Normal ordering

$$x^2 = N[x^2] + v = N[xx] + xx$$

"contraction"

$$= v$$

$$\langle 0 | x^2 | 0 \rangle = \langle 0 | N[xx] + xx | 0 \rangle$$

$$= xx = v$$

Wick's theorem: $x^n = N[x^n] + N[x^n]_1 + N[x^n]_2 + \cdots N[x^n]_{[n/2]}$

$$xxxx = N[xxxx]$$

$$+ N[xxxx] + N[xxxx] + N[xxxx] + N[xxxx] + N[xxxx] + N[xxxx]$$

6 one contraction

$$+ N[xxxx] + N[xxxx] + N[xxxx]$$

3

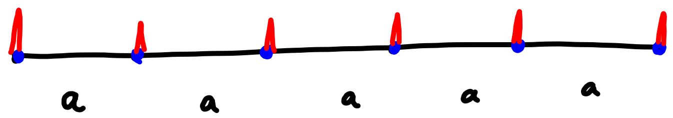
$\langle 0 | x^4 | 0 \rangle = 3 v^2$

$\langle 0 | x^6 | 0 \rangle = xxxxxx$

5 one contraction

$= 5 \cdot 3\, v^3$

Periodic potentials



$$V(x+a) = V(x)$$

$$|\psi(x+a)|^2 = |\psi(x)|^2 \Rightarrow \psi(x+a) = e^{i\delta}\psi(x)$$

$\delta = ka$ for some k

motivation: for plane waves

$$e^{ikx} \rightarrow e^{ik(x+a)} = e^{ika}e^{ikx}$$

In this case $\quad u_k(x) = e^{-ikx}\psi(x)$

$$u_k(x+a) = e^{-ikx}\cancel{e^{-ika}}\psi(x+a)$$

$$\qquad\qquad\qquad\qquad\qquad\qquad \| \;\cancel{e^{ika}}\psi(x)$$

$\Rightarrow u_k(x) \quad = u_k(x)$

is truly periodic.

Periodic

$$\psi(x) = e^{ikx}u_k(x) \qquad \text{Block's Theorem.}$$

$$\psi(x+a) = e^{i\delta}\psi(x) \qquad 0 \le \delta \le 2\pi$$

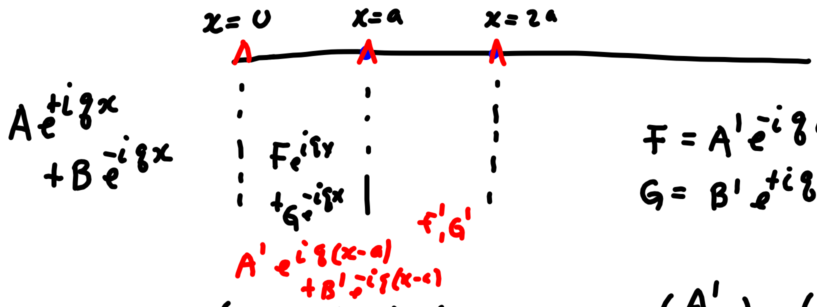
$$\delta = ka \qquad \text{or}$$

$$-\pi \le \delta \le \pi$$

can take

$$\boxed{-\frac{\pi}{a} \le k \le \frac{\pi}{a}} \longleftarrow -\pi \le ka \le \pi$$

the value of k can only be up to a multiple of $\frac{2\pi}{a}$



$$F = A' e^{-iqa} = A'\beta^{-1}$$
$$G = B' e^{+iqa} = B'\beta$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1+\gamma & \gamma \\ -\gamma & 1-\gamma \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix} \qquad \begin{pmatrix} A' \\ B' \end{pmatrix} = \begin{pmatrix} 1+\gamma & \gamma \\ -\gamma & 1-\gamma \end{pmatrix}\begin{pmatrix} F' \\ G' \end{pmatrix}$$

$$\begin{pmatrix} \beta^{-1} & 0 \\ 0 & \beta \end{pmatrix}\begin{pmatrix} A' \\ B' \end{pmatrix} \qquad \beta = e^{iqa}$$

$$= \begin{pmatrix} (1+\gamma)\beta^{-1} & \gamma\beta \\ -\gamma\beta^{-1} & \beta(1-\gamma) \end{pmatrix}\begin{pmatrix} A' \\ B' \end{pmatrix} = M^2 \begin{pmatrix} A'' \\ B'' \end{pmatrix}$$
$$= M^3 \begin{pmatrix} A''' \\ B''' \end{pmatrix} \quad \text{etc}$$

