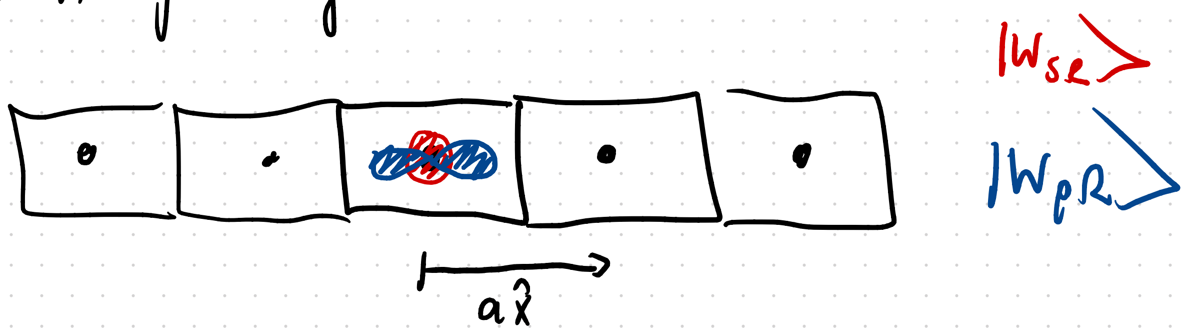
Lecture 20

Announcements: HW2 is graded, solutions posted
HW3 is due tonight
HW4 is posted

Recap 1D chain w/ inversion symmetry & Time-reversal symmetry



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

$$B(TRS) = \sigma^0 \mathcal{K}$$

Nearest Neighbor tb 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

$\mu_1 \pm t_1$ - ss hopping / p-p hopping

t_2: s-p hopping

Δ - relative on-site energy between s and p

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

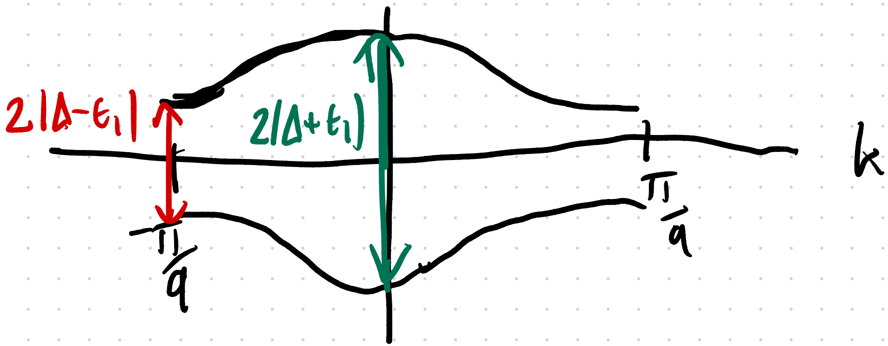
$\mu = 0$
$\mu_1 = 0$

There is a gap wherever if:

