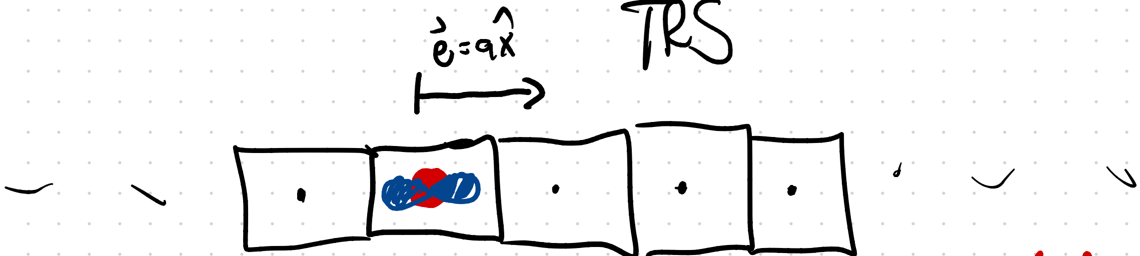
Lecture 20

Recap: 1D crystal w/ inversion & TRS



Basis Wannier functions

$|W_{s\vec{R}}\rangle$, $|W_{p\vec{R}}\rangle$

$i = s, p$

$\langle W_{iR} | W_{jR'} \rangle = \delta_{ij} \delta_{RR'}$

$B(I) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z$

$\langle W_{iR} | X | W_{jR'} \rangle = \delta_{ij} \delta_{RR'} R$

$B(T) = \sigma^0 K$

Nearest-Neighbor tight-binding model

$$h(k) = [\mu + \mu_1 \cos ka]\,\sigma^0 + (\Delta + t_1 \cos ka)\,\sigma^z + t_2 \sin ka\,\sigma^y$$

overall zero of energy

$t_{ss} = \frac{\mu_1 + t_1}{2}$ s-s hopping

$\frac{t_2}{2}$ s-p hopping

$t_{pp} = \frac{\mu_1 - t_1}{2}$ p-p hopping

Δ - relative on-site energy

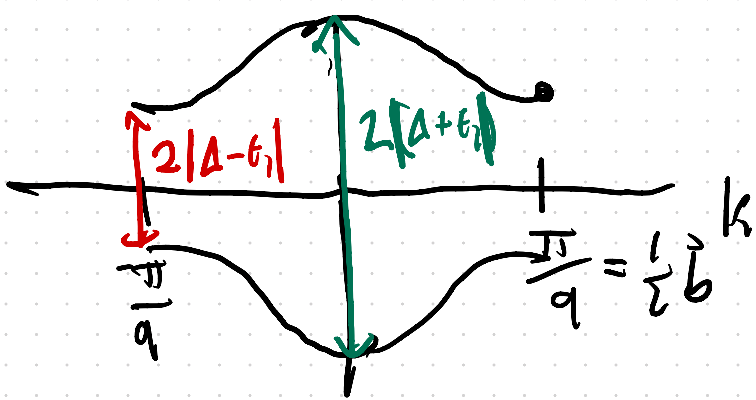
$$\varepsilon_\pm(k) = (\mu + \mu_1 \cos ka) \pm \sqrt{(\Delta + t_1 \cos ka)^2 + t_2^2 \sin^2 ka}$$

$\mu = 0$
$\mu_1 = 0$ wolog

When is there a gap between ε_+ and ε_-

$|\Delta| > |t_1|$ - gap

$t_2 \neq 0$, $|\Delta| \neq |t_1|$ - gap



one e^- per unit cell → insulator w/ one filled band

$$h(k) = (\Delta + t_1 \cos ka)\sigma^z + t_2 \sin ka\, \sigma^y$$

Little group irreps @ high-symmetry points

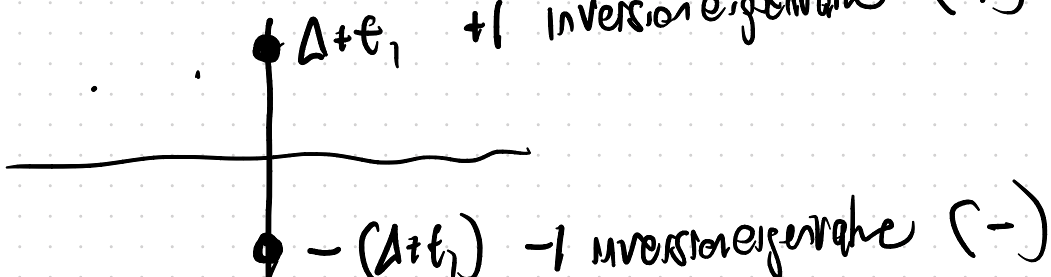
$$G = \langle \{I|0\}, \{E|a\hat{x}\}, TRS \rangle$$

