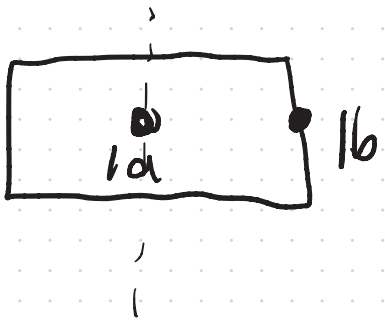
Lecture 27

Given: a set of orbitals at Wyckoff position $\bar{r}_n$ transforming in irrep ρ of $G_{\bar{r}_n}$

$$\rightarrow \langle \psi_{j\beta\bar{g}k} | U_g | \psi_{i\alpha k} \rangle = e^{-i\bar{g}k\cdot t'_{\alpha\beta}} \rho_{ji}(h_{\alpha\beta}) = B^{k}_{j\beta,i\alpha}(g)$$

$$g = t'_{\alpha\beta}\, g_\beta\, h_{\alpha\beta}\, g_\alpha^{-1}$$ for coset representatives $g_\alpha, g_\beta, h_{\alpha\beta} \in G_{\bar{r}_n}$

Example: Construct EBRs for a 1D inversion-symmetric chain:



$1a: (0) = \bar{r}_a$

$$G_{1a} = \langle \{ I | 0 \} \rangle$$
$$= \{ E, I \} \simeq T$$

Irreps

ρ	E	I
ρ_A	$+1$	$+1$
ρ_B	$+1$	-1

$G = T \rtimes G_{1a}$ only one coset

$$g_\alpha = \{E|0\}$$

$$\{I|0\} = \underset{\substack{\uparrow \\ t'_{\alpha\beta}}}{\{E|0\}}\,\underset{\substack{\uparrow \\ g_\alpha = g_\beta}}{\{E|0\}}\,\underset{\substack{\uparrow \\ h_{\alpha\beta}}}{\{I|0\}}\,\underset{\substack{\uparrow \\ g_\alpha^{-1}}}{\{E|0\}}$$

$$B^k_{1a}(\{I|0\}) = \begin{cases} \rho_A(\{I|0\}) \cdot & (A_{1a})\uparrow G \\ \rho_B(\{I|0\}) & (B_{1a})\uparrow G \end{cases}$$

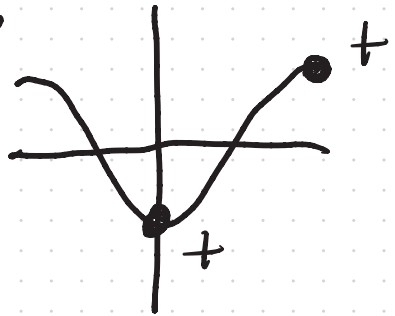
In this case $B^k_{1a}(\{I|0\})$ is k-independent

$k = 0$ vs $k = \pi$

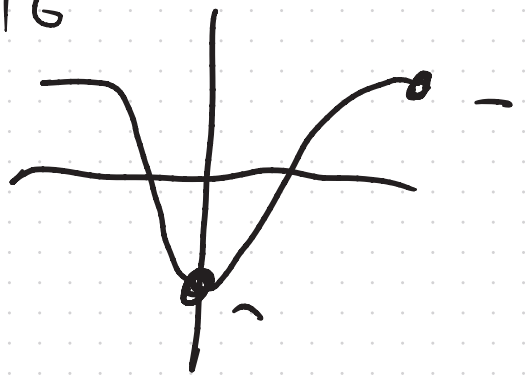
(A_{1g}) ÎG $+1$ $\quad$ $+1$

(B_{1g}) ÎG -1 $\quad$ -1

A_{1g} ÎG



B_{1g} ÎG



What about the 1b position:

$$1b: \left(\frac{a}{2}\right) = \overline{\Gamma}_6 \qquad \{I|a\}\overline{\Gamma}_6 = \overline{\Gamma}_6$$