wolog

$t_2 \neq 0 \quad |\Delta| \neq |t_1|$ – gap

$|\Delta| > |t_1|$ – gap



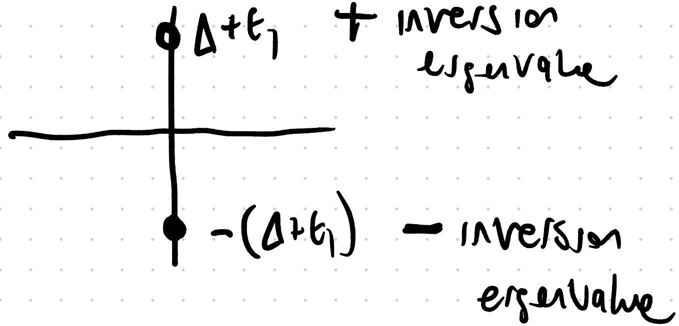
Little group representations

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

$k = 0 \; (\Gamma) \qquad G_\Gamma = G$

$k = \frac{\pi}{a} \; (X) \qquad G_X = G$

$$\Gamma: h(\Gamma) = (\Delta + t_1)\sigma^z \qquad B(I) = \sigma^z$$



$\Delta + t_1 > 0$: ε_- state has -1 inversion eigenvalue

ε_+ state has $+1$ inversion eigenvalue

$\Delta + t_1 < 0$: ε_+ state has -1 inversion eigenvalue

ε_- state has $+1$ inversion eigenvalue

X: $h(X) = (\Delta - t_1)\sigma^z$ $\qquad B(I) = \sigma^z$

$\Delta - t_1 > 0$: ε_- state has -1 inversion eigenvalue

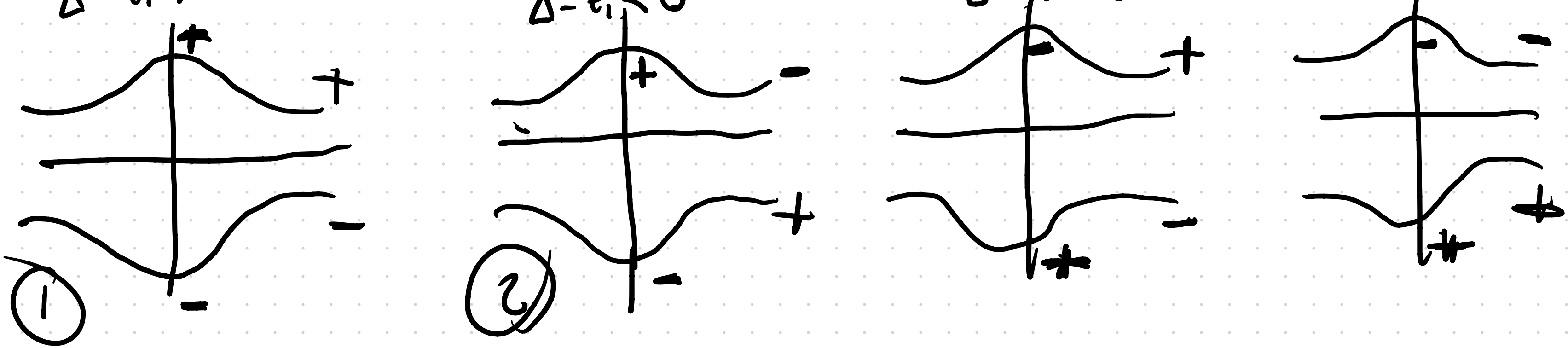
ε_+ state has $+1$ inversion eigenvalue

$\Delta - t_1 < 0$: ε_+ state has -1 inversion eigenvalue

ε_- state has $+1$ inversion eigenvalue

Summary:

$\Delta + t_1 > 0$, $\Delta - t_1 > 0$ | $\Delta + t_1 > 0$, $\Delta - t_1 < 0$ | $\Delta + t_1 < 0$, $\Delta - t_1 > 0$ | $\Delta + t_1 < 0$, $\Delta - t_1 < 0$

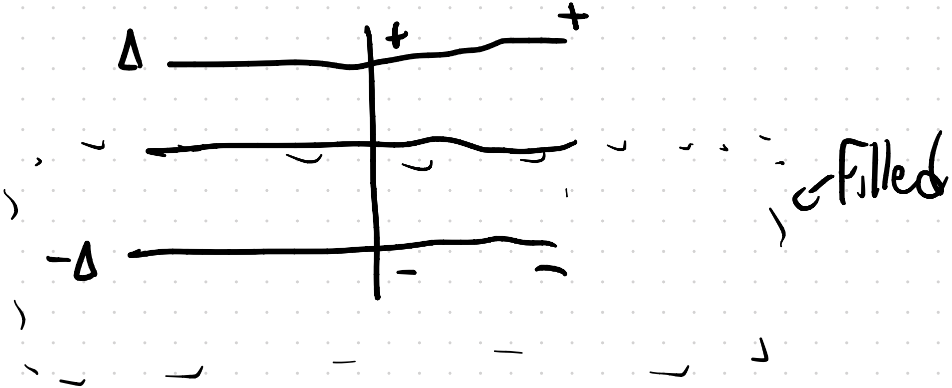


Lets look at two easy-to-solve limits to find Berry phase, polarization, Wannier functions

