$\mathbb{Z}_2$ Topological Invariant for TRI Insulators

As we noted before SO in general breaks the SU(2) symmetry of spins down to $\mathbb{Z}_2$. At the level of the bands $\mathbb{Z}_2$ is a parity. We need a topological invariant that does not require to have the U(1) subgroup present.

$\Rightarrow$ Classification of TRI top. insulators

Consider a TRI one-particle $\mathcal{H}$ with 2N occupied bands. $\mathcal{H}$ has Bloch states

$$|\psi_n(\vec{k})\rangle = e^{i\vec{k}\cdot\vec{r}}\,|u_n(\vec{k})\rangle$$

$|u_n(\vec{k})\rangle$ are periodic in the BZ and are eigenstates of the reduced Bloch Hamiltonian

$$H(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}}\,\mathcal{H}\,e^{i\vec{k}\cdot\vec{r}}$$

$\vec{G}$: reciprocal lattice vectors

$$|\psi_n(\vec{k}+\vec{G})\rangle = |\psi_n(\vec{k})\rangle \Rightarrow \text{BZ is a torus}$$

$$\Rightarrow |u_n(\vec{k}+\vec{G})\rangle = e^{-i\vec{G}\cdot\vec{r}}\,|u_n(\vec{k})\rangle$$

Time-reversal:

$$\Theta \equiv e^{i\pi S_y} K$$

spin reversal ($e^{i\pi S_y}$) complex conjugation (K)

For $S = 1/2 \Rightarrow \Theta^2 = -\mathbb{1}$

$$[\mathcal{H}, \Theta] = 0 \qquad (\text{TRI})$$

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

For each $\vec{k}$ there are two occupied bands

$\Rightarrow$ rank 2 vector bundle on BZ. $\Rightarrow \mathbb{Z}_2$ classification

Def. $2N \times 2N$ antisymmetric matrix

$$w_{m,n}(\vec{k}) = \langle u_m(-\vec{k}) | \Theta | u_n(\vec{k}) \rangle$$

$\mathbb{Z}_2$ invariants

$$\delta_i = [\det w(\vec{Q}_i)]^{1/2} / \text{Pf}(w)$$

Pfaffian (Pf)

$\vec{Q}_i = \frac{1}{2} \sum_j n_j \vec{b}_j$ — primitive lattice vectors $\quad / \quad \vec{Q}_i = -\vec{Q}_i + \vec{G}$ — reciprocal lattice vector ($\vec{G}$)

$$n_i = 0, 1$$

$$(\text{Pf}(w))^2 = \text{Det}\, w$$

2D: $(-1)^{\nu_0} = \prod_{i=1}^{4} \delta_i$ is the $\mathbb{Z}_2$ invariant (4 points)

3D: $(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i$ (8 points)

strong

$$(-1)^{\nu_k} = \prod_{n_k=1,\, n_{j\neq k}=0,1} \delta_{i=(n_1,n_2,n_3)}$$

weak

In the BHZ model $Q_i = (0,0), (\pi,0), (0,\pi), (\pi,\pi)$

$\delta(0,0) = -\mathrm{sgn}\, M$, $\delta(\pi,0) = -\mathrm{sgn}(M-2) = \delta(0,\pi)$

$\delta(\pi,\pi) = -\mathrm{sgn}(M-4)$

$$\Rightarrow (-1)^{\nu_0} = \delta(0,0)\,\delta(\pi,0)\,\delta(0,\pi)\,\delta(\pi,\pi)$$

$$= \mathrm{sgn}(M)\,\mathrm{sgn}(M-4)$$

$\Rightarrow \nu_0 = 0 \pmod 2$ for $\underline{M<0 \text{ (and } M<4\text{)}}$

(trivial) and $\underline{M>4}$

$\nu_0 = +1 \pmod 2$ If $\underline{0<M \text{ and } M<4}$

$\Rightarrow$ QSH regime

3D TRI Topological TI's

($Bi_{1-x}Sb_x$, HgTe (under strain), Bi_2Se_3, Bi_2Te_3 ...)