$\gamma = i\frac{mv_0}{q\hbar^2}$ "M" is $\det M = 1$

has two complex eigenvalue e^{ika}, e^{-ika}

$$\mathrm{tr}\, M = 2\cos(ka) = (1+\gamma)\beta^{-1} + \beta(1-\gamma) \qquad \beta = e^{iqa}$$
$$= \beta^{-1} + \beta + \gamma(\beta^{-1} - \beta)$$
$$= 2\cos(qa) - \gamma\, 2i\sin(qa)$$

$$\cancel{2}\cos(ka) = \cancel{2}\cos(qa) - i\frac{mv}{q\hbar^2}\cancel{2}i\sin(qa)$$

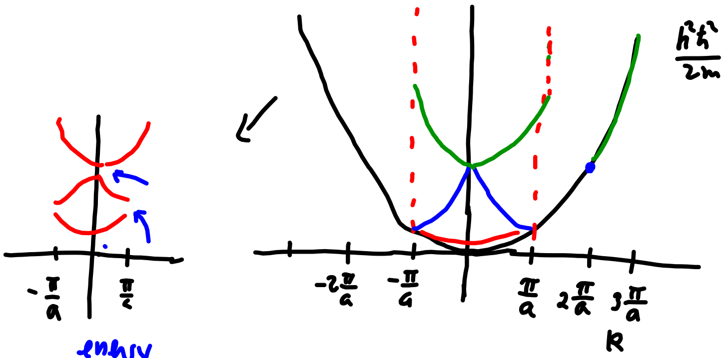
For a given k

$$\boxed{\cos(ka) = \cos(qa) + \frac{mva}{\hbar^2}\frac{\sin(qa)}{qa}}$$

find q $\Rightarrow$ $E = \frac{q^2\hbar^2}{2m}$ a function of k

for $v \ll 1$

$k \sim q$ $E \simeq k^2$



$E = \frac{k^2\hbar^2}{2m}$

no interaction

energy gaps

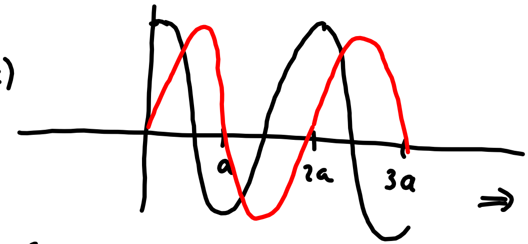
interaction

merely shift the energy near $\pm n\frac{\pi}{a}$ $\Rightarrow$ energy gap

at $\cos(kx)$ or $\sin(kx)$

$k = \frac{\pi}{a}$

$\cos(\frac{\pi}{a}x)$



$|\cos(\frac{\pi}{a}x)|^2$ has max at $x = na$

$|\sin(\frac{\pi}{a}x)|^2$ has zeros at $x = na$

$\Rightarrow$ two energy states at the band gap.

$V = \int \cos^2(kx)\, v(x)$
$\sin^2(kx)\, v(x)$

Since $\psi(x) = e^{ikx} u_k(x)$ for N atoms

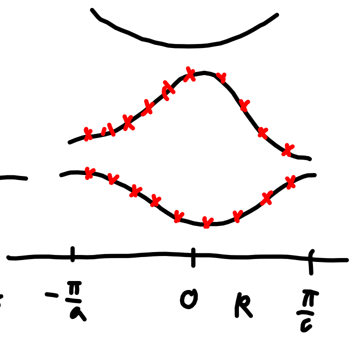
$\psi(L) = \psi(0)$ $L = Na$

$e^{ikL} = 1$ allow values for k

$kL = m 2\pi$ $m = 1, 2, 3, \cdots \frac{N}{2}$

$k = \frac{m 2\pi}{Na} = \frac{2m}{N}\frac{\pi}{a}$ $m = \frac{N}{2}$

$\Rightarrow$ N atoms $\Rightarrow$ N states of k



each band can hold 2N electrons

N state

filled bands are insulator

unfilled bands give conductors

Quantum Dynamics

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \qquad |\psi_i\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix}$$

