PHYS 4410

Quantum Mechanics 2

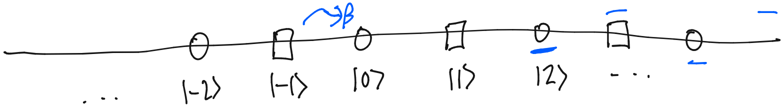
Spring 2023

Lecture 12

Metals and insulators

February 17

$\boxed{1}$



○ and □ inequivalent:

$$H = \sum_{n=-\infty}^{\infty}\Big[\underbrace{-\beta|n\rangle\langle n+1| - \beta|n+1\rangle\langle n|}_{\text{lec 11}} - (-1)^n\gamma\,|n\rangle\langle n|\Big].$$

$$H|n\rangle = -\beta|n-1\rangle - \beta|n+1\rangle \begin{cases} -\gamma|n\rangle & n \text{ even} \\ +\gamma|n\rangle & n \text{ odd} \end{cases}$$

$$H = H_\beta + H_\gamma$$

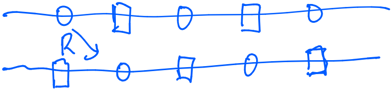
β-terms

γ-term (new for today)

2 Let $R = \sum_{n=-\infty}^{\infty} |n+1\rangle\langle n|$. Does $[H,R]=0$?

$[H,R]\neq 0$.

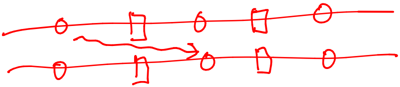
Intuitively:



$[H_\beta + H_\gamma, R] = \overbrace{\cancel{[H_\beta, R]}}^{0} + [H_\gamma, R]$ So $[H_\gamma, R]\neq 0$.

$$\left.\begin{aligned} H_\gamma R|n\rangle &= H_\gamma |n+1\rangle = -\gamma(-1)^{n+1}|n+1\rangle \\ RH_\gamma|n\rangle &= R[-\gamma(-1)^n|n\rangle] = -\gamma(-1)^n|n+1\rangle \end{aligned}\right\} \text{differ by } -1.$$

Fix:



$R\cdot R = R^2$.

You can check: $[H,R^2]=0$.

discrete translation sym: $\{1, R^2, R^4, \ldots, R^{-2}, R^{-4}, \ldots\}$
sub group of $\{1, R, R^2, \ldots\}$.

3 What are eigen values/vectors of R^2?

$$R^2 = \sum_{n=-\infty}^{\infty} |n+2\rangle\langle n|$$

$$\boxed{|0\rangle \xrightarrow{R^2} |2\rangle \xrightarrow{R^2} |4\rangle}$$

$$|1\rangle \xrightarrow{R^2} |3\rangle \xrightarrow{R^2} |5\rangle$$

Claim: $|k\rangle_e = \sum_{n \text{ even}} e^{ikn} |n\rangle$ $\qquad$ $|k\rangle_o = \sum_{n \text{ odd}} e^{ik(n-1)} |n\rangle$

always orthogonal

is equivalent to $(k \sim k + 2\pi)$

Have 2 eigenvectors for each k.

When $[H, R] = 0$, Brillouin zone: independent k are $0 \leq k < 2\pi$

$-\pi \leq k < \pi$

If $[H, R^2]$: $\sum_{n \text{ even}} e^{ikn} |n\rangle = \sum_{n \text{ even}} e^{in(k+\pi)} |n\rangle$ $\qquad$ $e^{2\pi i \times \text{integer}} = 1$

Now: $-\pi/2 < k \leq \pi/2$.

$\boxed{4}$ $\quad \underline{H|n\rangle = -\beta|n-1\rangle - \beta|n+1\rangle - \gamma(-1)^n|n\rangle}$

Since $[H, R^2]=0$, know e-vectors of H are $\underbrace{\text{e-vec. of } R^2.}_{c_e|\bar{k}\rangle_e + c_o|\bar{k}\rangle_o}$

c_e & c_o arbit.