(Fu & Kane, 2007; Zhang et al 2009)

Wilson fermion model : 4 ~~sp~~ states per site of a cubic lattice
2 parity, 2 spin

$$H = \sin\vec{p}\cdot\vec{\alpha} + M(\vec{p})\beta$$

$\vec{\alpha}, \beta$ are the 4 Dirac matrices

$$\{\alpha_i, \alpha_j\} = 0 = \{\alpha_i, \beta\}$$

$$\alpha_i^2 = \beta_i^2 = I \qquad \text{(Clifford)}$$

$$M(\vec{p}) = M + \cos p_1 + \cos p_2 + \cos p_3 - 3$$

("Wilson term")

Parities

$$\delta(0,0,0) = -\operatorname{sgn} M$$

$$\delta(\pi,0,0) = \delta(0,\pi,0) = \delta(0,0,\pi) = -\operatorname{sgn}(M-2)$$

$$\delta(\pi,\pi,0) = \delta(\pi,0,\pi) = \delta(0,\pi,\pi) = -\operatorname{sgn}(M-4)$$

$$\delta(\pi,\pi,\pi) = -\operatorname{sgn}(M-6)$$

$$\Rightarrow (-1)^{\nu_0} = \operatorname{sgn}(M)\operatorname{sgn}(M-2)\operatorname{sgn}(M-4)\operatorname{sgn}(M-6)$$

$$(-1)^{\nu_k} = \text{sgn}(M-2)\,\text{sgn}(M-6)$$

Strong $\mathbb{Z}_2$ TI: $0<M<2$ $\big(\nu_0 = 1 \pmod 2$, $(\nu_1,\nu_2,\nu_3) = (0,0,0) \bmod 2\big)$

$2<M<4$ $\big(\nu_0 = 1 \bmod 2$, $(\nu_1,\nu_2\nu_3) = (1,1,1) \bmod 2\big)$

Trivial TI: $\nu_0 = 0 \bmod 2$, $(\nu_1,\nu_2,\nu_3) = (0,0,0) \bmod 2$

<u>2nd quantized H</u>

$$H = \int_{BZ} \frac{d^3p}{(2\pi)^3} \sum_{\alpha,\beta} \Psi^\dagger_\alpha(\vec{p}) \underbrace{\left(\sin\vec{p}\cdot\vec{\alpha} + M(\vec{p})\beta\right)}_{H(\vec{p})}{}_{\alpha\beta}\, \Psi_\beta(p)$$

indices!

$$\gamma_0 = \beta, \quad \gamma^i = \beta\alpha^i, \quad \gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$$

$$\{\gamma_\mu, \gamma_\nu\} = 2 g_{\mu\nu}\mathbb{1}, \quad \{\gamma_\mu, \gamma_5\} = 0$$

$$g_{\mu\nu} = \text{diag}(1,-1,-1,-1)$$

$$\{\gamma_5, H(\vec{p})\} = 0$$

If $u^\pm_\alpha(\vec{p},\sigma)$ are the 4 Dirac spinors

with $E_\pm(p) = \pm\left(\sin^2\vec{p} + M^2(p)\right)^{1/2}$

$$\Rightarrow \gamma_5 u^\pm(p) = u^\mp(p)$$

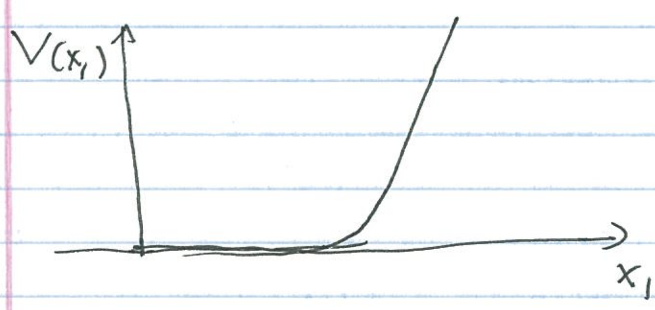
γ_5 maps positive energy states to negative e. states.