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$$

$$|\psi_i(t)\rangle = \left(e^{-i\hat{H}t/\hbar}\right)_{ij} |\psi_j(0)\rangle \qquad \langle\psi_i| = (\psi_1, \psi_2, \dots \psi_n)^*$$

$$\langle\psi_i(t)| = \langle\psi_j(0)| \left(e^{-i\hat{H}t/\hbar}_{ij}\right)^* \qquad \hat{H}^*_{ij} = H^+_{ji} = H_{ji}$$

$$= \langle\psi_j(0)|\, e^{i\hat{H}^*_{ij}t/\hbar}$$

$$= \langle\psi_j(0)|\, e^{i\hat{H}_{ji}t/\hbar}$$

The expectation of $\hat{A}$ ← Schrodinger picture of dynamics

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle$$

$$= \langle\psi(0)|\, e^{i\hat{H}t/\hbar}\, \hat{A}\, e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$$

$$= \langle\psi(0)|\, \hat{A}(t)\, |\psi(0)\rangle$$

$$\hat{A}(t) = e^{i\hat{H}t/\hbar}\, \hat{A}\, e^{-i\hat{H}t/\hbar}$$ ← Heisenberg picture of Q. dynamics.

The Heisenberg picture is closer to classical dynamics.

$$\frac{d}{dt}\hat{A}(t) = \frac{i}{\hbar} e^{i\hat{H}t/\hbar} [H, A]\, e^{-i\hat{H}t/\hbar} + \frac{\partial \hat{A}}{\partial t}$$

$$= \frac{-i}{\hbar} [A(t), H] + \frac{\partial \hat{A}}{\partial t}$$

$$i\hbar \frac{d}{dt}\hat{A} = [A(t), H] + \frac{\partial \hat{A}}{\partial t} i\hbar \qquad [\ ] \to i\hbar\{\ \}$$

classically $$\frac{d}{dt}\hat{A} = \{A(t), H\} + \frac{\partial \hat{A}}{\partial t}$$

If $\hat{H}$ has no explicit time-dependence

then $\dot{\hat{H}} = 0$ $\hat{H}$ unchange in time.

The evolution of $\hat{r}(t)$:

$$i\hbar \dot{\hat{r}} = [\hat{r}, \hat{H}] = [\hat{r}, \hat{p}^2]/2m$$

$$\hat{r}_i \hat{p}_j \hat{p}_j - \hat{p}_j \hat{p}_j \hat{r}_i = 2i\hbar p_i \qquad = 2i\hbar \frac{\hat{p}_i}{2m}$$

$$([\hat{r}_i, \hat{p}_j] + \hat{p}_j \hat{r}_i)\hat{p}_j$$

$$i\hbar \delta_{ij} \hat{p}_j = i\hbar \hat{p}_i$$

$$\boxed{\dot{\hat{r}}_i = \frac{\hat{p}_i}{m}}$$

Heisenberg operator obey classical equations.

can also prove $\boxed{\dot{\hat{p}}_i = -\vec{\nabla} V(\hat{r})}$

Quantum dynamics of Harmonic oscillator

$$a = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{p} \qquad i\hbar\,\dot{\hat{x}} = [\hat{x}, H]$$

$$\dot{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\dot{\hat{x}} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\dot{\hat{p}}$$

$$= -i\omega a \quad \Rightarrow \quad a(t) = e^{-i\omega t} a(0)$$

what is $\hat{x}(t)$

$$\mathrm{Re}\, a(t) = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}(t) = [\cos(\omega t) - i\sin(\omega t)]\,[\alpha\,\hat{x}(0) + i\beta\,\hat{p}(0)]$$

$$= \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}(t) = \cos\omega t\,\alpha\,\hat{x}(0) + \sin(\omega t)\,\beta\,\hat{p}(0)$$

$$\Rightarrow \quad \hat{x}(t) = \cos\omega t\,\hat{x}(0) + \frac{1}{m\omega}\sin(\omega t)\,\hat{p}(0)$$

$$[\hat{x}(0), \hat{x}(t)] = \frac{1}{m\omega}\sin(\omega t)\, i\hbar$$

operators at different times DO NOT commute generally