Topology in Band Theory

P715

Topology in band theory

Not all band insulators are "boring"! Topology in band theory $\Rightarrow$ protected edge modes, quantum Hall effect, and topological insulators.

(I) Berry phase and Berry curvature

Crucial in this chapter!

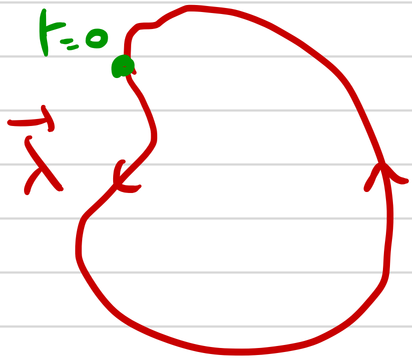
Vary parameter λ : $\quad H_0 \xrightarrow{\lambda} H_1$

. Start with $H_0 |\psi\rangle = E_0 |\psi\rangle$, vary λ slowly
$\lambda = 0$ $\quad \uparrow$ GS, or any eigenstate

. Adiabatic theorem: $|\psi(t)\rangle = |\psi(\lambda(t))\rangle$, eigenstate of H_λ
($|\psi(t)\rangle$ = instantaneous eigenstate)

. OK as long as we don't have level crossings.
(that's fine, QM naturally leads to avoided level crossings)

Now imagine a closed path in parameter space:



We end up with the same state (say the GS of H_0), $\underline{\underline{\text{BUT}}}$, up to a phase!

$$\boxed{|\psi\rangle \longrightarrow e^{i\gamma}|\psi\rangle}$$

(phase difference: physical!)

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

with $H(\lambda)|\psi_0(\vec{\lambda})\rangle = E_0(\vec{\lambda})\,|\psi_0(\vec{\lambda})\rangle$ GS (eigenstate) of $H(\vec{\lambda})$

- Adiabatic theorem:

$$|\psi(t)\rangle = e^{i\theta(t)}|\psi_0(\gamma(t))\rangle$$

$|n(\vec{\gamma}=0)\rangle = |\psi(t=0)\rangle = |\psi_0\rangle$, and $e^{i\theta(t=0)} = 1$

- $e^{i\theta(t)}$ includes $e^{-i/\hbar \int_0^t dt\, E_0(\vec{\lambda}(t))}$: ignore this, set $E_0 = 0$

- Plug $|\psi(t)\rangle = e^{i\theta(t)}|\psi_0(\vec{\gamma}(t))\rangle$ into the Schrödinger equation:

$$i\hbar\left(i\dot{\theta}\, e^{i\theta}|\psi_0\rangle + \dot{\vec{\lambda}}\cdot e^{i\theta}\frac{d}{d\vec{\lambda}}|\psi_0\rangle\right) = \underbrace{H(\vec{\lambda})\,e^{i\theta(t)}|\psi_0\rangle}_{=0}$$

we get: $i\dot{\theta} + \dot{\vec{\lambda}} \cdot \langle \psi_0 | \nabla_{\vec{\lambda}} | \psi_0 \rangle = 0$

$$\Rightarrow \quad \dot{\theta} = i\, \dot{\vec{\lambda}} \cdot \langle \psi_0 | \nabla_{\vec{\lambda}} | \psi_0 \rangle \equiv - \dot{\vec{\lambda}} \cdot \vec{A}$$

$$\boxed{\vec{A}(\vec{\lambda}) = -i \langle n | \nabla_{\vec{\lambda}} | n \rangle}$$

(Berry connection)
Here: $|n\rangle = |\psi_0\rangle$

$$\theta(t) = -\int_0^t dt\, \dot{\vec{\lambda}} \cdot \vec{A}$$

- If we take a closed path $\mathcal{C}$ in parameter space: $\theta(T) = \gamma$

$$\boxed{e^{i\gamma} = e^{-i \oint_{\mathcal{C}} \vec{A}(\vec{\lambda}) \cdot d\vec{\lambda}}}$$

Berry phase
(no dependence on time

- Gauge invariance: $|\psi_0'(\vec{\lambda})\rangle = e^{i\omega(\vec{\lambda})} |\psi_0(\vec{\lambda})\rangle$

Different choice of phase for GS of $H(\lambda)$.

$$\vec{A}' = -i \langle \psi_0' | \vec{\nabla}_{\vec{\lambda}} | \psi_0' \rangle = \vec{A} + \vec{\nabla}_{\vec{\lambda}} \omega$$

Recall E&M: $A_\mu' = A_\mu + \partial_\mu \omega$

$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$: gauge invariant

Berry curvature: (gauge invariant)

$$\boxed{F_{ij}(\vec{\lambda}) = \frac{\partial A_i}{\partial \lambda^j} - \frac{\partial A_j}{\partial \lambda^i}}$$

(in 3d for λ: $\vec{\nabla}_\lambda \times \vec{A}$)

. The Berry phase is also gauge invariant, since

$$\oint d\vec{\lambda} \cdot \vec{\nabla}_\lambda \omega = 0$$

Stokes theorem: $e^{i\gamma} = e^{-i\oint_{\mathcal{C}} \vec{A} \cdot d\vec{\lambda}} = e^{-i\int_S F_{ij}\, dS^{ij}}$

S: 2d surface in parameter space bounded by $\mathcal{C}$

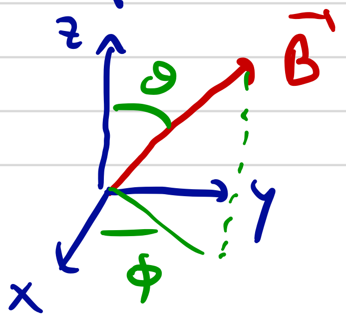
Example ①: Spin $\frac{1}{2}$

$\hat{H} = -\gamma \vec{B} \cdot \vec{S}$: $\vec{S} = \frac{\vec{\sigma}}{2}$; GS: $\hat{H}|-\rangle = -\frac{\gamma B}{2}$

$\hat{H}|+\rangle = +\frac{\gamma B}{2}$

. take $\vec{\lambda} = \vec{B}$: $\vec{A}$ and F_{ij} in space of $\vec{B}$ field