$$B(I) = \sigma^z$$

$k=0$ (Γ) $G_\Gamma = G$

$k = \frac{\pi}{a} = \frac{1}{2} b$ (X) $G_X = G$

Γ: $h(\Gamma) = (\Delta + t_1)\sigma_z$



$\Delta + t_1 > 0$; $\varepsilon_-(0)$ state has inversion eigenvalue -1

$\varepsilon_+(0)$ state has inversion eigenvalue $+1$

$\Delta + t_1 < 0$; $\varepsilon_+(0)$ state has inversion eigenvalue -1

$\varepsilon_-(0)$ state has inversion eigenvalue $+1$

X ; $h(X) = (\Delta - t_1)\sigma_z$

$B(I) = \sigma^z$

$V(b) = \sigma^0$

$\Delta - t_1 > 0$: $\varepsilon_-(X)$ state has inversion eigenvalue -1

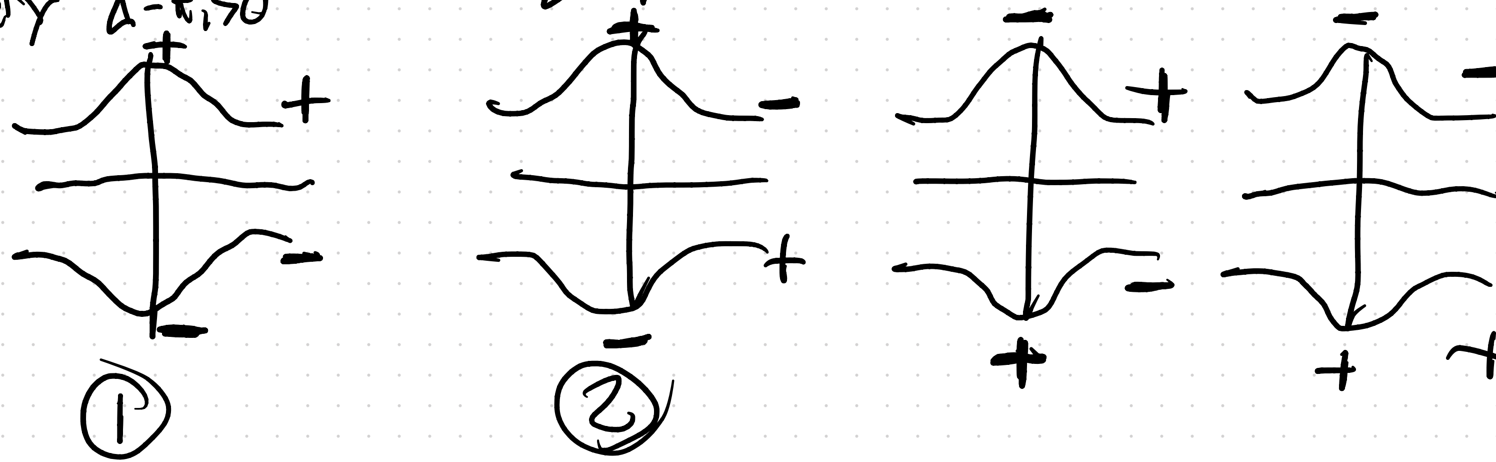
$\varepsilon_+(X)$ state has inversion eigenvalue $+1$