① $\Delta > 0 \qquad t_1 = t_2 = 0$

$$h(k) = \Delta \sigma^z = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} \qquad \varepsilon_\pm(k) = \pm\Delta$$

$$h(k)\vec{u}_{\pm k} = \varepsilon_\pm(k)\vec{u}_{\pm k} \qquad u_{+k} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad u_{-k} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



Tight-binding Berry connection: $A^{--} = i\, u^\dagger_{-,k} \cdot \dfrac{\partial \vec{u}_{-,k}}{\partial k}$

$= 0$

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

$\Rightarrow$ PxP has eigenvalues $\bar{r}_{n-} = na + \frac{a}{2\pi}\cancel{\varphi_{-}}^{\,0} = na$

$n \in \mathbb{Z}$

$\Rightarrow$ Wannier Functions are centered @ the origin of each unit cell

Lecture 14/15: Hybrid Wannier for 1 occupied band

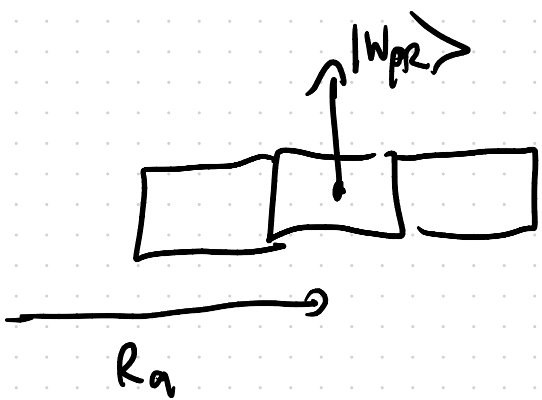
$$|W_{-R}\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk \, |\psi_{-k}\rangle e^{-ikR} e^{i\left[\int_0^k dk A^{-}(k) - \frac{ka}{2\pi}\varphi_{-}\right]}$$

For us $|\psi_{\underline{k}}\rangle = \sum_{i=s,p} u^i_{\underline{k}} |\chi_{ik}\rangle$

$= |\chi_{pk}\rangle$

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

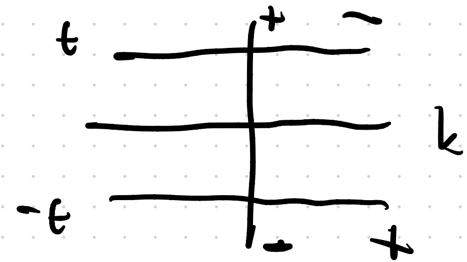
$= |W_{pR}\rangle$ - Wannier fn is just our basis function



More interesting:

(2) $\Delta = 0$ $\quad t_1 = t > 0$

$t_2 = t$



$$h(k) = (0 + t\cos ka)\sigma^z + t\sin ka\,\sigma^y$$

$$= t\,\hat{n}\cdot\vec{\sigma} \qquad \hat{n} = (0, \sin ka, \cos ka)$$

$$\theta = ka$$

Energies $\varepsilon_\pm = \pm t$

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

$$u_{+k} = \begin{pmatrix} \cos\frac{ka}{2} \\ i\sin\frac{ka}{2} \end{pmatrix} \qquad u_{-k} = \begin{pmatrix} \sin\frac{ka}{2} \\ -i\cos\frac{ka}{2} \end{pmatrix}$$

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

We can enforce this by multiply by $e^{-ika/2}$

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

Berry connection for u_{-k}

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

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

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

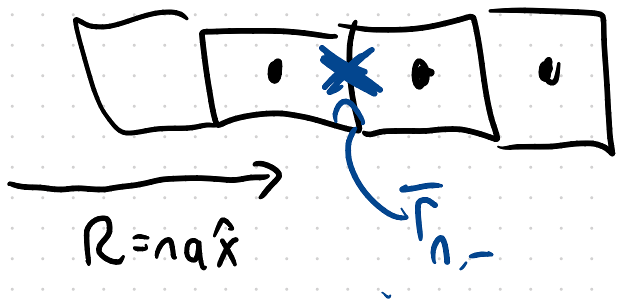
$$= \frac{i}{4}\left(2(-i)a\right) = \frac{a}{2}$$

