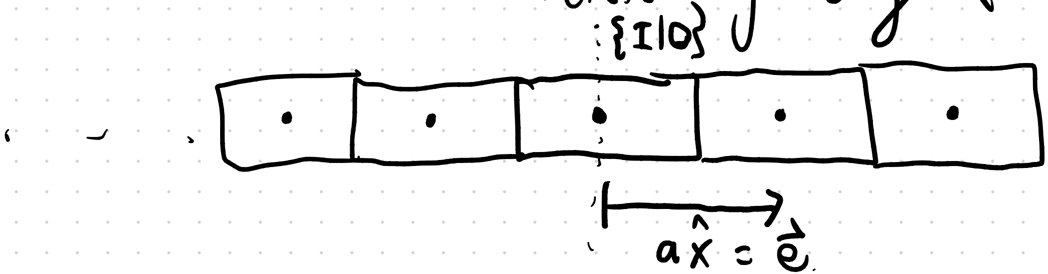
Lecture 19

Example: tight-binding model for a 1D chain w/ inversion symmetry (with time-reversal symmetry)



Inversion in 1D:

$x \to -x$

$$p\bar{1} = \langle \{E|a\hat{x}\}, \{I|0\} \rangle$$

two tight-binding basis orbitals $|W_{sR}\rangle$ $|W_{pR}\rangle$ centered at the origin of each unit cell

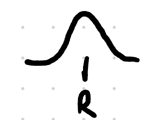
$$\langle W_{sR}|x|W_{sR}\rangle = R \qquad \langle r_s \rangle = 0$$

$$\langle W_{pR}|x|W_{pR}\rangle = R \qquad \langle r_p\rangle = 0$$

tight-binding limit $\langle W_{pR}|x|W_{sR'}\rangle = 0$

$$\Rightarrow \langle W_{iR}|x|W_{jR'}\rangle = \delta_{ij}\,\delta_{RR'}\,R \qquad i,j = s,p$$

Inversion symmetry: $W_{sR}(-x) = +W_{s\,-R}(x)$



$$W_{pR}(-x) = -W_{p\,-R}(x)$$

$$B^{ij}(\{I|0\}) = \begin{array}{cc} & \begin{array}{cc} s & p \end{array} \\ \begin{array}{c} s \\ p \end{array} & \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \end{array} = \sigma_z^{ij}$$

Time-reversal symmetry: $W^*_{SR}(x) = W_{SR}(x)$

$W^*_{pR}(x) = W_{pR}(x)$

$$B^{ij}(T) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \mathcal{K}$$ complex conjugation

$$= \sigma_0^{ij} \mathcal{K}$$

We want to construct $h^{ij}(k)$ satisfying:

1 Inversion $h(-k) = B^\dagger(I) h(k) B(I)$

$$= \sigma_z h(k) \sigma_z$$

② Time-reversal $h(-k) = h^*(k)$

$$\underline{h(k) = d_0(k)\sigma_0 + d_x(k)\sigma_x + d_y(k)\sigma_y + d_z(k)\sigma_z}$$

$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\boxed{\sigma_z \sigma_\mu \sigma_z = \begin{cases} \sigma_\mu, & \mu = 0, z \\ -\sigma_\mu, & \mu = x, y \end{cases}}$$

h Hermitian $\Rightarrow d_\mu(k)$ real

Inversion

$$\sigma_z h(k) \sigma_z = d_0(k)\sigma_0 - d_x(k)\sigma_x - d_y(k)\sigma_y + d_z(k)\sigma_z$$

$$= d_0(-k)\sigma_0 + d_x(-k)\sigma_x + d_y(-k)\sigma_y + d_z(-k)\sigma_z$$

$d_0(k), d_z(k)$ are even functions of k

$d_x(k), d_y(k)$ are odd functions of k

Time-reversal $h(-k) = h^*(k) = d_0(k)\sigma_0 + d_x(k)\sigma_x - d_y(k)\sigma_y + d_z(k)\sigma_z$

$$= d_0(-k)\sigma_0 + d_x(-k)\sigma_x + d_y(-k)\sigma_y + d_z(-k)\sigma_z$$

$$\boxed{\begin{array}{c} d_0(k), d_z(k), d_x(k) \text{ are even functions of } k \\ d_y(k) \text{ is an odd function of } k \end{array}}$$

$$\Rightarrow d_x(k) = 0$$

$[d_0(k)\sigma_0, h] = 0$ so it's a bit boring

wolog, $d_0(k) = 0$

$$h(k) = d_z(k)\sigma_z + d_y(k)\sigma_y$$

Last lecture: $V(\vec{b}) = e^{i\vec{b}\cdot\langle r_a\rangle}\delta_{ab} = \sigma_0$ for our choice of Wannier basis functions

$$h\left(k+\frac{2\pi}{a}\right) = h(k)$$

$$d_z(k) = \Delta + t_1 \cos ka + \ldots$$

$$d_y(k) = t_2 \sin ka + \ldots$$

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

In position space:

$$\langle W_{iR}|H|W_{jR'}\rangle = \frac{a}{2\pi}\int dk\, e^{ik(R-R')}h(k)$$

$$= \Delta \sigma_z \delta_{RR'} + \frac{1}{2} t_1 \sigma_z \left(\delta_{R',R+a} + \delta_{R',R-a} \right)$$

$$+ \frac{1}{2} t_2 (-i\sigma_y) \left(\delta_{R',R+a} - \delta_{R',R-a} \right)$$