$\Delta - t_1 < 0$: $\varepsilon_+(X)$ state has inversion eigenvalue -1

$\varepsilon_-(X)$ state has inversion eigenvalue $+1$

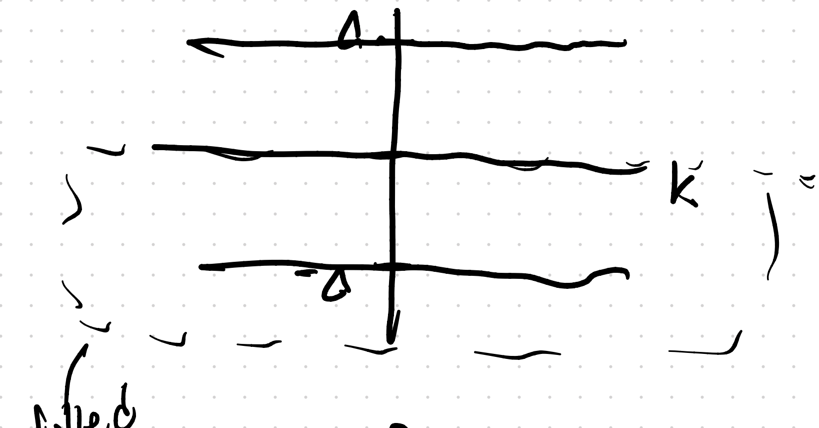
Summary

$\Delta + t_2 > 0$	$\Delta + t_2 > 0$	$\Delta + t_2 < 0$	$\Delta + t_2 < 0$
$\Delta - t_1 > 0$	$\Delta - t_1 < 0$	$\Delta - t_1 > 0$	$\Delta - t_1 < 0$



Look @ two easy to solve limits to find Berry phase, polarization, & Wannier functions & relate these to inversion eigenvalues

① $\Delta > 0,\ t_1 = t_2 = 0$ $\quad h(k) = \Delta\sigma^z = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix}$



$$h(k)\vec{u}_{\pm k} = \varepsilon_{\pm}(k)\vec{u}_{nk}$$

$$\vec{u}_{+k} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \vec{u}_{-k} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Berry connection $A^{-}(k) = i\vec{u}_{-k}^{\dagger} \cdot \dfrac{\partial u_{-k}}{\partial k} = 0$

Berry phase $\varphi_{--} = \int_0^{2\pi/a} dk\, A^{--}(k) = 0$

$P x P$ has eigenvalues $\lambda_n = na + \frac{a}{2\pi}\overset{0}{\cancel{\varphi_{--}(k)}} = na$

$n \in \mathbb{Z}$

$\Rightarrow$ Wannier functions for $-$ band are centered @ origin of the unit cell

Lecture 14/15: HWF for 1 occupied band

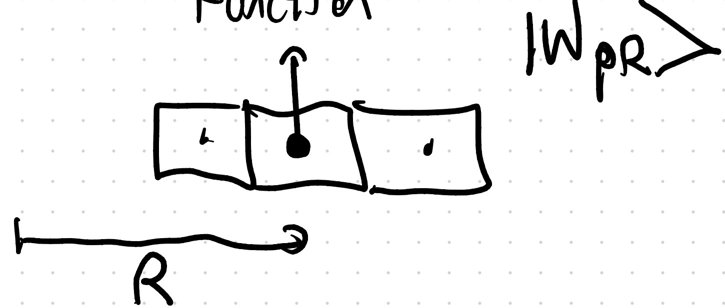
$$|W_{-R}\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk\, |\psi_{-k}\rangle e^{-ikR} e^{i\left[\int_0^k dk' \overset{0}{\cancel{A(k')}} - \frac{ka}{2\pi}\overset{0}{\cancel{\varphi_{--}}}\right]}$$

For us (tb) $|\psi_{-k}\rangle = \sum_{i=s,p} |\chi_{ik}\rangle u^{i}_{-k}$

$= |\chi_{pk}\rangle$

$$|W_{-R}\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk\, |\chi_{pk}\rangle e^{-ik\cdot R} = |W_{pR}\rangle$$

Wannier fn is just our position space basis function



② More interesting limit $\Delta = 0 \quad t_1 = t > 0$

$t_2 = t$

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

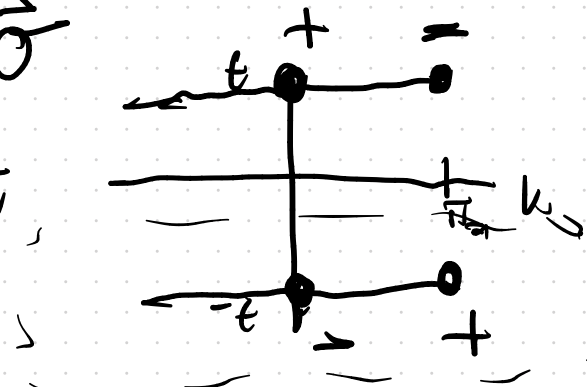
$$\hat{n} = (0, \sin ka, \cos ka)$$

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

$$\theta = ka$$

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

$$\varepsilon_{\pm}(k) = \pm t$$



Eigenstates:

spin in a B-field

$$u_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} \qquad u_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix}$$