Berry phase

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

This means PxP has eigenvalues $\hat{r}_{n-} = na + \frac{a}{2}$, $n \in \mathbb{Z}$

$\Rightarrow$ Wannier fns for $-$ Band are centered at the boundaries between unit cells



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

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

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

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

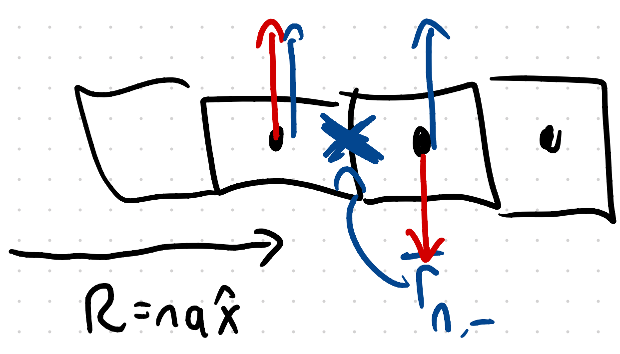
$$= \left(\frac{-i}{2}\right) \frac{a}{2\pi} \int_0^{2\pi/a} dk \Big[e^{-ik\cdot R} |\chi_{sk}\rangle + e^{-ik\cdot R} |\chi_{pk}\rangle$$

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

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

Centered at

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



Going beyond these two limits: What does I have to say about $P x P$

$$u_I P u_I^\dagger = P \quad \leftarrow \text{if } h \text{ is inversion symmetric}$$

$$u_I x u_I^\dagger = -x \quad \text{by definition}$$

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

$$P x P u_I |w\rangle = - u_I P x P u_I^\dagger u_I |w\rangle$$

$$= - u_I P x P |w\rangle$$

$$= - \bar{r} u_I |w\rangle$$

This means that the spectrum of PxP must map to itself under inversion symmetry

For a single band PxP has eigenvalues

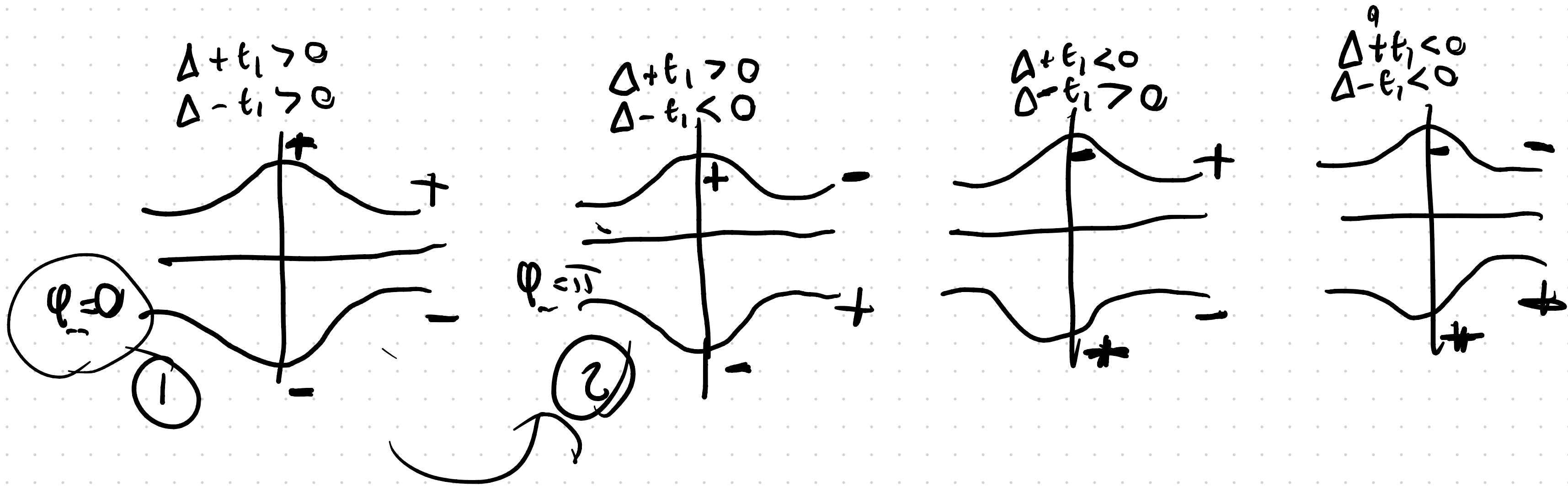
$$\left\{ na + \frac{\varphi a}{2\pi} , n \in \mathbb{Z} \right\}$$

