PHYS 4410

Quantum Mechanics 2

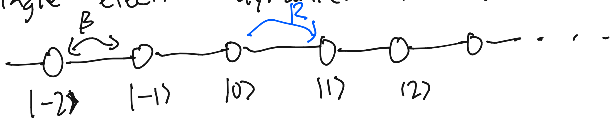
Spring 2023

Lecture 11

Discrete translation symmetry: infinite chain

February 13

1 Single electron dynamics in lattice:



$$H = -\beta \sum_{n=-\infty}^{\infty} \Big[\underbrace{|n\rangle\langle n+1|}_{\text{hop left}} + \underbrace{|n+1\rangle\langle n|}_{\text{hop right}} \Big]$$

Same strategy as Lec 10: look for symmetry (group)

$$\underset{\uparrow \text{ hop right}}{R} = \sum_{n=-\infty}^{\infty} |n+1\rangle\langle n| \qquad \{1, R, R^2, \dots, R^{-1}, R^{-2}, \dots\} = \mathbb{Z}$$

H & R share eigenvectors

$[H,R]|n\rangle = 0.$ $\qquad [H,R] = HR - RH$

Check: $[H,R] = 0.$

$$HR|n\rangle \quad = \quad RH|n\rangle$$

$$H|n+1\rangle \qquad\qquad R\left[-\beta|n-1\rangle - \beta|n+1\rangle\right]$$

$$-\beta|n\rangle - \beta|n+2\rangle \quad \overset{\checkmark}{=} \quad -\beta|n\rangle - \beta|n+2\rangle.$$

2 If $R|\lambda\rangle = \lambda|\lambda\rangle$:

$$|\lambda\rangle = \sum_{n=-\infty}^{\infty} c_n |n\rangle$$

$$\sum_{n=-\infty}^{\infty} c_n |n+1\rangle = \sum_{n=-\infty}^{\infty} (\lambda c_n)|n\rangle$$

$$\sum_{n=-\infty}^{\infty} |n\rangle \underbrace{\left(-\lambda c_n + c_{n-1}\right)}_{=0} = 0.$$

$$\underbrace{c_{n-1} = \lambda c_n,}$$

$$c_n = c_0 \cdot \lambda^{-n}$$

normalization?

$$|\lambda\rangle = \# \sum \lambda^{-n} |n\rangle$$

$|\lambda\rangle$ is not ever normalizable

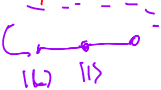
[cf free particle QM I]

Claim: R is unitary $(R^\dagger = R^{-1})$. so R's eigenvalues $|\lambda| = 1$,

so $\lambda = e^{-ik}$

k real

cf lec 10:



$$\lambda = e^{-2\pi i/L \cdot j}$$

$$j = 1, \ldots, L$$

discrete plane waves:

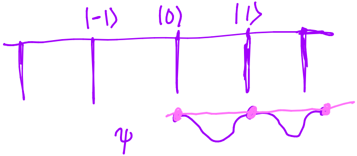
$$|\lambda\rangle = \sum_{n=-\infty}^{\infty} e^{ikn} |n\rangle$$

$\boxed{3}$ $|\bar{k}\rangle = \sum_{n=-\infty}^{\infty} e^{ikn} |n\rangle$ Take: $\underbrace{0 \le k < 2\pi}_{\text{Brillouin zone}}$

$$H|\bar{k}\rangle = -\beta \sum_{n=-\infty}^{\infty} e^{ikn} [\underbrace{|n+1\rangle}_{\sum |n'\rangle e^{ik(n'-1)}} + |n-1\rangle] = -\beta \sum_{n=-\infty}^{\infty} |n\rangle e^{ikn} [e^{-ik} + e^{ik}]$$

[used: $\cos x = \frac{1}{2}(e^{ix} + e^{-ix})$].

$$= \underbrace{-2\beta\cos(k)}_{E(k) = -2\beta\cos(k)} |\bar{k}\rangle$$



Why are other k's not different?

$$|\overline{k+2\pi}\rangle = |\bar{k}\rangle$$

$$\sum e^{i(k+2\pi)n} |n\rangle = \sum e^{ikn} |n\rangle \underbrace{e^{2\pi i n}}_{=1,}$$

n integer

Discrete translations:

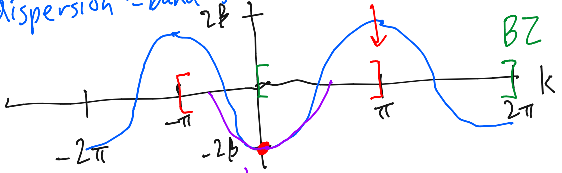
$x \to x + a$ $(a = 1)$

$k \sim k + \frac{2\pi}{a}$

"is equivalent to"

4 $E(k) = -2\beta\cos(ka)$: "single band metal".

dispersion = band structure



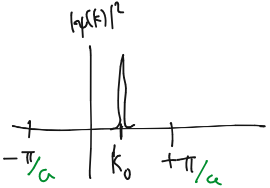
Taylor expand $E(k) = -2\beta + \beta a^2 \cdot k^2 + \dots$

If $k \ll \frac{2\pi}{a}$, $\approx E_{free}(k) = \underbrace{\cancel{-2\beta}}_{\text{offset}} + \frac{\hbar^2}{2m_{eff}} \cdot k^2$

Thus $\frac{\hbar^2}{2m_{eff}} = \beta a^2$

m_{eff} = "effective mass" for electron.

5 Think about wave packet...



$|\psi\rangle \sim \int dk \; \psi(k) \, |\tilde{k}\rangle$

If $\psi(k)$ tightly peaked:

wave packet travels at group velocity $v_g = \dfrac{d\omega}{dk}$

$e^{ikx - i\omega t}$

In QM:

$E = \hbar\omega$

$$v_g = \frac{d}{dk}\left[-2\beta\hbar\cos(ka)\right] = 2\beta\hbar a \sin(ka)$$

↳ Apply uniform force F:

$F = \dfrac{dp}{dt} = \hbar \dfrac{dk}{dt}$, so $k = \dfrac{F}{\hbar} t$ (if $t=0$, $k=0$)

$$v_g(t) = 2\beta\hbar a \cdot \sin\left(\frac{F}{\hbar} a \cdot t\right)$$

Bloch oscillations

6 $H = \sum_{n=-\infty}^{\infty} \left[-\beta \left(|n+1\rangle\langle n| + |n\rangle\langle n+1| \right) - \gamma \left[|n+2\rangle\langle n| + |n\rangle\langle n+2| \right) \right]$

$$H = -\beta R - \beta R^{-1} - \gamma R^{2} - \gamma R^{-2}$$

Check: $\underline{[H, R] = 0.}$

Eigenvectors of H: = Same as eigenvectors of R, $|\bar{k}\rangle$

Eigenvalues: $R|\bar{k}\rangle = e^{-ik}|\bar{k}\rangle$

$$H|\bar{k}\rangle = \left[-\beta e^{-ik} - \beta e^{ik} - \gamma e^{-2ik} - \gamma e^{2ik}\right]|\bar{k}\rangle$$

$$= \underbrace{\left[-2\beta\cos(k) - 2\gamma\cos(2k)\right]}_{E(k)}|\bar{k}\rangle$$