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

But theres a problem $\quad u_{\pm,k+\frac{2\pi}{a}} = u_{\pm,k}$

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

Berry connection

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

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

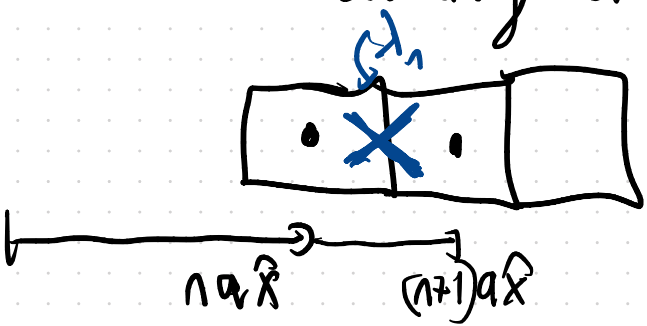
$$= \frac{i}{4}\left[ia\,e^{-ika}\left(\cancel{1}-e^{+ika}\right) - ia\,e^{-ika}\left(\cancel{1}+e^{+ika}\right)\right]$$

$$= \frac{i}{4}\left(-ia - ia\right) = \frac{a}{2}$$

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

PxP has eigenvalues $\lambda_n = na + \frac{a}{2\pi}\varphi_{--} = \left(n+\frac{1}{2}\right)a,\ n\in\mathbb{Z}$

$\Rightarrow$ in this limit Wannier functions are centered at the boundary of unit cell's



$$|\psi_{-k}\rangle = \sum_{i=s,p} |\chi_{ik}\rangle u^{i}_{-k}$$

$$= -\frac{i}{2}\left[(1-e^{-ika})|\chi_{sk}\rangle + (1+e^{-ika})|\chi_{pk}\rangle\right]$$

$$|W_{-R}\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk\, |\psi_{-k}\rangle e^{-ikR}\, e^{i\left[\int_0^k dk' \cancel{A}(k') - \frac{ka}{2\pi}\cancel{\phi}\right]}$$

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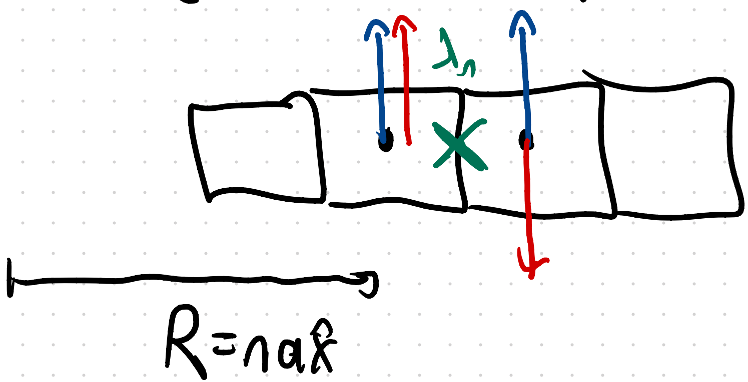
$$= \frac{a}{2\pi}\int_0^{2\pi/a} dk\, e^{-ikR}\left(-\frac{i}{2}\right)\left[(1-e^{-ika})|\chi_{sk}\rangle + (1+e^{-ika})|\chi_{pk}\rangle\right]$$

$$= \frac{-ia}{4\pi}\int_0^{2\pi/a} dk \Big[e^{-ik\cdot R} |\chi_{sk}\rangle + e^{-ik\cdot R} |\chi_{pk}\rangle$$

$$- e^{-ik\cdot(R+a)} |\chi_{sk}\rangle + e^{-ik\cdot(R+a)} |\chi_{pk}\rangle$$

$$= \frac{-i}{2} \Big(|W_{sR}\rangle + |W_{pR}\rangle + |W_{p\,R+a}\rangle - |W_{s\,R+a}\rangle \Big)$$



Going beyond flat band limits: What about $\mathcal{I}$

if $U_{\mathcal{I}} H U_{\mathcal{I}}^{\dagger} = H$

$\rightarrow U_{\mathcal{I}} P U_{\mathcal{I}}^{\dagger} = P$

$U_{\mathcal{I}} x U_{\mathcal{I}}^{\dagger} = -x$ by definition

$U_{\mathcal{I}} PxP U_{\mathcal{I}}^{\dagger} = -PxP$

if $|w\rangle$ is an eigenstate of PxP

$PxP|w\rangle = \bar{r}|w\rangle$

then $U_I|W\rangle$ is an eigenstate of PxP

$$PxP\,U_I|W\rangle = -U_I\,PxP|W\rangle = -\bar{r}\,U_I|W\rangle$$

$\Rightarrow$ the spectrum of PxP must be closed under inversion

For a single band, PxP has eigenvalues $\{na + \frac{a\varphi}{2\pi}, n \in \mathbb{Z}\}$