Nearest-neighbor tight binding model

Trick for diagonalizing $h(k)$:

$$h(k) = \sum_{i=1}^{n} d_i(k) \Gamma_i$$

$$\Gamma_i^\dagger = \Gamma_i \quad (d_i \text{ real})$$

$$\{\Gamma_i, \Gamma_j\} = 2\delta_{ij} \, \mathrm{Id}$$

$$[h(k)]^2 = \sum_{i=1}^{\wedge} \sum_{j=1}^{\wedge} d_i(k) d_j(k) \Gamma_i \Gamma_j$$

$$= \sum_{i=1}^{\wedge} \sum_{j=1} d_i(k) d_j(k) \left(\Gamma_i \Gamma_j + \Gamma_j \Gamma_i \right) \frac{1}{2}$$

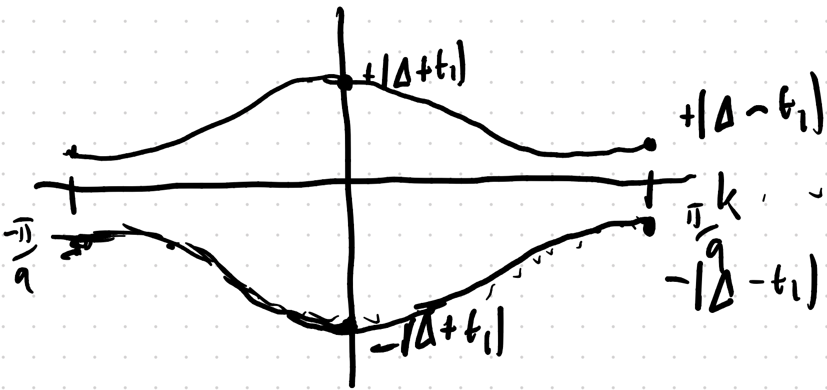
$$= \sum_{i=1}^{\wedge} \sum_{j=1}^{\wedge} d_i(k) d_j(k) \delta_{ij} \, \mathrm{Id} = \mathrm{Id} \left(\sum_{i=1}^{\wedge} [d_i(k)]^2 \right)$$

$h^2(k)$ has eigenvalues $\sum_{i=1}^{\wedge} (d_i(k))^2$

$\Rightarrow$ $h(k)$ has eigenvalues $\varepsilon_{\pm} = \pm \sqrt{\sum_{i=1}^{\wedge} [d_i(k)]^2}$

Our th model

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



$t_2 \neq 0$

$|\Delta| \neq |t_1|$ - there is an energy gap

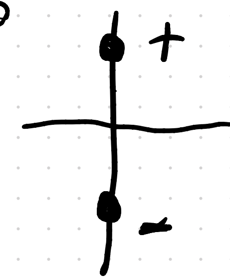
2x2	σ_x
	σ_y
	σ_z
4x4	$\sigma_x\tau_x$
	$\sigma_y\tau_x$
	$\sigma_z\tau_x$
	τ_y
	τ_z

Inversion eigenvalues:

Γ: $h(k=0) = (\Delta + t)\sigma_z$

$B(I) = \sigma_z$

$\Delta + t > 0$

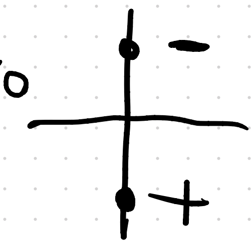


Inversion eigenvalue

$\Delta + t > 0$: negative ε state has negative I eigenvalue

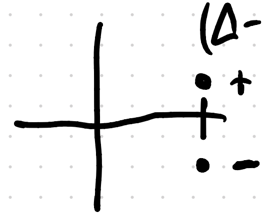
positive ε state has positive I eigenvalue

$\Delta + t < 0$

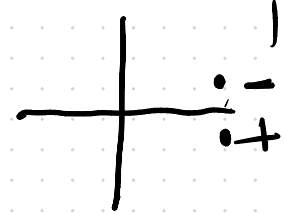


X: $h(k=\frac{\pi}{a}) = (\Delta - t)\sigma_z$

$(\Delta - t) > 0$



$(\Delta - t) < 0$



Next time: Berry phases & Wannier functions