. $\vec{B} = \begin{pmatrix} B \sin\theta \cos\phi \\ B \sin\theta \sin\phi \\ B \cos\theta \end{pmatrix}$ $\vec{\lambda} = (\phi, \theta)$



$$\hat{H} = \begin{pmatrix} -\frac{B\gamma}{2}\cos\theta & -\frac{B\gamma}{2} e^{-i\phi}\sin\gamma \\ -\frac{B\gamma}{2} e^{i\phi}\sin\gamma & \frac{1}{2}\frac{B\gamma}{2}\cos\theta \end{pmatrix}$$

GS: $|-\rangle = \begin{pmatrix} e^{-i\phi} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}$ in S^z basis $|\uparrow\rangle, |\downarrow\rangle$

$|+\rangle = \begin{pmatrix} e^{-i\phi} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$ (avoid $\theta = \pi$)

We have: $A_\theta = -i \langle - | \frac{\partial}{\partial\theta} | - \rangle = 0$

$$A_\phi = -i \langle - | \frac{\partial}{\partial\phi} | - \rangle = -i \langle - | \left(-i e^{-i\phi} \sin\frac{\theta}{2} |\uparrow\rangle \right)$$

$$= -\sin^2\frac{\theta}{2}$$

Berry curvature: $F_{\phi,\theta} = \frac{\partial A_\phi}{\partial\theta} = -\frac{\sin\theta}{2}$

in $\vec{B}$ space: $\frac{\partial}{\partial\vec{B}} = \frac{\partial}{\partial B}\vec{e_r} + \frac{1}{B}\frac{\partial}{\partial\theta}\vec{e_\theta} + \frac{1}{B\sin\theta}\frac{\partial}{\partial\phi}\vec{e_\phi}$

$$\vec{A} = -i \langle - | \frac{\partial}{\partial\vec{B}} | - \rangle = \frac{1}{B\sin\theta} A_\phi \vec{e_\phi} = -\frac{\sin^2\theta/2}{B\sin\theta}\vec{e_\phi}$$

$$\vec{F} = \vec{\nabla}_{\vec{B}} \times \vec{A} = \frac{1}{B\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{-\sin^2\theta/2}{B} \right)\vec{e_r} = \frac{1}{B^2\sin\theta} F_{\phi,\theta}\vec{e_r}$$

curl in spherical coordinates

$$= -\frac{1}{2B^2}\vec{e_r}$$

$\vec{e_r} = \hat{B} = \vec{B}/|\vec{B}|$

$$\boxed{\vec{\nabla}_{\vec{B}} \times \vec{A} = -\frac{1}{2B^2}\vec{e_n}}$$

"Magnetic monopole!"
charge $q = -\frac{1}{2}$

$$\int_{S^2} (\vec{\nabla}_{\vec{B}} \times \vec{A}).\vec{ds} = \int_0^\pi d\theta\, 2\pi \cancel{B^2} \left(-\frac{1}{2\cancel{B^2}}\right) \sin\theta$$

$$= -2\pi = 4\pi q$$

For any γ:

$$e^{i\gamma} = e^{-i\int_S \vec{F}.\vec{ds}} = e^{i\Omega/2}$$

Ω solid angle

But we can equally choose S': covering solid angle

$$\Omega' = 4\pi - \Omega$$

$$e^{i\gamma'} = e^{-i\frac{(4\pi-\Omega)}{2}} = e^{i\gamma}$$

surface has opposite orientation now!
$\vec{ds}$ points inwards

$$\Rightarrow \quad e^{+iq(4\pi-\Omega)} = e^{-iq\Omega}$$

$$\Rightarrow 2q \in \mathbb{Z}$$ Charge quantization (Dirac)

$$\Rightarrow \boxed{\int F_{ij}\, ds^{ij} = 2\pi c}$$

$c \in \mathbb{Z}$
Chern number

Example ②: Chern insulator

periodic $\vec{r} \in \Lambda$

Bloch e^-: $\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}.\vec{x}} u_{\vec{k}}(\vec{x})$ (fows on given band)

$$\hat{H}_{\vec{k}} = e^{-i\vec{k}.\vec{x}} \hat{H} e^{+i\vec{k}.\vec{x}} = \frac{(\vec{p}+\hbar\vec{k})^2}{2m} + V(\vec{r})$$

$$\hat{H}_{\vec{k}} |u_{\vec{k}}\rangle = E_{\vec{k}} |u_{\vec{k}}\rangle$$

BZ: periodic (Square or cubic lattice: Torus T^2, T^3)
Phase can wind as we move around the BZ!

$$\boxed{\begin{aligned} \vec{A} &= -i \langle u_{\vec{k}} | \nabla_{\vec{k}} | u_{\vec{k}} \rangle \\ \vec{F} &= \vec{\nabla}_{\vec{k}} \times \vec{A} \end{aligned}}$$

in 2d:

$$C = \frac{1}{2\pi} \int_{BZ} dk_x dk_y \, F$$

$$F = \frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y}$$

Chern insulator: Two bands, most general form:

$$H_{\vec{k}} = \vec{d}(\vec{k}).\underbrace{\vec{\sigma}}_{\text{band space}} + \varepsilon(\vec{k}) \mathbb{1},$$

Take $\vec{k} \in BZ \sim T^2$ in 2d

$$= \begin{pmatrix} \varepsilon + d_z & d_x - i d_y \\ d_x + i d_y & \varepsilon - d_z \end{pmatrix}$$

- Two bands of energy $\varepsilon(\vec{k}) \pm |\vec{d}(\vec{k})|$
- Insulator: fill lower band

<u>Example</u> : $H_{\vec{k}} = \sin k_x \, \sigma_x + \sin k_y \, \sigma_y + (2 - m - \cos k_x - \cos k_y)\sigma^z$

$$\overset{\text{low } k}{\simeq} (k_x \sigma_x + k_y \sigma_y) - m \quad \sigma_z$$

2-component Dirac Hamiltonian in 2+1 d !

$$C = \begin{cases} -1 & 0 < m < 2 \\ 1 & 2 < m < 4 \\ 0 & m < 0 \\ & m > 4 \end{cases}$$

$$\vec{n} : \overset{\vec{k}}{\uparrow}\!T^2 \longrightarrow S^2 : \text{Bloch sphere}$$

In general, one can show:

$$\boxed{C = \int_{BZ} \frac{d^2\vec{k}}{4\pi}\, \vec{n}\cdot\left(\frac{\partial \vec{n}}{\partial k_x} \times \frac{\partial \vec{n}}{\partial k_y}\right)}$$

with $\vec{n} = \dfrac{\vec{d}(k)}{|\vec{d}|} \in$ Bloch sphere

<u>Example 3</u> : Dirac fermion in 2+1d (Not lattice model here!)

