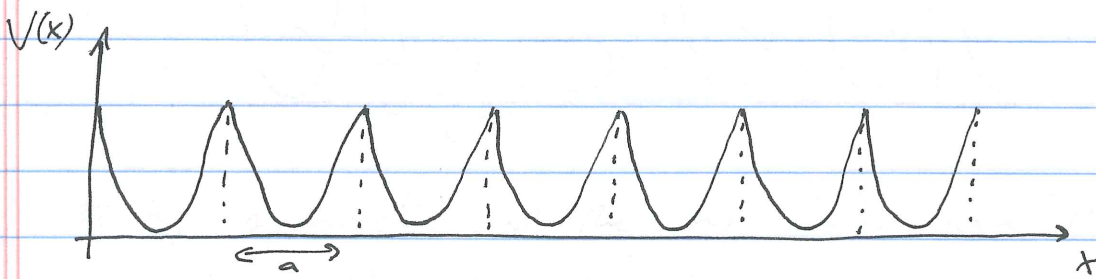
Tuesday, April 2, 2013

Lattice translation symmetry

We examine how discrete translation symmetry affects the energy eigenstates (in a solid state system)

We consider a 1D periodic potential with lattice period $\Delta x = a$ so that $V(x \pm a) = V(x)$.



the translation operator: $\tau(\Delta x)|x\rangle = |x+\Delta x\rangle$

$\Rightarrow \langle x|\tau^\dagger(\Delta x) = \langle x+\Delta x|$

$$\Rightarrow \langle x|\tau^\dagger(\Delta x)\, X\, \tau(\Delta x)|x\rangle = \langle x+\Delta x|\, X\, |x+\Delta x\rangle$$

$$= x + \Delta x$$

$$\Rightarrow \tau^\dagger(a)\, V(x)\, \tau(a) = V(x+a) = V(x)$$

Recall, that $\tau(\Delta x) = e^{-i\frac{P\Delta x}{\hbar}}$ (P: operator, Δx: scalar)

$\tau(\Delta x)$ is unitary, but not Hermitian $\tau^\dagger(\Delta x) = \tau^{-1}(\Delta x)$

Also $\langle x|\tau(\Delta x) = \langle x-\Delta x|$

$$\tau(\Delta x)|p\rangle = \underbrace{e^{-\frac{ip\Delta x}{\hbar}}}_{\text{complex eigenvalue}}|p\rangle$$

Also $[\tau(\Delta x), P] = 0$ and $\left[\tau(\Delta x), \frac{P^2}{2m}\right] = 0$

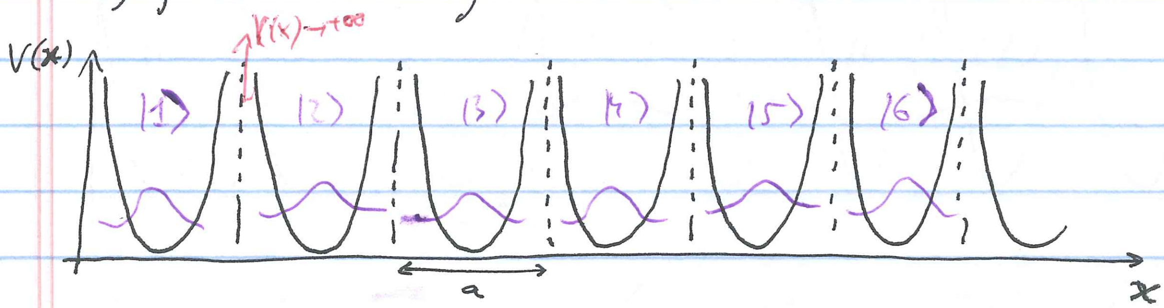
$[\tau(\Delta x), V(x)] \neq 0$ but $[\tau(a), V(x)] = 0$

$\tau(a)\tau^\dagger(a)V(x)\tau(a) = \tau(a)V(x) \Leftrightarrow V(x)\tau(a) = \tau(a)V(x)$

thus for $H = \dfrac{P^2}{2m} + V(x)$, we have $[\tau(a), H] = 0$

Deep periodic potential

we consider a periodic potential of deep wells with negligible tunneling between wells.