$$G_{1b} = \{\{E|0\}, \{I|a\}\} \subseteq T$$

Irreps

ρ	E	I
ρ_A	$+1$	$+1$
ρ_B	$+1$	-1

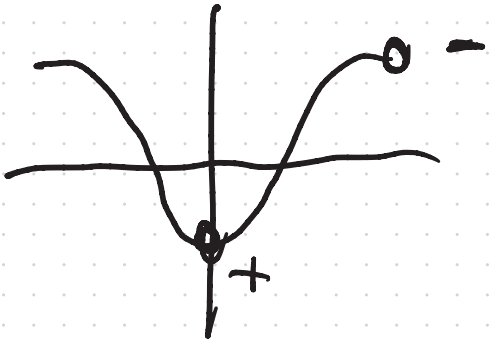
$$\{I|0\} = \underset{\substack{\parallel \\ t}}{\{E|-a\}} \underset{\substack{\cap \\ G_{1b}}}{\{I|a\}}$$

$$B^{k}_{1b}(\{I|0\}) = e^{-i(Ik)\cdot(-a)} \begin{cases} \rho_A(\{I|a\}) \\ \rho_B(\{I|a\}) \end{cases}$$

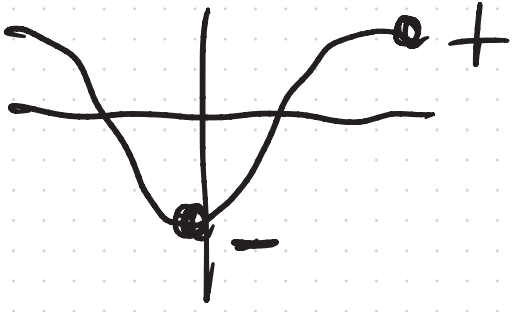
$$= \begin{cases} e^{-ika} & A \\ -e^{-ika} & B \end{cases}$$

	$k=0$	$k=\pi/a$
$(A_{1b})\uparrow G$	$+1$	-1
$B_{1b})\uparrow G$	-1	$+1$

$(A)_{1b}$ PG



(B_{1b}) PG



Recall: For the 1d Chain

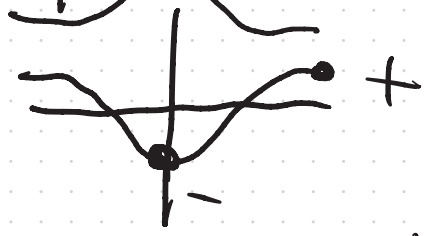
$$h(k) = (\Delta + t_1 \cos ka)\sigma_z + t_2 \sin ka\, \sigma_y$$

$\Delta > t_1 > 0$

WFs localized at $\bar{r}_- = 0$

(B_{1a}) ↑ G

$t_1 > \Delta > 0$



WFs localized at $\bar{r}_- = a/2$

(B_{1b}) ↑ G

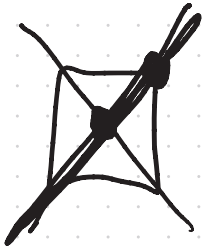
What about all bands?

$s + p$ @ $\bar{r} = 0$

$(A_{1g}) \uparrow G \qquad (B_{1g}) \uparrow G$

both bands together: $A_{1g} \uparrow G \oplus B_{1g} \uparrow G$

$\equiv A_{1b} \uparrow G \oplus B_{1b} \uparrow G$



$= \eta_{2c} \uparrow G$

$\parallel$

$\eta_{2c} \uparrow G_{1g} \uparrow G$

$G_{2c} = \{\{E|0\}\} \qquad \eta_{2c}(E) = 1$

$$\eta_{2c} \uparrow G_{1a} = \rho_A \oplus \rho_B$$ regular representation

$$\eta_{2c} \uparrow G_{1b} = \rho_A \oplus \rho_B$$

$$\eta_{2c} \uparrow G_{1b} \uparrow G$$

equivalent Band reps

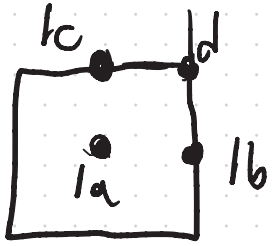
this means that $A_{1a} \uparrow G \oplus B_{1a} \uparrow G \equiv A_{1b} \uparrow G \oplus B_{1b} \uparrow G$

unocc $\Delta > t_1$ occ unocc $t_1 > \Delta$ occ

Lets generalize now to 2D (spinless)