$$H = \vec{d}(\vec{k}) \cdot \vec{\sigma} \qquad \vec{d} = (k_x, k_y, m)$$

$$\vec{A} = -i\langle u_{\vec{k}} | \vec{\nabla}_{\vec{k}} | u_{\vec{k}} \rangle$$

$$E_\pm = \pm \sqrt{\vec{k}^2 + m^2}$$

$$F = \partial_{k_x} A_y - \partial_{k_y} A_x$$

$$\vec{n} = \begin{pmatrix} k_x / \sqrt{k^2 + m^2} \\ k_y / \sqrt{k^2 + m^2} \\ m / \sqrt{k^2 + m^2} \end{pmatrix} \quad \text{and} \quad = \frac{1}{2}\, \vec{n} \cdot \left(\partial_{k_x} \vec{n} \times \partial_{k_y} \vec{n}\right)$$

$$= \frac{1}{2} \frac{m}{(\vec{k}^2 + m^2)^{3/2}}$$

No BZ here

$$C = \int_0^\infty \frac{\cancel{2\pi} k\, dk}{\cancel{2\pi}} \frac{m}{2(k^2+m^2)^{3/2}} = \frac{1}{2}\frac{m}{|m|} = \frac{1}{2}\,\mathrm{sign}(m)$$

$$\boxed{C = \frac{\mathrm{sign}(m)}{2}}$$

Half integer! Because of continuum

" π Berry phase "

Important physical consequences

II Semi-Classical equations of motion (revisited) and anomalous Hall effect

Adiabatic perturbation theory (corrections to adiabatic theorem): $\vec{\lambda} = \vec{\lambda}(t)$

start in eigenstate $|n(0)\rangle$

eigenstate of $H(\lambda(t))$

$$|\psi_n(t)\rangle = \underbrace{e^{-i/\hbar \int_0^t E_n(\vec{\lambda}(t))dt}}_{\text{"Usual" Dynamical phase}} \; \underbrace{e^{-i\int_0^t dt\, \vec{A}\cdot\dot{\vec{\lambda}}}}_{\text{Berry phase}} \times \Big(|n(t)\rangle$$

$$+ \; i\hbar \sum_{m\neq n} \frac{\langle m(t)|\vec{\nabla}_{\vec{\lambda}}|n(t)\rangle}{E_m(t) - E_n(t)} \cdot \dot{\vec{\lambda}}\; |m(t)\rangle + \dots$$

correction

"Perturbation theory" in $-i\hbar\frac{\partial}{\partial t} = -i\hbar\vec{\nabla}_\lambda \cdot \dot{\vec{\lambda}}$

- Consider: Bloch e^- in small $\vec{E}$ field

choose $\vec{A}_e = -\vec{E}t$ so $\vec{E} = -\frac{\partial \vec{A}_e}{\partial t}$

"real" gauge potential

$$H = \frac{(\vec{p} - e\vec{E}t)^2}{2m} + V(\vec{x}) \longrightarrow H_{\vec{k}} = \frac{(\vec{p} + \hbar\vec{k}(t))^2}{2m} + V(\vec{x})$$

with $\vec{k}(t) = \vec{k} - \frac{e\vec{E}t}{\hbar}$

$$H_{\vec{k}} |u^n_{\vec{k}}\rangle = E^n_{\vec{k}} |u^n_{\vec{k}}\rangle \qquad n = \text{band index}$$

Velocity: $\vec{v}^n_{\vec{k}} = \langle \psi^n_{\vec{k}} | \frac{\vec{p}}{m} | \psi^n_{\vec{k}} \rangle = \langle u^n_{\vec{k}} | \frac{\vec{p} + \hbar\vec{k}}{m} | u^n_{\vec{k}} \rangle$

$$= \langle u^n_{\vec{k}}(t) | \frac{1}{\hbar} \frac{\partial H_{\vec{k}}}{\partial \vec{k}} | u^n_{\vec{k}}(t) \rangle$$

As before, except here:

$\vec{k} = \vec{k}(t)$ everywhere

up to phases

$$|u^n_{\vec{k}}(t)\rangle \simeq |u^n_{\vec{k}(t)}\rangle + i\hbar \sum_{m\neq n} \frac{\langle u^m_{\vec{k}} | \vec{\nabla}_{\vec{k}} | u^n_{\vec{k}} \rangle \cdot \dot{\vec{k}}}{E^m_k - E^n_k} |u^m_{\vec{k}}\rangle$$

adiabatic theorem

$$\Rightarrow \vec{v}^n_{\vec{k}} = \langle u^n_{\vec{k}} | \frac{1}{\hbar} \frac{\partial H_{\vec{k}}}{\partial \vec{k}} | u^n_{\vec{k}} \rangle$$

$$- i \sum_{m\neq n} \frac{\langle u^n_{\vec{k}} | \vec{\nabla}_{\vec{k}} H_{\vec{k}} | u^m_{\vec{k}} \rangle \langle u^m_{\vec{k}} | \vec{\nabla}_{\vec{k}} u^n_{\vec{k}} \rangle}{E^n_{\vec{k}} - E^m_{\vec{k}}} \cdot \dot{\vec{k}} + h.c.$$

$\vec{k} = \vec{k}(t)$ everywhere

Now: $\langle u_k^n | u_k^m \rangle = \delta^{nm} \Rightarrow \langle \frac{\partial u_k^n}{\partial \vec{k}} | u_k^m \rangle = -\langle u_k^n | \frac{\partial u_k^m}{\partial \vec{k}} \rangle$

$$\langle u_{\vec{k}}^n | H_{\vec{k}} | u_k^m \rangle = E_{\vec{k}}^n \delta^{nm} \Rightarrow \langle \frac{\partial u^n}{\partial \vec{k}} | u_k^m \rangle E_k^m + \langle u^n | \vec{\nabla}_k H | u^m \rangle$$
$$+ E_k^n \langle u_{\vec{k}}^n | \frac{\partial}{\partial \vec{k}} u_k^m \rangle$$
$$= \vec{\nabla}_k E_{\vec{k}}^n \delta^{nm}$$

$$\Rightarrow \langle u_{\vec{k}}^n | \vec{\nabla}_{\vec{k}} H_{\vec{k}} | u_{\vec{k}}^m \rangle = \frac{\partial}{\partial \vec{k}} E_{\vec{k}}^n \delta^{nm}$$
$$+ (E_{\vec{k}}^n - E_{\vec{k}}^m) \langle \frac{\partial u^n}{\partial \vec{k}} | u_k^m \rangle$$

