqrt{2}}\left[\psi_0^+ \pm \frac{\Delta}{|\Delta|}\psi_0^- \right]$$

Vortex and Majorana fermion

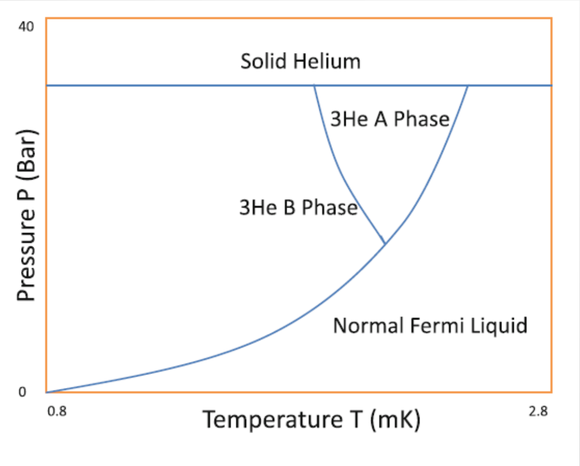
$$\Psi_{j=0} = \begin{pmatrix} f(r)e^{-i\theta/2} \\ g(r)e^{+i\theta/2} \end{pmatrix} \qquad \phi(r) = \sqrt{r}\begin{pmatrix} f \\ g \end{pmatrix}$$

$$\left[i\Delta\partial_r\sigma_x + \left(-\mu - \frac{\hbar^2}{2m}\partial_r^2 \right)\sigma_z \right]\phi(r) = E\phi(r)$$

It is exactly equivalent to the 1D modified Dirac equation! There are one zero energy modes near r=R for mB>0. Due to the particle-hole symmetry, the real bound state has one half near the centre and one half near the boundary.

The quasi-particle is a linear combination of particle and holes: its creation operator is equal to its annihilation operator, i.e., Majorana fermion.

Superfluid He-3: A and B phase



$$\Delta_+(\mathbf{k}) = \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}') \langle c_{-\mathbf{k}',\uparrow} c_{\mathbf{k}',\uparrow} \rangle$$

$$\Delta_0(\mathbf{k}) = \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}') \langle c_{-\mathbf{k}',\uparrow} c_{\mathbf{k}',\downarrow} \rangle$$

$$\Delta_-(\mathbf{k}) = \sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}') \langle c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\downarrow} \rangle$$

He-3 B phase

$$\Delta_{+1}(\mathbf{k}) = \Delta(-k_x + i k_y);$$
$$\Delta_0(\mathbf{k}) = \Delta k_z;$$
$$\Delta_{-1}(\mathbf{k}) = \Delta(k_x + i k_y).$$

$$\psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k},\uparrow}^\dagger, c_{\mathbf{k},\downarrow}^\dagger, c_{-\mathbf{k},\downarrow}, -c_{-\mathbf{k},\uparrow})$$

$$H_{\text{eff}} = \Delta\left(k_x\alpha_x + k_y\alpha_y + k_z\alpha_z\right) + \xi_{\mathbf{k}}\beta$$

He-3 A phase: Equal Spin Pairing

$$H_\uparrow = \frac{1}{2}\sum_{\mathbf{k}} (c_{\mathbf{k},\uparrow}^\dagger, c_{-\mathbf{k},\uparrow}) \left(\Delta k_x \sigma_x - \Delta k_y \sigma_y + \xi_{\mathbf{k}} \sigma_z\right) \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{-\mathbf{k},\uparrow}^\dagger \end{pmatrix}$$

$$\xi_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2) - \left(\mu - \frac{\hbar^2 k_z^2}{2m}\right)$$

Model for Weyl Semimetal

$$H = \begin{bmatrix} \mathcal{M}_{\mathbf{k}} & A(k_x - ik_y) \\ A(k_x + ik_y) & -\mathcal{M}_{\mathbf{k}} \end{bmatrix}$$

$$\mathcal{M}_{\mathbf{k}} = M_0 - M_1(k_x^2 + k_y^2 + k_z^2)$$

It is a massive Dirac equation with mass $M_0 - M_1 k_z^2$

or an effective model for A-phase of liquid He3 superfluidity.

