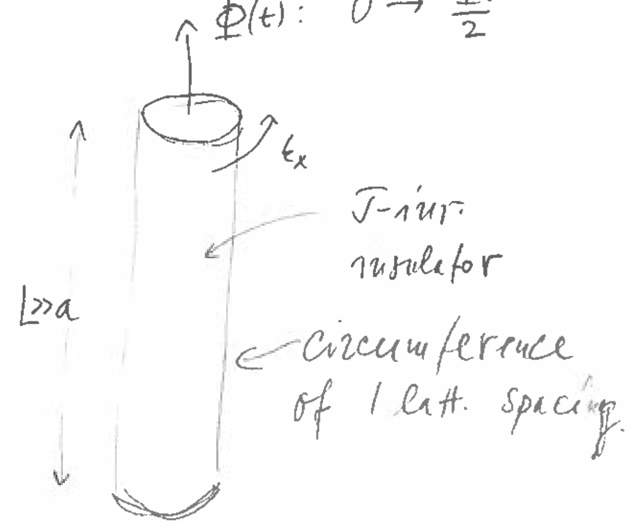
Mathematics of the $\mathbb{Z}_2$ invariant

Fu & Kane, PRB 74, 195312 (2006)

- Physical meaning
- Can it be calculated in the bulk?

The $\mathbb{Z}_2$ invariant is related to a quantity called "Time-reversal polarization" analogous to charge polarization in 1D systems.



Allowed values of momenta k_x

$$e^{ik_x\cdot(x+a)} = e^{i\chi}e^{ik_x\cdot x}$$

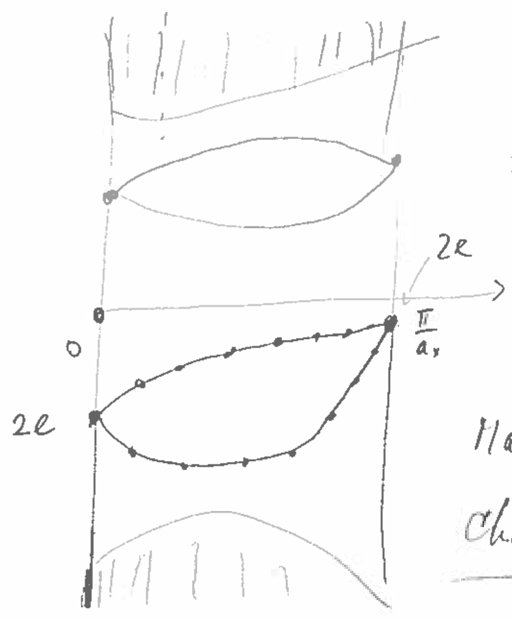
Aharonov-Bohm phase.

$$\Rightarrow \quad k_x = \frac{\chi}{a} \qquad \chi = \frac{e}{\hbar c}\int_0^a \vec{A}\cdot d\vec{\ell}$$

$$= \frac{2\pi}{a}\frac{\Phi(t)}{\Phi_0} \qquad = \frac{e}{\hbar c}\Phi(t)$$

$$= 2\pi\frac{\Phi(t)}{\Phi_0}$$

$$\Phi_0 = \frac{hc}{e} \quad \text{(flux quantum}$$

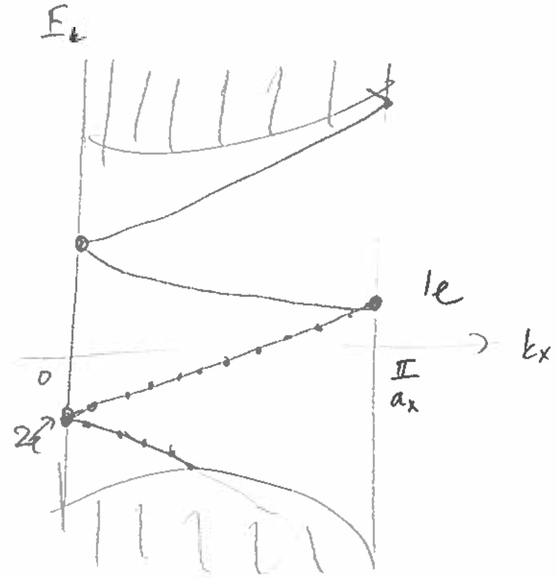


$$\Phi(t):\ 0 \to \frac{\Phi_0}{2}$$

$$k_x = 2\pi\frac{\Phi(t)}{\Phi_0}$$

$\nearrow$ TR polarization is ZERO

Many body ground state degeneracy does not change as $\Phi(t)$ goes from $0 \to \frac{1}{2}\Phi_0$

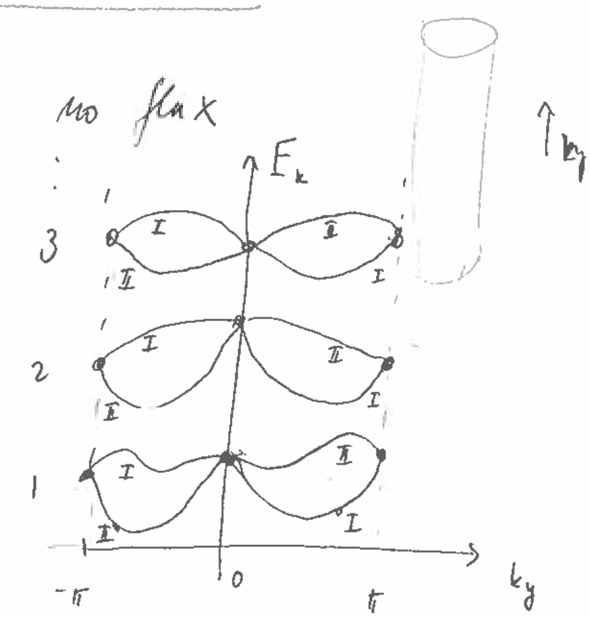


Many-body ground state degeneracy has changed.

TR polarization is non-zero.

TR polarization calculated from the bulk

Consider an INFINITE cylinder with no flux



TRS implies:

$$|u^{I}_{-k\alpha}\rangle = -e^{i\chi_{k\alpha}}\,\Theta\,|u^{II}_{k\alpha}\rangle$$

1)

$$|u^{II}_{-k\alpha}\rangle = e^{i\chi_{-k\alpha}}\,\Theta\,|u^{I}_{k\alpha}\rangle \qquad \alpha = 1,2,3\ldots$$

$$\Theta = i s_y K \quad (J\text{-operator}), \quad \Theta^2 = -1$$

$$\Theta|u^{I}_{-k\alpha}\rangle = e^{-i\chi_{+k\alpha}}\,|u^{II}_{k\alpha}\rangle$$

Define "partial" polarization

$$P^s = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, \mathcal{A}^s(k)\,, \qquad s = I, II$$

$$\mathcal{A}^s(k) = i \sum_{\alpha\in occ} \langle u^s_{k\alpha} | \nabla_k | u^s_{k\alpha}\rangle$$

- P^s is gauge invariant, but depends on arbitrary label s

Massage:

$$P^I = \frac{1}{2\pi}\int_0^{\pi} dk \left[\mathcal{A}^I(k) + \mathcal{A}^I(-k)\right]$$

$$\mathcal{A}^I(-k) = -i \sum_{\alpha}^{(1)\leftarrow occ} \langle \theta u^{II}_{k\alpha} | e^{-i\chi_{k\alpha}} \nabla_k e^{i\chi_{k\alpha}} | \theta u^{II}_{k\alpha} \rangle$$

$$= \mathcal{A}^{II}(k) - \sum_\alpha{}' \nabla_k \chi_{k\alpha}$$

$\Downarrow$

$$\boxed{P^I = \frac{1}{2\pi}\left[\int_0^{\pi} dk\, \mathcal{A}(k) - \sum_n{}' (\chi_{\pi\alpha} - \chi_{0\alpha})\right]} \qquad \mathcal{A}(k) = \mathcal{A}^I(k) + \mathcal{A}^{II}(k)$$

Define a unitary matrix for each k

$$w_{mn}(k) = \langle u_{-km} | \theta | u_{kn}\rangle\,, \qquad w^\dagger w = \mathbb{1} \quad \text{check!}$$

Using Eq (1) we deduce the following structure for $w_{mn}(k)$:

$$w(k) = \mathrm{diag}\left(W_1(k), W_2(k), \ldots W_N(k)\right) \qquad W_\alpha(k) = \begin{pmatrix} 0 & e^{i\chi_{k\alpha}} \\ -e^{i\chi_{k\alpha}} & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & e^{i\chi} \\ -e^{i\chi} & 0 \end{pmatrix}\begin{pmatrix} 0 & -e^{-i\chi} \\ e^{i\chi} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

At TR momenta, $k = 0, \pi$, $w(k)$ is ANTISYMMETRIC and can be characterized by a Pfaffian.

- <u>Digression on Pfaffians</u>

For every $2N \times 2N$ antisymmetric (complex) matrix A one can define a Pfaffian, such that

$$\det(A) = [Pf(A)]^2 \qquad \text{or} \qquad Pf(A) = \pm\sqrt{\det(A)}$$

For a 2×2 matrix $\quad A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}, \quad Pf(A) = a$

$$A' = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix}, \quad Pf(A') = -a$$

$$\det(A) = \det(A') = a^2$$

Recursive def:

$$Pf(A) = \sum_{j=2}^{2N} (-1)^j a_{1j}\, Pf(A_{\hat{j}\hat{1}})$$

$A_{\hat{j}\hat{1}}$ is matrix A with both 1^{st} and j-th row and column removed.

Useful relations

$$Pf[XAX^T] = \det(X)\, Pf(A)$$

$$Pf[A^T] = (-1)^N\, Pf(A)$$

$$Pf[\lambda A] = \lambda^N\, Pf(A)$$

Back to physics:

It is easy to show that

$$\exp\left[i\sum_\alpha (\chi_{\pi\alpha} - \chi_{0\alpha})\right] = \frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}$$

$$\Rightarrow \quad P^{I} = \frac{1}{2\pi}\left(\int_0^\pi dk\, \mathcal{A}(k) + i\ln\left[\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right]\right)$$

Similarly

$$P^{II} = \frac{1}{2\pi}\left[\int_{-\pi}^{0} dk\, \mathcal{A}(k) - i\ln\left[\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right]\right]$$

Charge polarization

$$P = P^{I} + P^{II} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, \mathcal{A}(k) \qquad \checkmark$$

TR Polarization

$$P_\theta = P^{I} - P^{II} = \frac{1}{2\pi}\left\{\int_0^\pi dk\, \mathcal{A}(k) - \int_{-\pi}^{0} dk\, \mathcal{A}(k) + 2i\ln\left[\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right]\right\}$$

$$= \frac{1}{2\pi i}\left\{\int_0^\pi dk\, \mathrm{Tr}\left[w^+ \nabla_k w\right] - 2\ln\left(\frac{\mathrm{Pf}[w(\pi)]}{\mathrm{Pf}[w(0)]}\right)\right\} \qquad \text{check!}$$

$$\mathrm{Tr}\left[w^+ \nabla_k w\right] = \mathrm{Tr}\left[\nabla_k \ln w\right] = \nabla_k \mathrm{Tr}\ln(w) = \nabla_k \ln\det(w)$$

$$\nabla_k \ln w = w^{-1}\nabla_k w = w^+ \nabla_k w \qquad (w \text{ is unitary})$$

$$\int_0^{\pi} dk\ \mathrm{Tr}\left[W^{+}\nabla_k W\right] = \int_0^{\pi} dk\ \nabla_k \ln\det(W) = \ln\frac{\det[W(\pi)]}{\det[W(0)]}$$

$$\underbrace{P_\theta = \frac{1}{2\pi i}\left\{\ln\frac{\det[W(\pi)]}{\det[W(0)]} - 2\ln\frac{\mathrm{Pf}[W(\pi)]}{\mathrm{Pf}[W(0)]}\right\}}$$

Now since $\det(W) = \mathrm{Pf}^2(W)$ it would appear that $P_\theta = 0$.

(Denote $z = \dfrac{\mathrm{Pf}[W(\pi)]}{\mathrm{Pf}[W(0)]}$, $P_\theta = \dfrac{1}{2\pi i}\left[\ln z^2 - 2\ln z\right]$)

Since z is complex, one must be careful

Note W is unitary ($W^{+}W = 1$), thus $|\det(W)| = |\mathrm{Pf}(W)| = 1$

$$1 = \det(W^{+}W) = \det(W^{+})\det(W) = [\det(W^{T})]^{*}\det(W) = |\det(W)|^2$$

$\Rightarrow \quad |z| = 1 \qquad z = e^{i\varphi}$

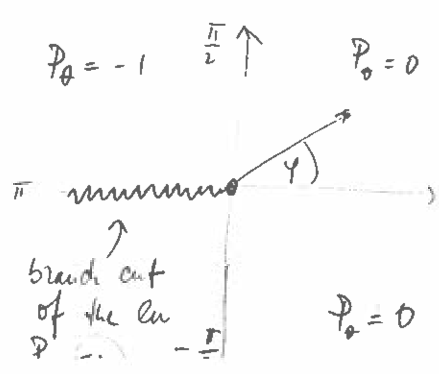
$\ln e^{i\alpha} = i\alpha$, $\alpha \in (-\pi, \pi)$

$\varphi \in (\frac{\pi}{2}, \pi)$: $2\ln e^{i\varphi} = 2i\varphi$

but $\ln e^{2i\varphi} = \ln e^{2i\varphi - 2\pi i} = 2i\varphi - 2\pi i$

$$P_\theta = \frac{1}{2\pi i}\left[\ln(e^{2i\varphi}) - 2\ln(e^{i\varphi})\right] = \cancel{\frac{1}{2\pi i}\left(i\arg(2\varphi) - 2i\arg(\varphi)\right)}$$

$$= \begin{cases} 0 & -\frac{\pi}{2} < \varphi < \frac{\pi}{2} \\ -1 & \frac{\pi}{2} < \varphi < \pi \\ +1 & -\pi < \varphi < -\frac{\pi}{2} \end{cases}$$



P_Θ = integer but only even and odd values are distinct

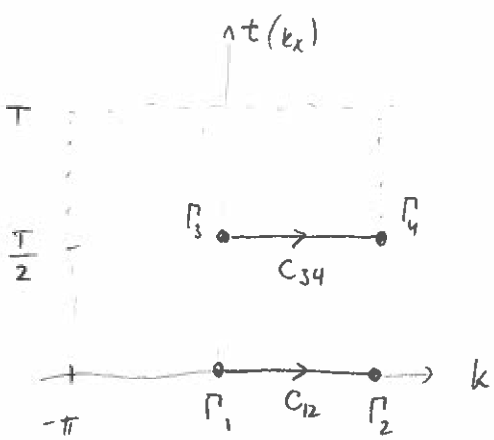
$P_\Theta = 0, 1$ $\qquad$ $\mathbb{Z}_2$ index

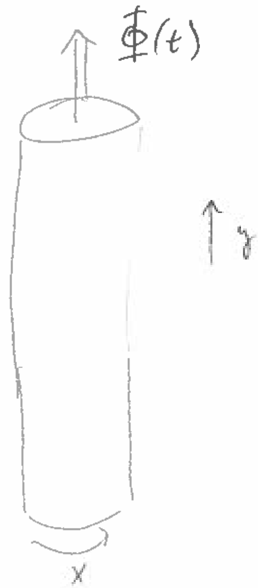
$$\boxed{(-1)^{P_\Theta} = \frac{\sqrt{\det[w(0)]}}{Pf[w(0)]} \cdot \frac{\sqrt{\det[w(\pi)]}}{Pf[w(\pi)]}}$$

TR polarization in a 1D system

The branches of $Pf[w] = \pm\sqrt{\det[w]}$ must be chosen such that the branch chosen at $k=0$ evolves continuously into the branch chosen at $k=\pi$.

Back to 2D system





$\mathbb{Z}_2$ index: $\qquad \nu = \left[P_\Theta\left(\frac{T}{2}\right) - P_\Theta(0)\right] \bmod 2$

$$\boxed{(-1)^\nu = \prod_{i=1}^{4} \delta_i, \quad \delta_i = \frac{\sqrt{\det w(\Gamma_i)}}{Pf\, w(\Gamma_i)} = \pm 1}$$

$\mathbb{Z}_2$ index for a 2D insulator.