We thus have:

$$\vec{v}_{\vec{k}}^n = \frac{1}{\hbar} \frac{\partial E_{\vec{k}}^n}{\partial \vec{k}} - i \left[\sum_m \langle \frac{\partial u_k^n}{\partial \vec{k}} | u_k^m \rangle \langle u_k^m | \frac{\partial u_k^n}{\partial t} \rangle - h.c. \right]$$

$= 1$

Now: $\vec{F}^n = \vec{\nabla}_{\vec{k}} \times \vec{A}^n = -i \langle \underbrace{\vec{\nabla}_{\vec{k}} u^n}_{\vec{b}} | \times | \underbrace{\vec{\nabla}_{\vec{k}} u^n}_{\vec{c}} \rangle$

$$\underbrace{\dot{\vec{k}}}_{\vec{a}} \times \vec{F}^n = \vec{b}(\vec{a} \cdot \vec{c}) - (\vec{a} \cdot \vec{b}) \vec{c}$$

$$= -i \left(\langle \vec{\nabla}_k u^n | \partial_t u^n \rangle - \langle \partial_t u^n | \vec{\nabla}_{\vec{k}} u^n \rangle \right)$$ and $\dot{\vec{k}} = -\frac{e\vec{E}}{\hbar}$

$$\Rightarrow \boxed{\vec{v}_k^n = \frac{1}{\hbar} \frac{\partial E_{\vec{k}}^n}{\partial \vec{k}} - \frac{e\vec{E}}{\hbar} \times \vec{F}^n}$$

"anomalous" velocity!

$\perp \vec{E} \rightarrow$ Hall effect! even if $\vec{B} = \vec{0}$!

In general, if $\vec{B}$ and $\vec{E} \neq \vec{0}$:

$$\boxed{\begin{aligned} \dot{\vec{x}} &= \frac{1}{\hbar} \nabla_{\vec{k}} E^n_{\vec{k}} + \dot{\vec{k}} \times \vec{F}^n \\ \hbar \dot{\vec{k}} &= -e\vec{E} - e\dot{\vec{x}} \times \vec{B} \end{aligned}}$$

New term!

$\vec{F}^n = \vec{\nabla}_k \times \vec{A}$

"B field in $\vec{k}$ space"!

Current in filled band

: take $\vec{B} = \vec{0}$, $\vec{E} = \begin{pmatrix} 0 \\ E \\ 0 \end{pmatrix}$, 2d system

Focus on spinless case ($\vec{B}$ field)

$$\vec{j} = -e \int_{BZ} \frac{d^2\vec{k}}{(2\pi)^2} \vec{v}_k$$

$$F = F_z = \partial_{k_x} A_y - \partial_{k_y} A_x$$

$$= -\underbrace{e \int_{BZ} \frac{d^2k}{(2\pi)^2} \frac{\vec{\nabla}_k E}{\hbar}}_{0} + \frac{e^2}{\hbar} \int_{BZ} \frac{d^2k}{(2\pi)^2} \underbrace{\vec{E} \times \vec{F}}_{\begin{pmatrix} 0 \\ E \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ F \end{pmatrix}}$$

$$= \frac{e^2}{\hbar} \int_{BZ} \frac{d^2k}{2\pi} E F \vec{e}_x$$

: Hall response!

$$\Rightarrow \boxed{\sigma_{xy} = \frac{e^2}{\hbar} C}$$

with $C = \int_{BZ} \frac{d^2k}{2\pi} F$

Chern number

Quantized Hall conductivity

TKNN: Thouless - Kohomoto - Nightingale - den Nijs invariant

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} \left[\langle \partial_{k_y} u^n_{\vec{k}} | \partial_{k_x} u^n_{\vec{k}} \rangle - h.c. \right]$$

sum over filled bands

Note: . $C \in \mathbb{Z}$, integer, can't change continuously! Robust

. Quantum Anomalous Hall effect: QAH

quantized Hall response even if $\vec{B} = 0$!

simplest "Topological insulator"

. $\vec{F}$ requires non trivial conditions to be non zero:

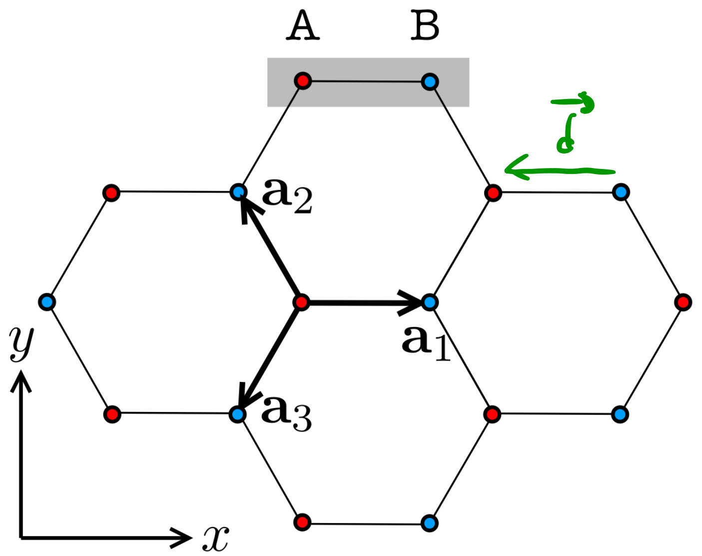
if crystal has inversion symmetry $\left(u^n_{-\vec{k}}(-\vec{x}) = u^n_{\vec{k}}(\vec{x})\right)$ and time reversal symmetry $\left(u^{n*}_k = u^n_{-k} = u^n_k\right)$ then $\vec{F} = \vec{0}$

C: 4 e^- in outer shell (6 total)

half filled

III Graphene and Haldane model

: Tight binding model for π (p_z) orbitals



See HW2.