$$C_2 : (x, y) \to (-x, -y)$$

p2



$G_{1a} = \langle \{C_2|0\} \rangle$

$G_{1b} = \langle \{C_2|a\hat{x}\} \rangle$

$G_{1c} = \langle \{C_2|b\hat{y}\} \rangle$

$G_{1d} = \langle \{C_2|a\hat{x}+b\hat{y}\} \rangle$

All these have the same irreps

	E	C_2
A	+1	+1
B	+1	-1

We want $B^k(\{C_2|0\})$

Eight possibilities

$$A_{1a} = +1 \qquad B_{1a} = -1$$

$$A_{1b} = e^{-ik_x a} \qquad B_{1b} = -e^{-ik_x a}$$

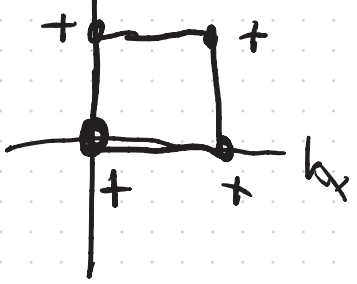
$$A_{1c} = e^{-ik_y b} \qquad B_{1c} = -e^{-ik_y b}$$

$$A_{1d} = e^{-i(k_x a + k_y b)} \qquad B_{1d} = -e^{-i(k_x a + k_y b)}$$

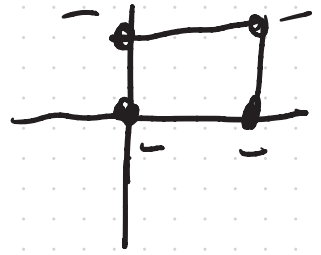
In the BZ

k_y

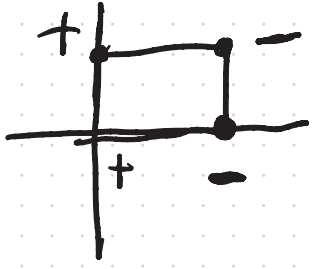
A_{1a}



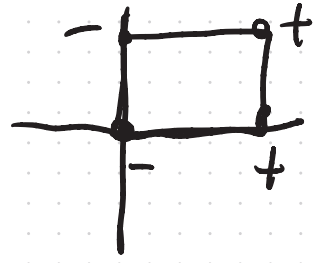
B_{1a}



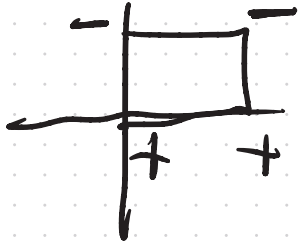
A_{1b}



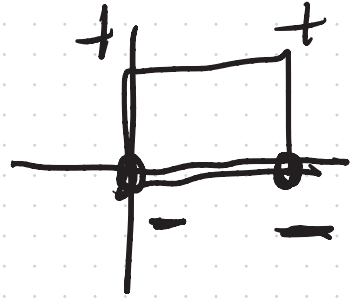
B_{1b}



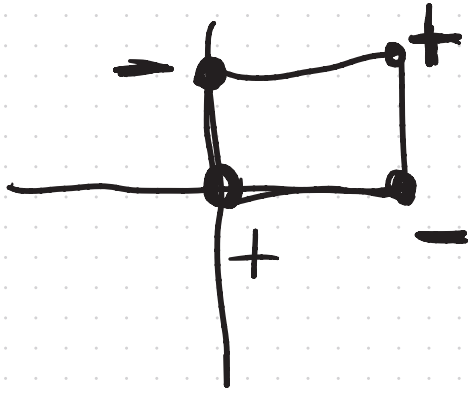
A_{1c}



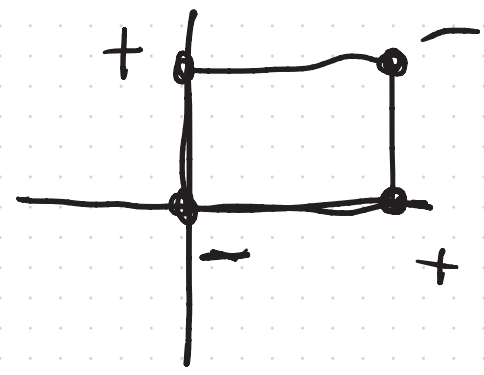
B_{1c}



A_{1d}



B_{1d}



These are the eight possible configurations of C_2 eigenvalues compatible w/ having a single exponentially localized Wannier function