S. Q. Shen, Topological Insulators (Springer, Berlin, 2012)

$M_0 M_1 > 0$ $\quad\quad \mathcal{M}_{\mathbf{k}} = M_1[k_c^2 - k_x^2 - k_y^2 - k_z^2]$

There exist two crossing points at $(0, 0, \pm k_c)$

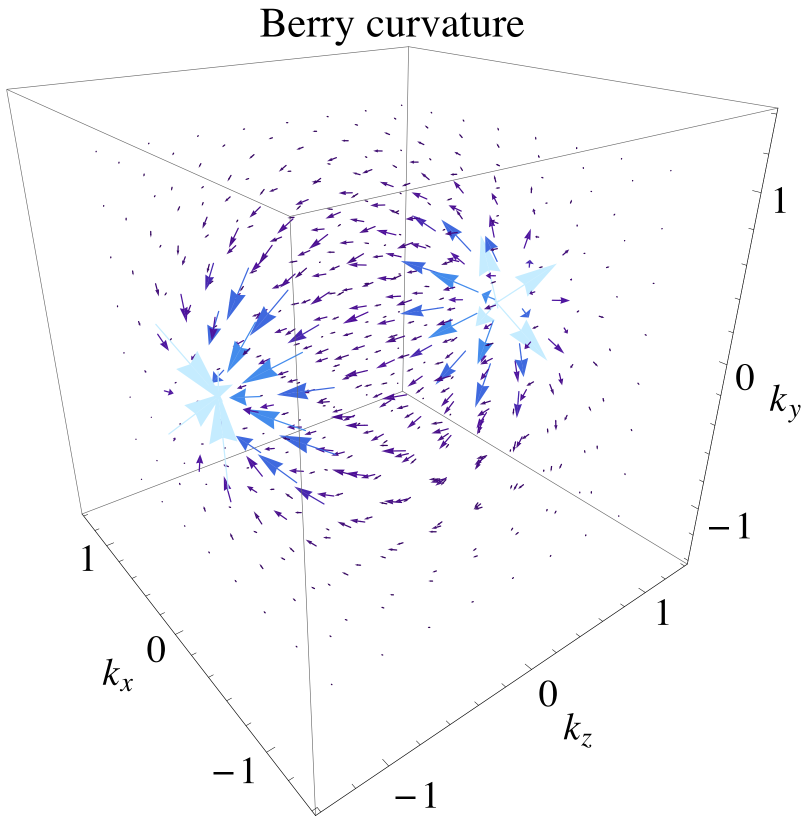
Near the two points the model is reduced to

$$H_\pm = \mathbf{M}_\pm \cdot \sigma$$

$$\mathbf{M}_\pm = \left(A\widetilde{k}_x, A\widetilde{k}_y, \mp 2M_1 k_c \widetilde{k}_z\right)$$

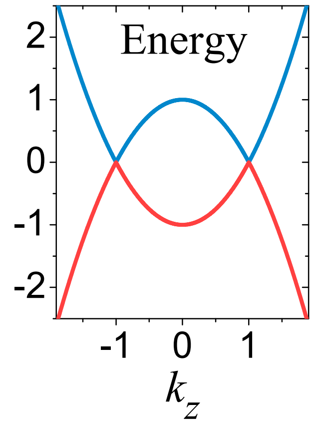
Berry Curvature

$$\mathbf{\Omega}(\mathbf{k}) = \frac{A^2 M_1}{E_+^3}\left[k_z k_x, k_z k_y, \frac{1}{2}\left(k_z^2 - k_c^2 - k_x^2 - k_y^2\right)\right]$$



$$\Omega(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}(\mathbf{k})$$

$$\mathbf{A}(\mathbf{k}) = \langle u(\mathbf{k})|\, \nabla_{\mathbf{k}}\, |u(\mathbf{k})\rangle$$