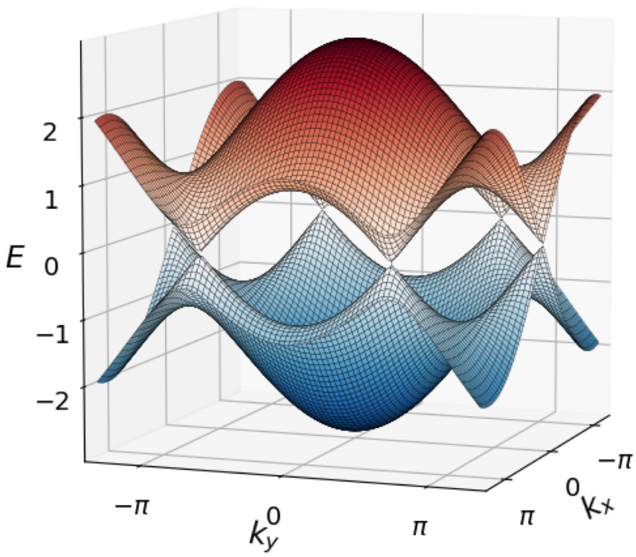
In basis $\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$

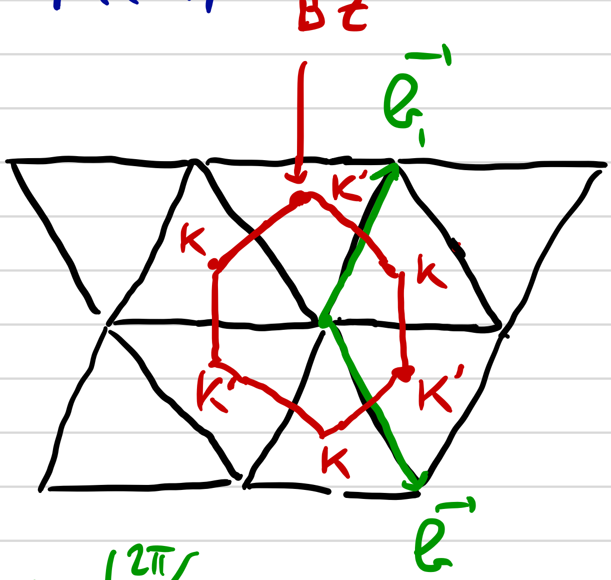
$$H_{\vec{k}} = \begin{pmatrix} 0 & h(\vec{k}) \\ h(\vec{k})^\dagger & 0 \end{pmatrix}$$

with $$h(\vec{k}) = -t \sum_{j=1}^{3} \underbrace{e^{i\vec{k}\cdot\vec{a_j}}}_{\cos(\dots) + i\sin(\dots)}$$

$$\Rightarrow \quad H_{\vec{k}} = -t \sum_{j=1}^{3} \left(\sigma^x \cos(\vec{k}\cdot\vec{a_j}) - \sigma^y \sin(\vec{k}\cdot\vec{a_j}) \right)$$

Energy spectrum : $E(\vec{k}) = \pm |h(\vec{k})|$





$$\vec{b_1} = \begin{vmatrix} 2\pi/3a \\ 2\pi/\sqrt{3}a \end{vmatrix} \qquad \vec{b_2} = \begin{vmatrix} 2\pi/3a \\ -2\pi/\sqrt{3}a \end{vmatrix}$$

$\nearrow$ out of the 6

- Two inequivalent Dirac points at $\vec{K}, \vec{K}'$

$$\vec{K} = \begin{vmatrix} 2\pi/3 \\ +\frac{2\pi}{3\sqrt{3}} \end{vmatrix} \qquad \vec{K}' = \begin{vmatrix} 2\pi/3 \\ -2\pi/3\sqrt{3} \end{vmatrix}$$

- Fill lower band: $E_F = 0$ Semi Metal

- $\vec{k} = \vec{K} + \delta\vec{k}$: $\boxed{E(k) \simeq \pm \hbar v_F |\delta\vec{k}|}$ Linear dispersion with $v_F = \frac{3ta}{2\hbar}$

$$R(\vec{k}) \simeq \hbar v_F (i\,\delta k_x - \delta k_y)$$

$$\Rightarrow H(\vec{k}) = -\hbar v_F \underbrace{(\delta k_x \sigma^y + \delta k_y \sigma^x)}_{\substack{\text{Dirac Hamiltonian!} \\ k_x \leftrightarrow k_y \text{ by } \pi/2 \text{ rotation}}}$$

- Near $\vec{K}'$: $H(\vec{k}) = -\hbar v_F (\delta k_x \sigma^y - \delta k_y \sigma^x)$

(different "helicity")

spin $\downarrow$ 2×2 $\swarrow$ "valley": K, K'

$\uparrow$

- Low energy physics of Graphene = 4 massless Dirac fermions

- σ^z term: protected by $A \leftrightarrow B$

Ex: Boron Nitride = BN $\Rightarrow$ same lattice insulator.

. Density of states: $g(E)\,dE = \underset{\text{spin}}{2} \times \underset{K,K'}{2} \times \frac{k\,dk}{(2\pi)^2} 2\pi$

$\frac{3ta}{2}|k| = E \quad \Rightarrow \quad g(E)\,dE = \frac{2}{\pi}\left(\frac{2}{3ta}\right)^2 |E|\,dE$

$\Rightarrow \quad \boxed{g(E) = \frac{8}{9\pi t^2 a^2} |E|}$ (vanishing d.o.s)

(took $\hbar = 1$ here)

. Different from usual Fermi liquid!

Can't use Sommerfeld Expansion (No Fermi Surface)

$$E(T) = \int_{-\infty}^{+\infty} dE\, \frac{E\, g(E)}{1+e^{\beta E}}$$

$$= \int_{-\infty}^{0} dE\, g(E) \left[1 - \frac{e^{\beta E}}{1+e^{\beta E}} \right] E + \int_{0}^{\infty} dE\, \frac{E\, g(E)}{1+e^{\beta E}}$$

$$= \underbrace{\int_{-\infty}^{0} dE\, g(E) E}_{E_0} - \int_{-\infty}^{0} dE\, \frac{g(E) E}{1+e^{-\beta E}} + \int_{0}^{\infty} dE\, \frac{E\, g(E)}{1+e^{\beta E}}$$

$E_0 =$ divergent constant (because of low energy approx)

$$= E_0 + 2\int_0^{\infty} dE\, \frac{E\, g(E)}{1+e^{\beta E}} \qquad \text{since } g(E) = g(-E)$$

$$= E_0 + CT^3 + \dots \qquad x = \beta E$$

$\Rightarrow$ $\boxed{C_v \sim T^2}$ $\neq$ Fermi gas with Fermi surface!