$$H\left[c_e|\bar{k}\rangle_e + c_o|\bar{k}\rangle_o\right] = H\sum_{m=-\infty}^{\infty} e^{2ikm}\left[c_e|2m\rangle + c_o|2m+1\rangle\right]$$

$$= \sum_{m=-\infty}^{\infty} e^{2ikm}\Big[-\beta c_e|2m-1\rangle - \beta c_e|2m+1\rangle - \gamma c_e|2m\rangle$$
$$-\beta c_o|2m\rangle - \beta c_o|2m+2\rangle + \gamma c_o|2m+1\rangle\Big]$$

e.g. $\displaystyle\sum_{m=-\infty}^{\infty} e^{2ikm}(-\beta c_e)|2m-1\rangle \xrightarrow{m=m'+1} \sum_{m'=-\infty}^{\infty} e^{2ik}\cdot e^{2ikm'}(-\beta c_e)|2m'+1\rangle$

$$= \sum_{m=-\infty}^{\infty} e^{2ikm}\Big[-\gamma c_e|2m\rangle + \gamma c_o|2m+1\rangle - \beta c_e(1+e^{2ik})|2m+1\rangle$$
$$-\beta c_o(1+e^{-2ik})|2m\rangle\Big]$$

$$= \left(-\gamma c_e - \beta c_o(1+e^{-2ik})\right)|\bar{k}\rangle_e + \left(\gamma c_o - \beta(1+e^{2ik})\right)|\bar{k}\rangle_o.$$

$\boxed{5}$ $H|\psi\rangle = E|\psi\rangle$, where $|\psi\rangle = c_1|\bar{k}\rangle_e + c_2|\bar{k}\rangle_o$

$$E c_e = -\gamma c_e - \beta(1+e^{-2ik})c_o$$
$$E c_o = +\gamma c_o - \beta(1+e^{2ik})c_e .$$

$$E\begin{pmatrix} c_e \\ c_o \end{pmatrix} = \underbrace{\begin{pmatrix} -\gamma & -\beta(1+e^{-2ik}) \\ -\beta(1+e^{2ik}) & \gamma \end{pmatrix}}_{Z}\begin{pmatrix} c_e \\ c_o \end{pmatrix}$$

Find E by: $\det(E\mathbb{1} - Z) = 0 = \det\begin{pmatrix} E+\gamma & \beta(\ ) \\ \beta(\ ) & E-\gamma \end{pmatrix}$

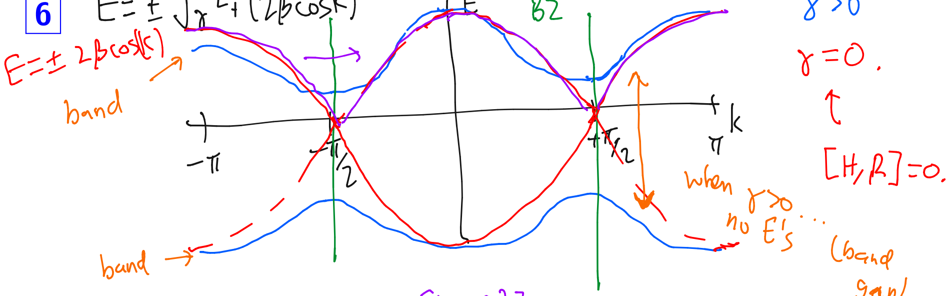
$$= (E+\gamma)(E-\gamma) - \beta^2(1+e^{-2ik})(1+e^{2ik})$$
$$= E^2 - \gamma^2 - \beta^2(2+2\cos(2k))$$

or: $E^2 = \gamma^2 + 4\beta^2\cos^2(k)$

Thus: $E = \pm\sqrt{\gamma^2 + (2\beta\cos k)^2}$.

6

$E = \pm\sqrt{\gamma^2 + (2\beta\cos k)^2}$



go from $[H_\beta, R] = 0$ to $[H_\beta, R^2] = 0$

- cut BZ in half
- 2x bands

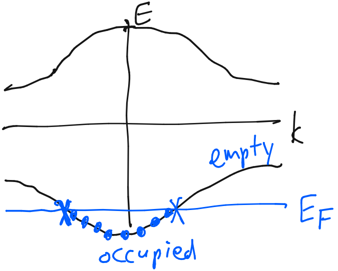
} relabeling same states.

(half translational)

break R-trans $\longrightarrow$ R^2-trans symmetry:
- 2x bands
- 1/2 BZ
- open a gap

7 If $\gamma \neq 0$:

Many mobile electrons...
(ignore electrons...)
ground state: fill in all lowest energy states



metal: $E = E_F$ & $E(k)$ intersect.
- any $\Delta E > 0$ kicks system out of ground state.

insulator: $E = E_F$ & $E(k)$ not intersect