Non-Zero Chern Number as a Function of kz

$$n_c(k_z) = -(1/2\pi) \iint dk_x dk_y \Omega(\mathbf{k}) \cdot \hat{z}$$

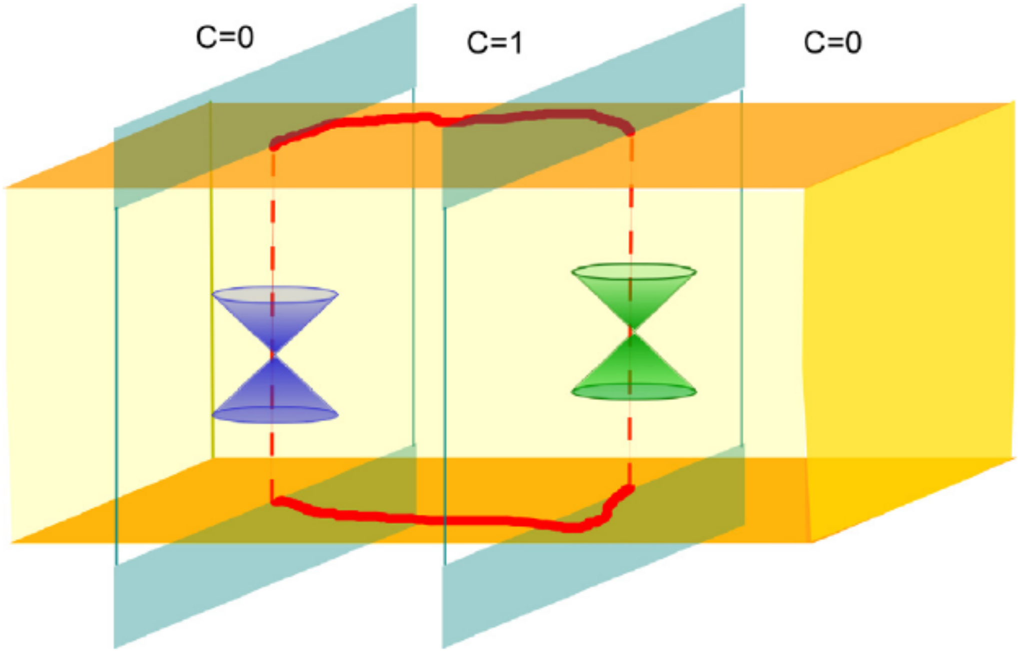
$$n_c(k_z) = -\frac{1}{2}[\text{sgn}(M_0 - M_1 k_z^2) + \text{sgn}(M_1)]$$

For $M_0/M_1 > 0$

$$n_c(k_z) = -\frac{1}{2}\text{sgn}(M_1)\left[\text{sgn}(k_c^2 - k_z^2) + 1\right]$$

The Chern number is 1 or -1 when kz is between the two Weyl nodes and the system is half filled.

Weyl Semimetal



Hosur & Qi, 2014

Fig. 1. (Color online.) Weyl semimetal with a pair of Weyl nodes of opposite chirality (denoted by different colors green and blue) in a slab geometry. The surface has unusual Fermi arc states (shown by red curves) that connect the projections of the Weyl points on the surface. *C* is the Chern number of the 2D insulator at fixed momentum along the line joining the Weyl nodes. The Fermi arcs are nothing but the gapless edge states of the Chern insulators strung together.

Sau-Lutchyn-Tewari-Das Sarma Model For Topological Superconductor

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} c^{\dagger}_{\mathbf{k},\sigma} \left(\epsilon(k)\sigma_0 + \alpha(k_x\sigma_y - k_y\sigma_x) + V_Z\sigma_z\right)_{\sigma\sigma'} c_{\mathbf{k},\sigma'}$$

$$V = \sum_{\mathbf{k}} \left(\Delta c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow} + h.c.\right)$$

We first perform a unitary transformation to diagonalize H_0

$$\begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta_{\mathbf{k}}}{2} & -e^{-i\varphi_{\mathbf{k}}}\sin\frac{\theta_{\mathbf{k}}}{2} \\ e^{i\varphi_{\mathbf{k}}}\sin\frac{\theta_{\mathbf{k}}}{2} & \cos\frac{\theta_{\mathbf{k}}}{2} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k},+} \\ a_{\mathbf{k},-} \end{pmatrix}$$

$$V_1 = \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k},c} a^{\dagger}_{\mathbf{k},+} a^{\dagger}_{-\mathbf{k},-} + h.c.\right),$$

$$V_2 = -\frac{1}{2}\sum_{\mathbf{k},\nu} \left(\Delta_{\mathbf{k},\nu} a^{\dagger}_{\mathbf{k},\nu} a^{\dagger}_{-\mathbf{k},\nu} + h.c.\right)$$