. <u>Can we gap out Graphene in a topological way?</u>

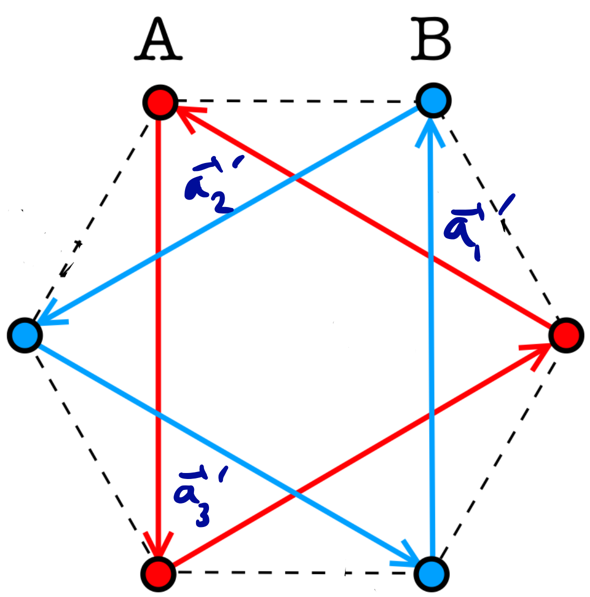
Guess : break sublattice symmetry (A vs B)

$$H \to H + m\,\sigma^z$$

$$E(k) = \pm\sqrt{|R|^2 + m^2}$$

but trivial bands...

. Need to break Time reversal and sublattice symm:



"Haldane model"

(Nobel prize 2016!)

$t' e^{\pm i\varphi}$ hopping

between $A \leftrightarrow A$ sites
$B \leftrightarrow B$

. Has a Chern insulator phase with "edge modes"!
("Quantum Hall without B field")

. Realized in cold atoms (Esslinger group, 2014)

• This modifies the low energy Dirac Hamiltonians to:

$$\underset{\text{K point}}{H(\vec{k})} = -\hbar v_F\left(\delta k_x \sigma^y + \delta k_y \sigma^x\right) + (m + 3\sqrt{3}t'\sin\varphi)\sigma^z$$

$$\underset{\text{K' point}}{H(\vec{k})} = -\hbar v_F\left(\delta k_x \sigma^y - \delta k_y \sigma^x\right) + \underbrace{(m - 3\sqrt{3}t'\sin\varphi)}_{\text{"mass" term}}\sigma^z$$

• We can understand the phase diagram by looking at the change in Chern number: $m \to \infty$ trivial phase, $C = 0$

(Not C directly!) $\varphi > 0$ $\sigma_{xy} = 0$

• At $m = 3\sqrt{3}t'\sin\varphi$, K' gap closes: mass > 0 → mass < 0

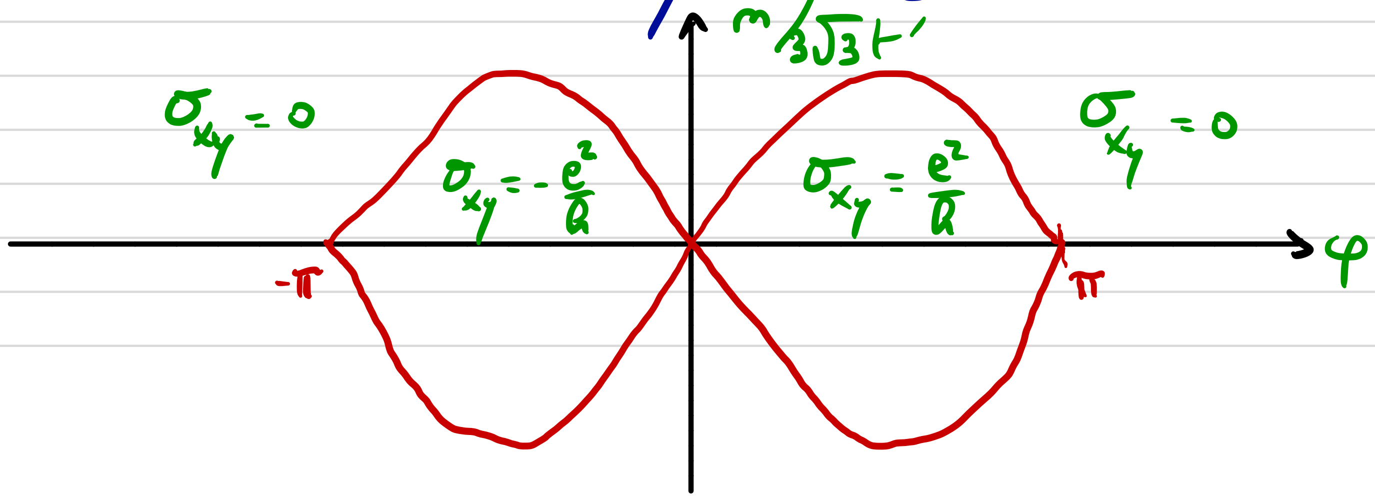
σ^x, σ^y terms have ≠ signs, $C = -\frac{1}{2}\,\mathrm{sign}(m)$ → $C_{K'} = -\frac{1}{2} \to C_{K'} = +\frac{1}{2}$

$$\Rightarrow \Delta C = +1 \Rightarrow \sigma_{xy} = \frac{e^2}{h}$$

• At $m = -3\sqrt{3}t'\sin\varphi$: K point gap closes, mass > 0 → mass < 0

$C_K = +\frac{1}{2} \to C = -\frac{1}{2}$

$$\Rightarrow \Delta C = -1 \Rightarrow \sigma_{xy} = 0 \text{ again}$$



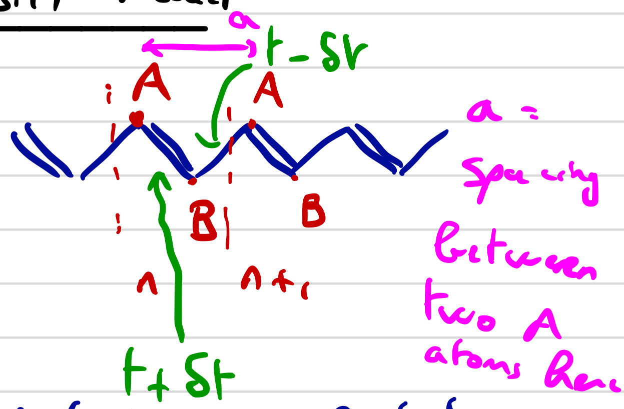
IV Edge modes and SSH model

What's special about topological phases → edge modes!