Edge states

I) Integer QH state

Consider ~~a~~ N electrons on a plane with a $\perp \vec{B}$ confined to a region ~~B~~ by a potential $V(\vec{r})$

Let $V(\vec{r}) \equiv V(x_1)$



Single particle states (lowest Landau level) $\psi_n(x_1, x_2) = \pm 1\, e^{ik_n x_2}$ ~~B~~

$e^{-\frac{B}{2}(x_1 - k_n/B)^2}$

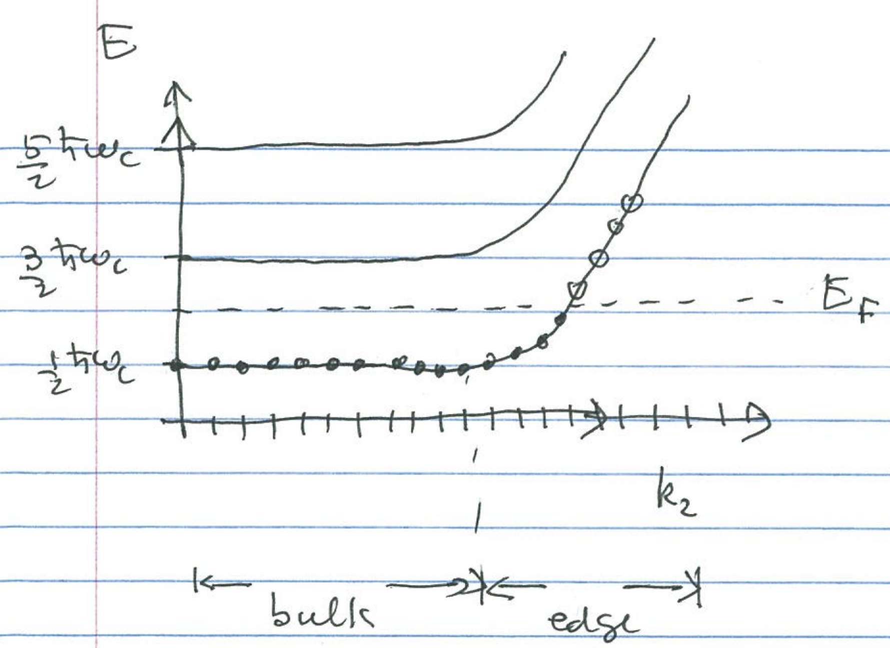
$k_n = \dfrac{2\pi n}{L_2}$ (PBC's on x_2)

$$\Rightarrow \Psi(x_1, x_2) = \sqrt{\frac{B}{\sqrt{\pi} L_2}} \sum_{n=-\infty}^{+\infty} a_n\, e^{ik_n x_2}\, e^{-\frac{B}{2}(x_1 - k_n/B)^2}$$

$$\{a_n, a_m^\dagger\} = \delta_{n,m}$$

1st order shift

$$\Rightarrow E_0(\vec{k}) = \frac{1}{2}\hbar\omega_c + \langle 0, k | V(x_1) | 0, k \rangle + \cdots$$



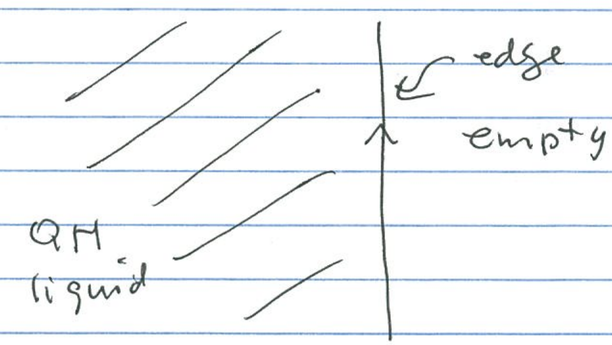
For a linear potential $V(x_1) = V x_1$

$$\Rightarrow (V = -E)$$

$$\Rightarrow E_0(k) = \frac{E}{B} k$$

$$\Rightarrow v_F = \frac{\partial E_0}{\partial k} = \frac{e}{c} \frac{|\vec{E}|}{|B|}$$

$\Rightarrow$



edge states propagates only along the direction determined by the sgn(B)

$\Rightarrow$ The only low energy states are at the edge (bulk is gapped)