All have an even # of negative eigenvalues

$$h(k) = (\Delta + t_1 \cos k_x)\sigma_z + t_2 \sin k_x \sigma_y$$
$$+ \Delta \cos k_y \sigma_z + t_2 \sin k_y \sigma_x$$

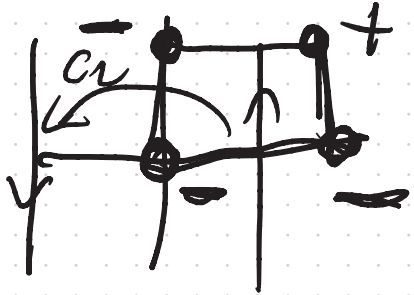
$$\sigma_z h(-\vec{k}) \sigma_z = h(k)$$ C_2 symmetric

$$h(k_x, k_y=0) = (2\Delta + t_1 \cos k_x)\sigma_z + t_2 \sin k_x \sigma_y$$

$$h(k_x, k_y=\pi) = t_1 \cos k_x \sigma_z + t_2 \sin k_x \sigma_y$$

if $2\Delta > t_1$ $h(k_x, k_y=0)$ is the Bloch ham. for a 1D chain in one of our two phases;

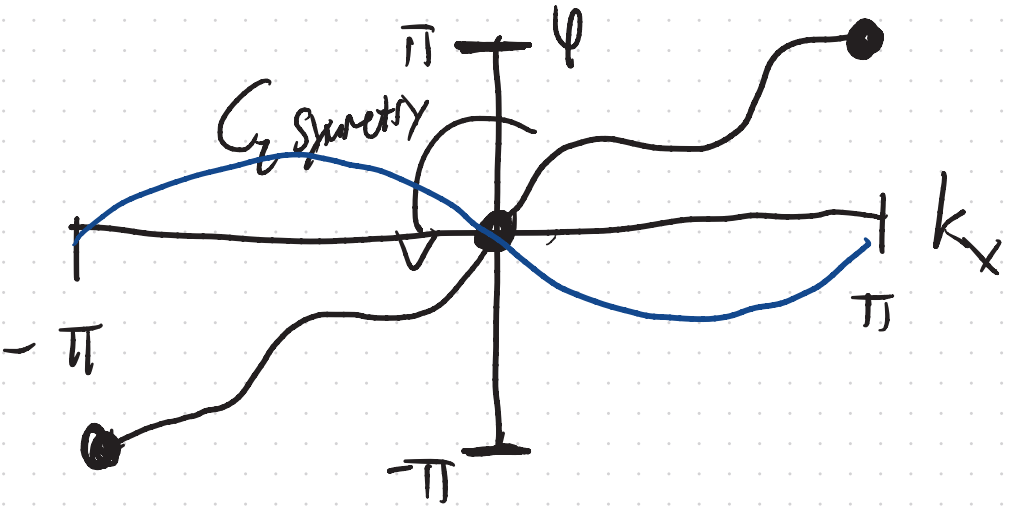
$h(k_x, k_y=\pi)$ is the other phase



$h(k_x, k_y)$ has an occupied band that cannot be one of our EBRs

$\rightarrow$ the occupied band does not have symmetric, exponentially localized Wannier functions

Wilson loop $\quad W_{2\pi\hat{y} \leftarrow 0}(k_x)$



$W_{k_x R_y}(y)$ has center given by $R_y + \frac{\varphi(k_x)}{2\pi}$

$$W_{k_x+2\pi R_y}(y) = W_{k_x R_y+1}(y)$$ Not periodic

$\rightarrow$ we can't FT to get localized Wannier functions

ν - the # of times $W_{2\pi y=0}(k_x)$ winds from $-\pi$ to π

$$\nu = \frac{1}{2\pi} \oint d^2k \, \mathrm{tr}\, \Omega_n(k)$$ Chern #

Berry curvature