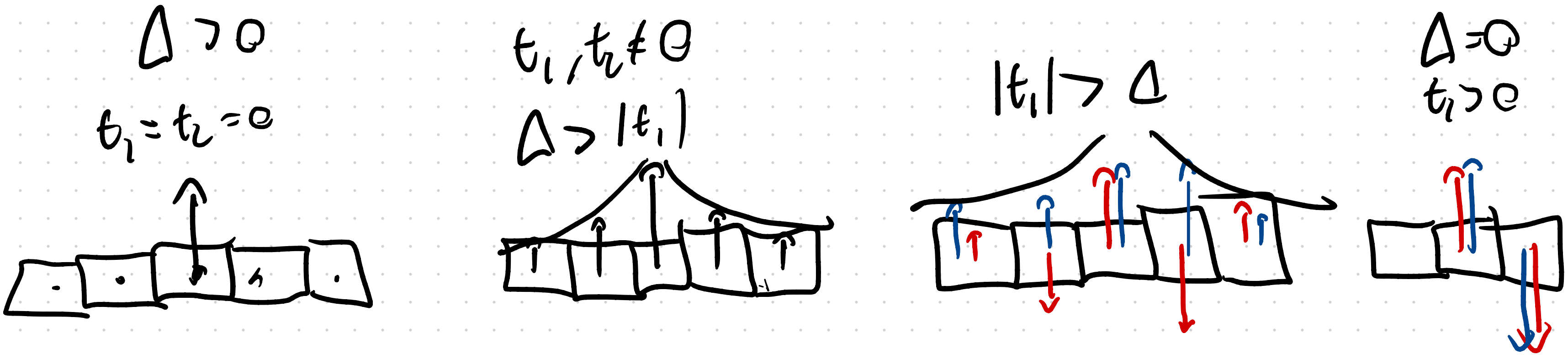
$$-\left(na + \frac{\varphi a}{2\pi}\right) \stackrel{?}{=} \left(ma + \frac{\varphi a}{2\pi}\right)$$ if we have inversion symmetry

$$\varphi = (m-n)\pi \mod 2\pi$$

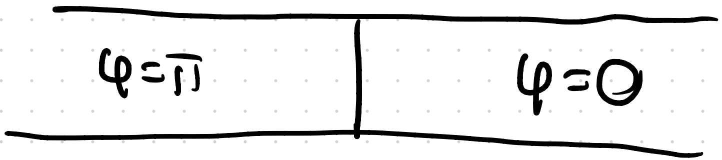
$$\varphi = 0 \text{ or } \pi \mod 2\pi$$

$\boxed{\text{For a single band w/ inversion symmetry, } \varphi \text{ is quantized and is either } 0 \text{ or } \pi \text{ mod } 2\pi}$


$\Delta + t_1 > 0$
$\Delta - t_1 > 0$
$\varphi = 0$
1
$\Delta + t_1 > 0$
$\Delta - t_1 < 0$
$\varphi = \pi$
2
$\Delta + t_1 < 0$
$\Delta - t_1 > 0$
$\Delta + t_1 < 0$
$\Delta - t_1 < 0$


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

Observables



$$\Delta p = \frac{ea}{2} \mod ea$$

→ bound charge density (charge)

$$\rightarrow \; q_{\text{boundry}} = e/2$$