Let's see this in the simplest example of topological insulator:

Su Schrieffer Heeger (SSH) model

Model for polyacetylene:



We solved this model already! (phonon chapter) Peierls instability

choose sign of t

$$E\phi_n^A = +(t-\delta t)\,\phi_{n-1}^B + (t+\delta t)\,\phi_n^B$$

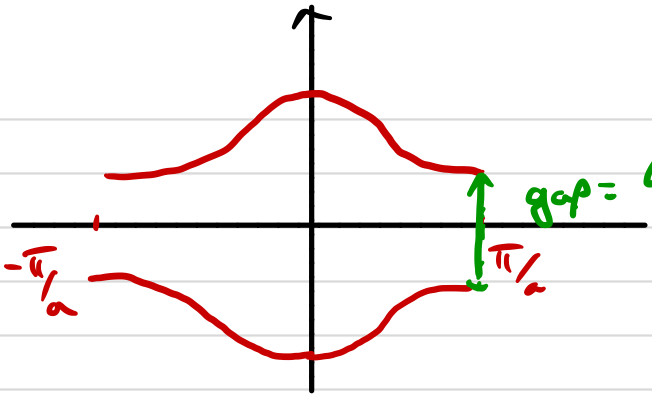
$$E\phi_n^B = +(t+\delta t)\,\phi_n^A + (t-\delta t)\,\phi_{n+1}^A$$

$$H_k \begin{pmatrix} \phi_k^A \\ \phi_k^B \end{pmatrix} = E \begin{pmatrix} \phi_k^A \\ \phi_k^B \end{pmatrix}$$

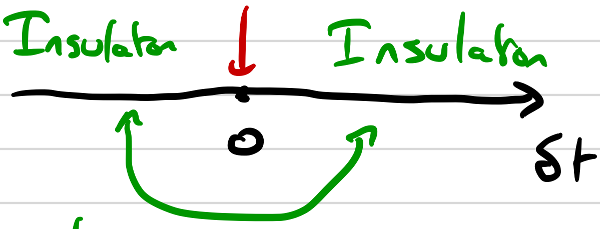
$$H_k = \begin{pmatrix} 0 & +(t+\delta t) + (t-\delta t)e^{-ika} \\ +(t+\delta t) + (t-\delta t)e^{+ika} & 0 \end{pmatrix}$$

$$= \left[(t+\delta t) + (t-\delta t)\cos ka\right]\sigma^x + (t-\delta t)\sin ka\,\sigma^y$$

$$= \vec{d}(\vec{k}) \cdot \vec{\sigma}$$



gap closes



$\neq$ phases of matter!

$$E_\pm = \pm\sqrt{(t+\delta t)^2 + (t-\delta t)^2 + 2(t+\delta t)(t-\delta t)\cos ka}$$

$$ka = \pi : \quad E_\pm = \pm\sqrt{(2\,\delta t)^2} = \pm 2|\delta t|$$

Eigenvectors : $|k_\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm e^{-i\phi(k)} \\ 1 \end{pmatrix}$

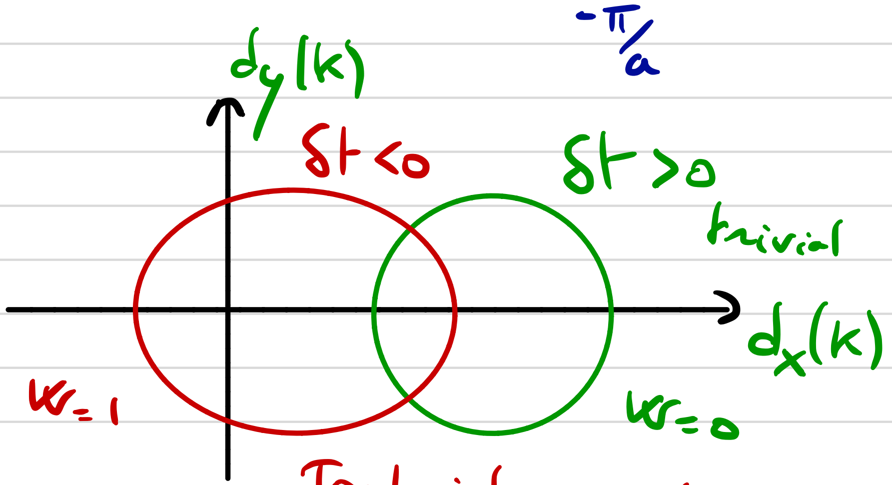
$$\phi(k) = \arctan\left(\frac{\overbrace{(t-\delta t)\sin ka}^{d_y(k)}}{\underbrace{(t+\delta t) + (t-\delta t)\cos ka}_{d_x(k)}}\right)$$

different convention here

$$A_- = +i\langle k_-|\frac{d}{dk}|k_-\rangle = +\frac{1}{2}\frac{d\phi}{dk}$$

Topological invariant: $W = \int_{-\pi/a}^{\pi/a}\frac{dk}{\pi}A_- = \frac{\phi(\pi/a) - \phi(-\pi/a)}{2\pi}$

"winding number"



Topological : winds around origin!

$\mathcal{C}$: $\vec{d}(k)$ vector as $\vec{k}$ winds around BZ

$W = 1$ if $\mathcal{C}$ circles the origin: $\delta t < 0$

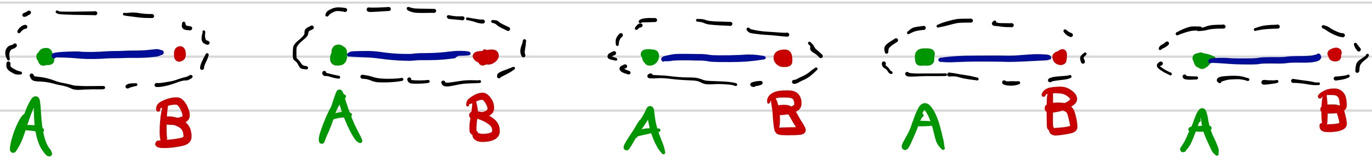
Topological

$= 0$ if $\mathcal{C}$ doesn't, $\delta t > 0$

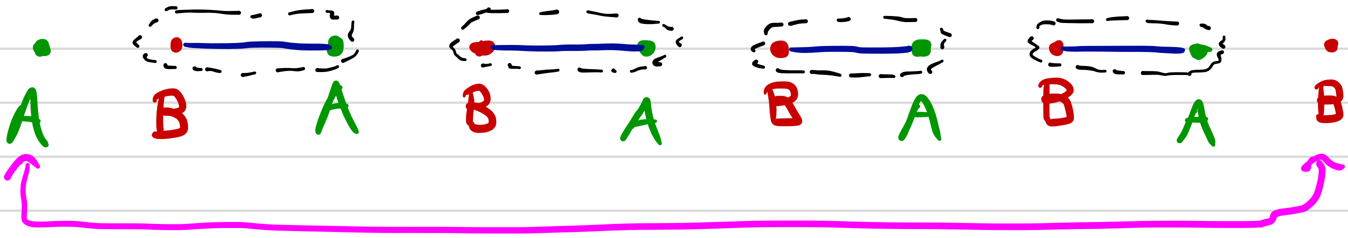
Topological invariant: transition for $\delta t = 0$ (gap closing)

Edge modes $\quad \delta t \to \infty \quad$ (take $t = 1$)

Dimer



$\delta t \to -\infty$



Unpaired sites: edge modes!

Continuum version: Focus on $k = \frac{\pi}{a} + q$, q small

$$H_k = \Big[(t+\delta t) + (t-\delta t)\underbrace{\cos ka}_{-\cos qa \simeq -1}\Big]\sigma^x + (t-\delta t)\underbrace{\sin ka}_{\simeq qa}\sigma^y$$

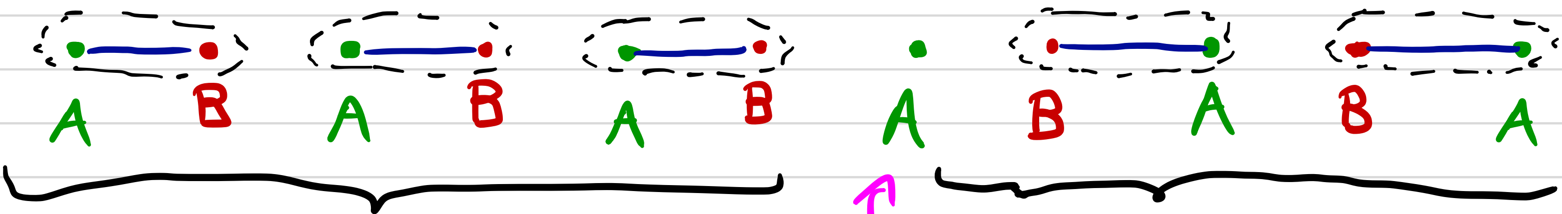
$$\simeq 2\delta t\, \sigma^x + t\, q a\, \sigma^y \quad (\text{take } \delta t \ll t).$$

$q \to -i\hbar \partial_x$: $\boxed{H = -i\hbar v_F \partial_x \sigma^y + m \sigma^x}$

$v_F = ta$ $\quad m = 2\delta t$

Dirac equation (again) with $m<0$ for $\delta t<0$

Let's consider a Domain Wall (DW):



region with $\delta t > 0$

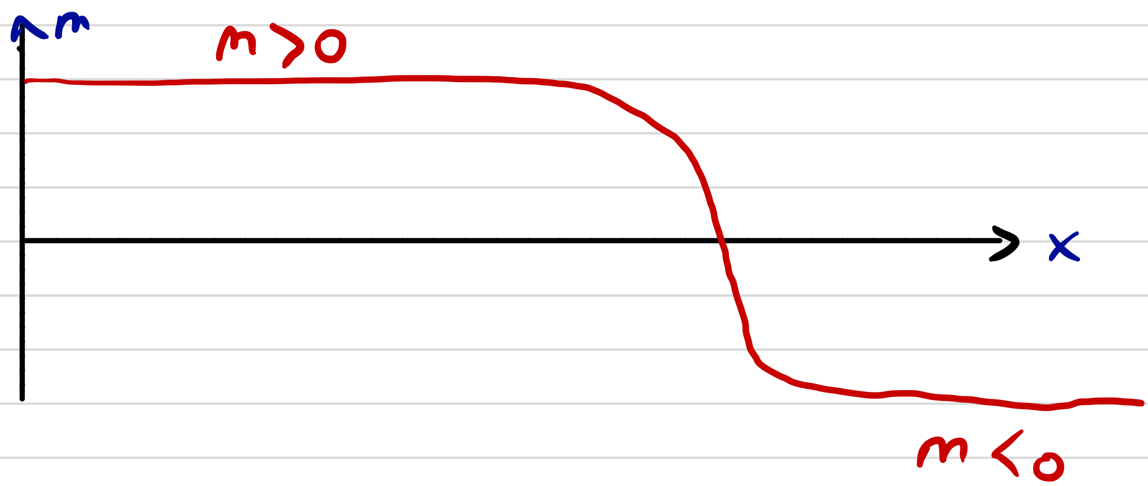
Trivial

"free zero mode"

region with $\delta t < 0$

Topological

Continuum version



Look for zero mode: $H\Psi = 0$

$$\Rightarrow \sigma^y i v_F \hbar \partial_x \Psi = \sigma^x m(x) \Psi$$

$$\Rightarrow \hbar i v_F \partial_x \Psi = \underbrace{\sigma^y \sigma^x}_{-i\sigma^z} m(x)\, \Psi$$

$$\Rightarrow \partial_x \Psi = -\sigma^z \frac{m(x)}{\hbar v_F} \Psi$$

We find: $\Psi(x) = C \exp\left(-\sigma^z \int_0^x \frac{m(x)}{\hbar v_F} dx\right) \Psi(0)$

$$= C \exp\left(+ \int_0^x \frac{m(x)}{\hbar v_F} dx \right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

eigenvalue -1

eigenvector of σ^z

$$\Rightarrow \boxed{\Psi(x) = C \exp\left(+ \int_0^x \frac{m(x)}{\hbar v_F} dx \right) \begin{pmatrix} 0 \\ 1 \end{pmatrix}}$$

- Exponentially localized solution, near DW.
- Exists only if $m(x)$ changes sign!

(Otherwise, not normalizable)