$$-\left(na + \frac{a\varphi}{2\pi}\right) \overset{?}{=} \left(ma + \frac{\varphi a}{2\pi}\right)$$

$$(m-n)a = \frac{\varphi a}{\pi}$$

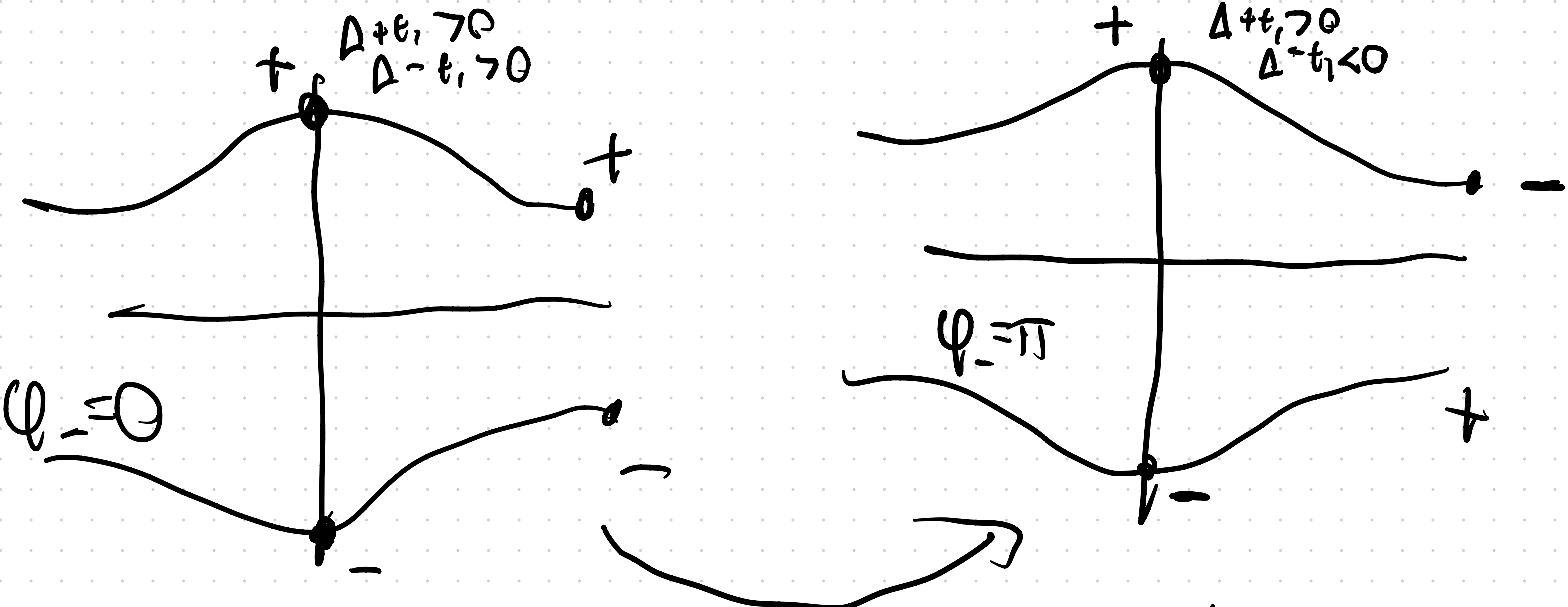
The spectrum of PXP is inversion symmetric if and only if $\varphi = (m-n)\pi \mod 2\pi$

$$\downarrow$$

$$\varphi = 0 \text{ or } \pi \mod 2\pi$$

For a single band w/ inversion symmetry, φ is quantized and is either 0 or π

①



$|\Delta|=|t_1|$

$\Delta>0$
$t_1=t_2=0$

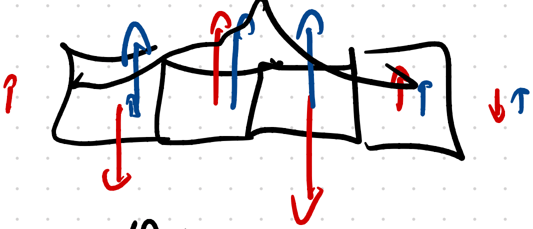
$\longrightarrow$

$\Delta>|t_1|$
$t_1,t_2\neq 0$

$\rightarrow$ gapless

$\varphi=0$ $\qquad$ $\varphi=0$

$\rightarrow$ $|t_1|>\Delta$
$\Delta\neq 0$



$\varphi = \pi$

$\longrightarrow$

$A = 0$