Let $j(x_2)$ be the operator that measures the charge localized on some small region Λ near the edge

$$j(x_2) = \int_{-\infty}^{+\infty} dx_1 \, f_\Lambda(x_1) \, \psi^\dagger(x_1, x_2) \, \psi(x_1, x_2)$$

~~cutoff~~ cutoff function

$\Rightarrow$ Fourier Transf.

$$j(x_2) = \sum_{n=-\infty}^{+\infty} e^{-ik_n x_2} \, j_n$$

$$j_n = \sum_{m=-\infty}^{+\infty} a^\dagger_{m+n} \, a_m \, e^{-\frac{B}{4} k_n^2}$$

very small away from the F.S. (regulator)

The fermions are chiral (right moving) with $\varepsilon(k) = v_F k$

$$\Rightarrow H = \int dx_2 \, \psi_R^\dagger(x_2) \, (-i v_F \partial_2) \, \psi_R(x_2)$$

One can prove that

$$[j_n, j_m] = -n \, \delta_{n+m,0} \Leftrightarrow [j(x_2), j(x'_2)] = -\frac{i}{2\pi} \partial_2 \delta(x_2 - x'_2)$$

Let $|0\rangle$ be the Gnd State

Coherent state: $|\theta(x_2)\rangle = e^{i\int dx_2 \, \theta(x_2)\, j(x_2)} |0\rangle$

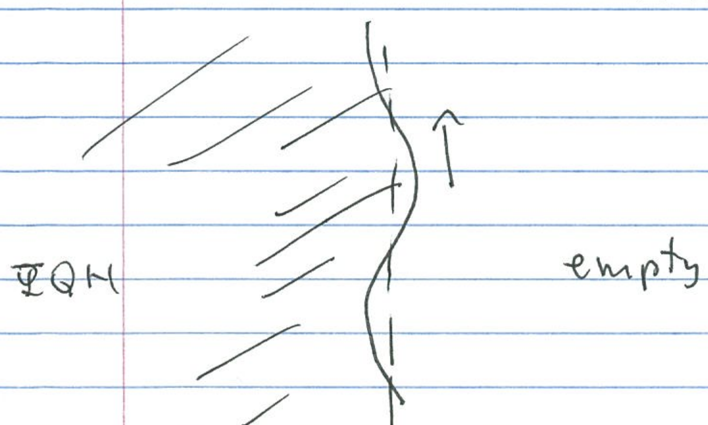
$j(x_2)|0\rangle = 0$ (normal ordering)

$\Rightarrow j(x_2)|\theta(x_2)\rangle = \frac{1}{2\pi} \partial_2 \theta(x_2) |\theta(x_2)\rangle$

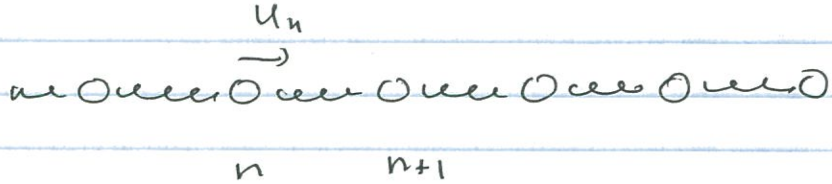
$$e^{-i\int dx_2' \, \theta(x_2')\, j(x_2')} \, j(x_2) \, e^{+i\int dx_2' \, \theta(x_2')\, j(x_2')}$$

$$= j(x_2) + \frac{1}{2\pi} \partial_2 \theta(x_2)$$

$\Rightarrow |\theta(x_2)\rangle$ is a distortion of the edge that travels at v_F



Polyacetylene and Fractional Charge



"$(CH)_n$"

one Spin $1/2$ fermion at each site (half-filling)

$$H = -\sum_{n,\sigma}\left(t_{n,n+1}\,\psi^{\dagger}_{n,\sigma}\,\psi_{n+1,\sigma} + h.c.\right)$$

$$+ \sum_{n} \frac{D}{2}\left(u_{n+1}-u_n\right)^2 + \sum_{n} \frac{P_n^2}{2M}$$

ions

$$[u_m, P_n] = i\,\delta_{m,n}$$

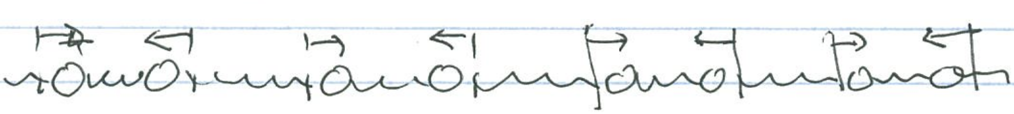
$$\{\psi_{n,\sigma}, \psi^{\dagger}_{n',\sigma'}\} = \delta_{n,n'}\,\delta_{\sigma\sigma'}$$

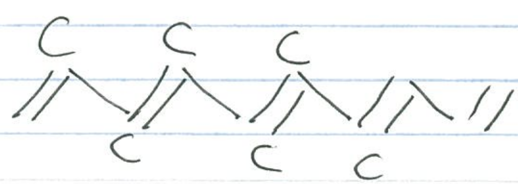
If $|u_{n+1}-u_n| \ll a$

$$t_{n,n+1} \cong t - \alpha\,(u_{n+1}-u_n)$$

electron-phonon coupling

$$\langle u_n\rangle = (-1)^n \Delta \qquad \text{(dimerization)}$$





period 2 CDW

$$\psi_{n,\sigma} = e^{i\pi n/2}\,\psi_{R,\sigma}(x) + e^{-i\pi n/2}\,\psi_{L,\sigma}(x)$$

$$p_F = \frac{\pi}{2}$$

$$\psi_{1,\sigma} = \frac{1}{\sqrt{2}}\left(-\psi_{R,\sigma} + \psi_{L,\sigma}\right)$$

$$\psi_{2,\sigma} = \frac{1}{\sqrt{2}}\left(\psi_{R,\sigma} + \psi_{L,\sigma}\right)$$

$$u_n = u_0(x) + (-1)^n \Delta$$

acoustic phonon   optical phonon

$$Q = 2p_F = \pi$$

Eff. Low Energy Theory

$$\mathcal{H} = \psi^{\dagger}_{a,\sigma}(x)\left(-i v_F \sigma_1 \partial_x\right)\psi_{a,\sigma}(x)$$

$$+ g\,\Delta(x)\,\bar{\psi}_\sigma(x)\,\psi_\sigma(x) + \frac{1}{8Ma_0^2}\,\Pi^2(x)$$

$$+ \frac{1}{2}\Delta^2(x) \quad ; \quad \left[\Delta(x), \Pi(y)\right] = i\delta(x-y)$$

discrete chiral symmetry : $\psi \to \gamma_5 \psi$, $\Delta \to -\Delta$

$$\gamma_5 = \alpha = \sigma_1,\ \gamma_0 = \beta = \sigma_3,\ \gamma_1 = i\sigma_2 ;$$

$v_F = 2t$, $g = \frac{\alpha}{\sqrt{Dt}}$

M: mass of CH group (heavy) ("adiabatic")

If $M \to \infty \Rightarrow \Delta(x)$ is classical $\Rightarrow$ MFT

$$\Delta_0 = \frac{2\Lambda v_F}{g} e^{-\pi v_F/g^2} \qquad \Lambda \approx \frac{\pi}{a_0}$$

Anti-adiabatic limit: $M \to 0$

$$\mathcal{L} = \bar{\psi}_\sigma(x)\, i\gamma^\mu \partial_\mu \psi_\sigma(x) + g^2 \left(\bar{\psi}_\sigma(x) \psi_\sigma(x)\right)^2$$

(N=2 Gross-Neveu model)

~~B~~ RG: $\beta(g) = a_0 \frac{\partial g}{\partial a_0} = \frac{(N-1)}{\pi} g^3 + \dots$

$(N=2) \Rightarrow$ marginally relevant
(assymptotically free)

$\Rightarrow \langle \bar{\psi}_\alpha \psi_\sigma \rangle \neq 0 = g \langle \Delta \rangle$

Soliton: domain wall of the dimerized state

$$\Delta(x) \xrightarrow[x \to \pm\infty]{} \pm \Delta_0$$

$g\,\Delta(x)$ is a slowly varying mass