$$\Delta_{k,c} = \Delta V_z / \Lambda_k$$

The second transformation is to diagonalize the part of s-wave pairing

$$\begin{pmatrix} a_{\mathbf{k},+} \\ a^{\dagger}_{-\mathbf{k},-} \end{pmatrix} = \begin{pmatrix} \cos\frac{\gamma_{\mathbf{k}}}{2} & -\sin\frac{\gamma_{\mathbf{k}}}{2} \\ \sin\frac{\gamma_{\mathbf{k}}}{2} & \cos\frac{\gamma_{\mathbf{k}}}{2} \end{pmatrix} \begin{pmatrix} b_{\mathbf{k},+} \\ b^{\dagger}_{-\mathbf{k},-} \end{pmatrix}$$

$$H = \sum_{\mathbf{k},\nu=\pm} \left[\left(\sqrt{\epsilon(k)^2 + \Delta^2_{\mathbf{k},c}} + \nu\Lambda_{\mathbf{k}} \right) b^{\dagger}_{\mathbf{k},\nu} b_{\mathbf{k},\nu} - \frac{1}{2} \sum_{\mathbf{k},\nu} \left(\Delta_{\mathbf{k},\nu} b^{\dagger}_{\mathbf{k},\nu} b^{\dagger}_{-\mathbf{k},\nu} + h.c. \right) \right]$$

The result: the model is equivalent to two p-wave pairing superconductors, one is always topological trivial, and the other is possibly nontrivial with the condition $\sqrt{\mu^2 + \Delta^2} < |V_z|$

$$H = \frac{1}{2} \sum_{\mathbf{k},\nu=\pm} \psi^{\dagger}_{\mathbf{k},\nu} \left[\frac{\alpha\Delta}{\Lambda_{\mathbf{k}}} (k_y\sigma_x - \nu k_x\sigma_y) + \left(\sqrt{\epsilon(k)^2 + \Delta^2_{\mathbf{k},c}} + \nu\Lambda_{\mathbf{k}} \right) \sigma_z \right] \psi_{\mathbf{k},\nu}$$

S. Q. Shen, Topological Insulator, (Springer, 2012)

Equation and Basis

$$H_{eff} = vp \cdot \alpha + (mv^2 - Bp^2)\beta$$

The Dirac equation has a physical meaning only on a physical basis:

$$H = \sum \Psi_p^+ H_{eff}(p) \Psi_p$$

Summary

$$H = vp \cdot \alpha + (mv^2 - Bp^2)\beta$$

1. The modified Dirac equation has a boundary solution with the condition: mB>0;
2. Non-topological impurity: in-gap bound state;
3. Topological impurity: vortex-induced zero-energy state, Majorana fermion

References:
•Shen, Shan and Lu, SPIN 1, 33 (2011)
•Shen, Topological Insulators, (Springer, Berlin-Heidelberg, 2012)

Springer Series in Solid-State Sciences 174

Shun-Qing Shen

Topological Insulators

Dirac Equation in Condensed Matters

Topological insulators are insulating in the bulk, but process metallic states around its boundary owing to the topological origin of the band structure. The metallic edge or surface states are immune to weak disorder or impurities, and robust against the deformation of the system geometry. This book, *Topological insulators,* presents a unified description of topological insulators from one to three dimensions based on the modified Dirac equation. A series of solutions of the bound states near the boundary are derived, and the existing conditions of these solutions are described. Topological invariants and their applications to a variety of systems from one-dimensional polyacetalene, to two-dimensional quantum spin Hall effect and p-wave superconductors, and three-dimensional topological insulators and superconductors or superfluids are introduced, helping readers to better understand this fascinating new field.

This book is intended for researchers and graduate students working in the field of topological insulators and related areas.

Shun-Qing Shen is a Professor at the Department of Physics, the University of Hong Kong, China.

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Topological Insulators

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Shun-Qing Shen

Topological Insulators

Dirac Equation in Condensed Matters

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Quantum States of Matter

Spontaneous Symmetry Breaking & Order Parameters	Topological Invariant & Topological Quantum Phase
Ferromagnetism	Integer Quantum Hall Effect
Antiferromagnetism	Fractional Quantum Hall Effect
Superconductivity	Quantum Spin Hall Effect
Charge or spin density wave	3D Topological Insulator
…….	……….

Free energy: