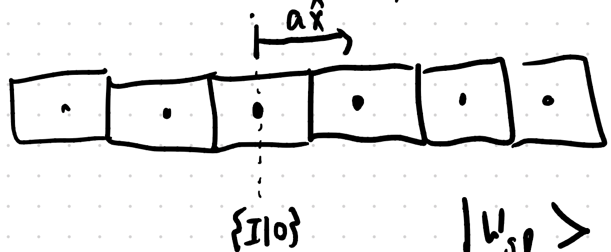
Lecture 20

1D Chain w/ Inversion & Time-reversal symmetry



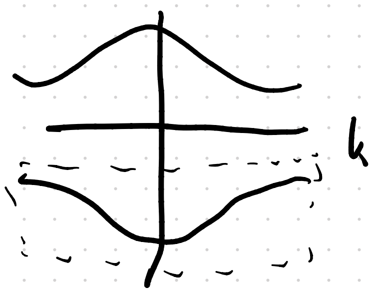
$|w_{sR}\rangle$

$|w_{pR}\rangle$

$$h(k) = (\Delta + t_1 \cos ka)\,\sigma_z + t_2 \sin ka\, \sigma_y$$

$$B(I) = \sigma_z$$

$$B(T) = \mathcal{K}$$



Energies: $\varepsilon_{\pm}(k) = \pm\sqrt{(\underline{\Delta + t_1 \cos ka})^2 + (t_2 \sin ka)^2}$

$t_2 \neq 0$

$\Delta = t_1 \rightarrow$ energy gap closes

$\Delta = -t_1$

Lets compute the Berry phase for the negative energy band in two limits:

1. $t_1 = t_2 = 0, \ \Delta > 0$

$$h(k) \to \Delta \sigma_z = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} \qquad \varepsilon_{\pm}(k) = \pm \Delta$$

$$h(k) u_{\pm k} = \varepsilon_{\pm}(k) u_{\pm k}$$

$$u_{+k} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad u_{-k} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\psi_{\pm k}\rangle = \sum_a u^a_{\pm k} |\chi_{ak}\rangle = |\chi_{s_p \vec{k}}\rangle$$

tight-binding Berry connection: $A^{--} = i u^{\dagger}_{-k} \frac{\partial}{\partial k} u_{-k} = 0$

tight-binding Berry phase: $\varphi = \int_0^{2\pi/a} dk\, A^{--} = 0$

What does this mean?

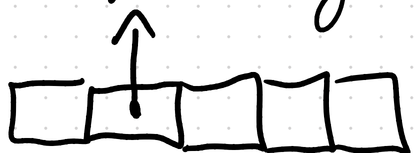
PxP eigenvalues: $na + \frac{a}{2\pi}\hat{\cancel{\varphi}}^{\,0} \quad n \in \mathbb{Z}$

→ Wannier functions are centered at the origin of each unit cell

$|\psi_{\pm k}\rangle = \sum_a u^a_{\pm k} |\chi_{ak}\rangle = |\chi_{{s \atop p} \vec{k}}\rangle$

$|\psi_{-k}\rangle = |\chi_{pk}\rangle = \sum_n e^{ik(na)} |W_{p\, na}\rangle$

$|W_{-na}\rangle = |W_{pna}\rangle$ - Wannier fns in this limit are just tight-binding basis functions.



$|W_{R}\rangle = |W_{pna}\rangle$

$t_1 = t_2 = 0$

$\Delta > 0$

② $\Delta = 0$, $t_1 = t_2 = t > 0$

$$h(k) = (0 + t\cos ka)\sigma_z + t\sin ka\,\sigma_y$$

$$\varepsilon_\pm = \pm\sqrt{(t\cos ka)^2 + (t\sin ka)^2} = \pm|t|$$

$$h(k) = t\,\hat{n}\cdot\vec{\sigma}$$

$$\hat{n} = (\sin\theta_k\cos\varphi_k, \sin\theta_k\sin\varphi_k, \cos\theta_k)$$

$$u_{+k} = \begin{pmatrix} \cos \frac{\theta_k}{2} \\ e^{i\varphi_k} \sin \theta_k/2 \end{pmatrix}$$

$$\theta_k = ka$$
$$\varphi_k = \pi/2$$

$$u_{-} = \begin{pmatrix} \sin \theta_k/2 \\ -e^{i\varphi_k} \cos \theta_k/2 \end{pmatrix}$$

$$u_{-k} = \begin{pmatrix} \sin \frac{ka}{2} \\ -i\cos \frac{ka}{2} \end{pmatrix} e^{-ika/2}$$

$$\left[u_{+k} = \begin{pmatrix} \cos ka/2 \\ i \sin ka/2 \end{pmatrix} e^{-ika/2} \right]$$

We need $u_{\pm,k+\frac{2\pi}{a}} \overset{!}{=} u_{\pm,k}$

$$u_{-k} = \frac{-i}{2}\begin{pmatrix} 1-e^{-ika} \\ 1+e^{-ika} \end{pmatrix} \checkmark$$

$$A^{--} = i\, u_{-k}^{\dagger} \frac{\partial}{\partial k} u_{-k}$$

$$= i\left[\frac{i}{2}\left(1-e^{ika},\, 1+e^{ika}\right)\right]\left[-\frac{i}{2}\begin{pmatrix} ia e^{-ika} \\ -ia e^{-ika} \end{pmatrix}\right]$$

$$= \frac{i}{4}\left[\cancel{iae^{-ika}} - ia - \cancel{iae^{-ika}} - ia\right] = \frac{a}{2}$$

Berry phase: $\varphi = \int_0^{2\pi/a} dk\, A^{--} = \frac{a}{2}\left(\frac{2\pi}{a}\right) = \pi$

Physically: PxP eigenvalues $na + \frac{a}{2\pi}\varphi \quad n \in \mathbb{Z}$

$na + \frac{a}{2}$

Wannier functions in this limit are centered at the boundary between unit cells

Bloch eigenstates

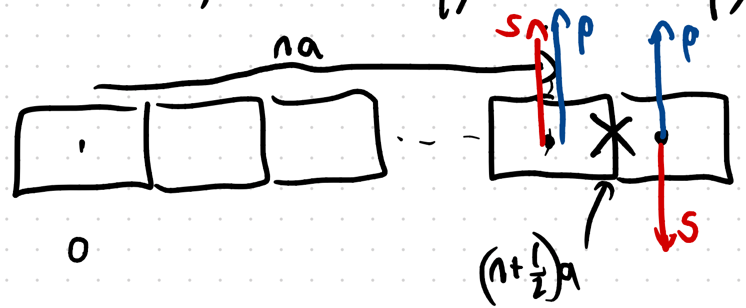
$$|\psi_{-k}\rangle = \sum_{a\,n} u^{a}_{-k} e^{ikna} |W_{a\,na}\rangle$$

$$= -\frac{i}{2} \sum_{n} e^{ikna} \Big(|W_{s,na}\rangle - e^{-ika} |W_{s,na}\rangle$$

$$+|W_{p,na}\rangle + e^{-ika}|W_{p,na}\rangle\Big)$$

$$= \frac{-i}{2}\sum e^{ikna}\Big(|W_{s,na}\rangle - |W_{s,(n+1)a}\rangle + |W_{p,na}\rangle + |W_{p,(n+1)a}\rangle\Big)$$

$$|W_{-,na}\rangle = \frac{-i}{2}\Big(|W_{s,na}\rangle + |W_{p,na}\rangle + |W_{p,(n+1)a}\rangle - |W_{s,(n+1)a}\rangle\Big)$$



Inversion symmetry & Wannier centers:

PxP

P is invariant under inversion

$x \to -x$ under inversion

if we have inversion symmetry, and if $|w\rangle$ is an eigenvector of PxP

$$PxP|w\rangle = r|w\rangle$$

then $U_I|w\rangle$ is also an eigenvector of PxP w/ eigenvalue

$$PxP\,U_I|w\rangle = r_I U_I|w\rangle$$

$$r_I = -r$$

The spectrum of PxP is closed under inversion

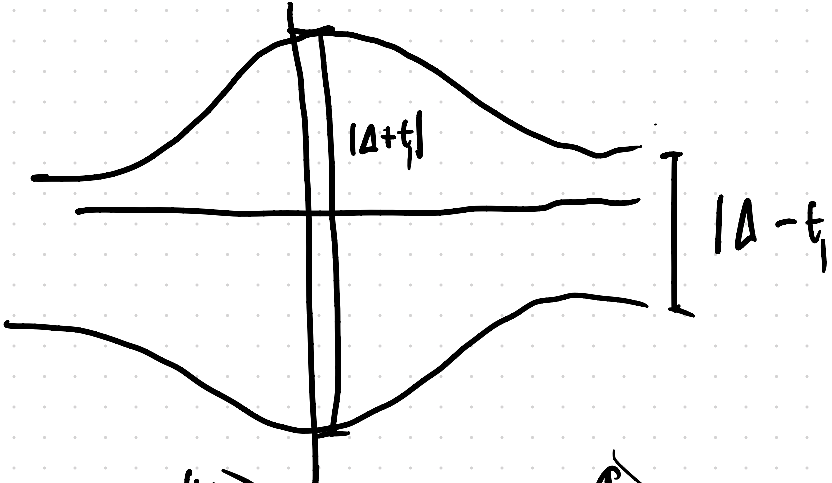
For a single occupied band: $\left\{ na + \frac{a\varphi}{2\pi}, n \in \mathbb{Z} \right\}$

for this to be closed under inversion,

$$-na - \frac{a\varphi}{2\pi} = ma + \frac{a\varphi}{2\pi}$$

$$\Rightarrow \varphi = \begin{cases} 0 \\ \pi \end{cases}$$

$\boxed{\text{Inversion symmetry quantizes the Berry phase for a single occupied band}}$



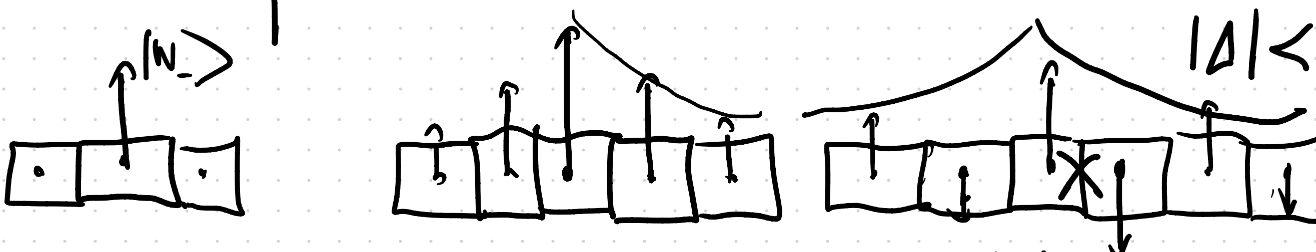
$t_1=t_2=0 \quad \Delta\neq 0$

$\varphi=0$

$t_2\neq 0$

$|\Delta|>|t_1| \to \varphi=0$

$|\Delta|<|t_1| \to \varphi=\pi$



$t_1=t_2=0$ $\qquad |\Delta|>|t_1|$, $t_2=0$ $\qquad |\Delta|<|t_1|$

Tight-Binding Wilson loop

Projection operator in terms of H

$$P=\sum_{n\ \text{occupied}} |\psi_n\rangle\langle\psi_n|$$

tight-binding projection operator

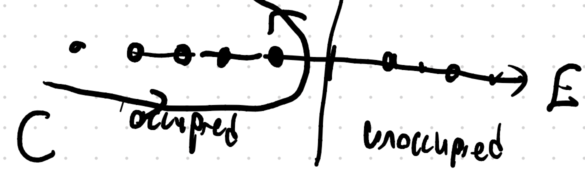
$$\tilde{P}_{ab}(\vec{k}) = \sum_{n=1}^{N_{occ}} u^{a}_{nk}\left(u^{b}_{nk}\right)^{*}$$

$$W^{nm}_{k_\mu \leftarrow 0}(\vec{k}_\perp) = \vec{u}^{\dagger}_{nk_\mu,k_\perp} \cdot \prod_{k'_\mu}^{k_\mu \leftarrow 0} \tilde{P}(k'_\mu,k_\perp) \cdot \vec{u}_{m0,k_\perp}$$

$$= P e^{i\int dk'_\mu A^{+b}_\mu (k'_\mu, k_\perp)}$$

Symmetries: $g = \{\bar{g} | \vec{s}\}$

$$U_g|\chi_{ak}\rangle = |\chi_{b\,\bar{g}k}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k\cdot\vec{s}}$$



$$1 = \frac{1}{2\pi i}\oint \frac{dz}{z-E_n}$$

$$P = \frac{1}{2\pi i}\oint_C \frac{1}{z-H}\,dz$$

$$= \frac{1}{2\pi i}\sum_{n}^{\text{all states}}\oint_C dz\,\frac{|\psi_n\rangle\langle\psi_n|}{z-E_n}$$