By symmetry all the $|n\rangle$ states have the same energy E_0: $H|n\rangle = E_0|n\rangle \iff |n\rangle$ are energy eigenstates

Note: $\tau(a)|n\rangle = |n+1\rangle$ | $\langle x|n\rangle = f(x-na)$

$\Rightarrow |n\rangle$ is not an eigenstate of $\tau(a)$ | $\langle x|\tau(a)|n\rangle = \langle x-a|n\rangle = f(x-(n+1)a)$

Since $[\tau(a), H] = 0$, ~~___~~ there should be a common basis of eigenstates for $\tau(a)$ and H:

→ Consider the state

$$|\phi\rangle = \sum_{n=-\infty}^{+\infty} e^{in\phi} |n\rangle$$

clearly $H|\phi\rangle = E_0|\phi\rangle$

$$\tau(a)|\phi\rangle = \sum_{n=-\infty}^{+\infty} e^{in\phi}\, \tau(a)|n\rangle = \sum_{n=-\infty} e^{in\phi} |n+1\rangle = \sum_{n'=-\infty} e^{i(n'-1)\phi} |n'\rangle$$

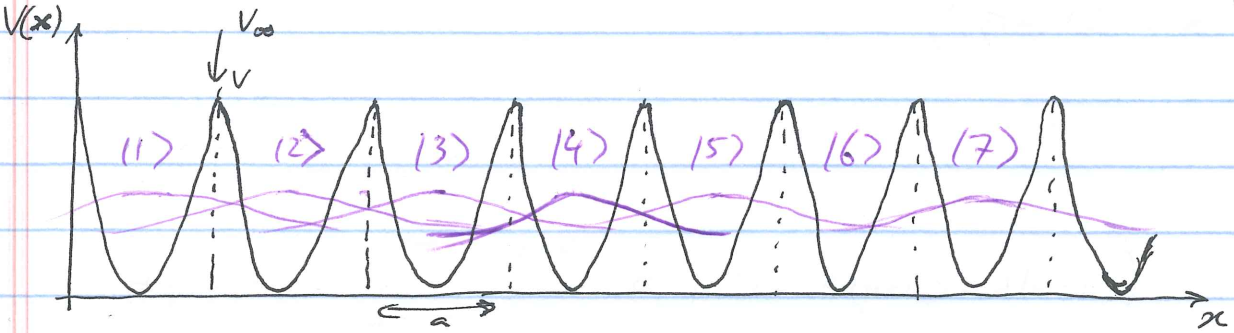
$n' = n+1$

$$= e^{-i\phi} \sum_{n'=-\infty}^{+\infty} e^{in'\phi} |n'\rangle$$

$$= e^{-i\phi} |\phi\rangle \Rightarrow |\phi\rangle \text{ are eigenstates of } H \text{ and } \tau(a)$$

Moderate Depth periodic potential

We consider a periodic potential of wells with ~~small~~ modest tunneling between adjacent sites.



The $|n\rangle$ states are the localized states obtained by smoothly ramping down the barrier heights from $+\infty$ to a finite ~~E~~ value V_{max}.

observations: ~~The $|n\rangle$ are no longer eigenstates of H~~

- the $|n\rangle$ states overlap $\Rightarrow \langle n|n+1\rangle \neq 0$ (i.e. not orthonormal)
- the $|n\rangle$ states are no longer eigenstates of H, but we will
  ↳ define $\langle n|H|n\rangle = E_0'$ (true for all n by ~~not the same~~ translational symmetry)
- $\langle n'|H|n\rangle \neq 0$
  ↳ we will choose to work in the tight binding approx.

See Sakurai & Napolitano section 4.3

Cohen-Tannoudji Complement F_{XI}

$\langle n|n+1\rangle \neq 0$ but $\langle n|n+2\rangle \simeq 0$

(overlap of ~~1st~~ nearest neighbor well wave-functions but not next-to-nearest neighbor wells)

we define
$$\begin{cases} \langle n\pm1|H|n\rangle = -A & A \in \mathbb{R} \\ \langle n\pm m|H|n\rangle \simeq 0 & m = 2,3,4,\dots \end{cases}$$

$$\Rightarrow H|n\rangle = E_0'|n\rangle - A|n+1\rangle - A|n-1\rangle$$

$$H = \begin{array}{c|c} & \begin{matrix} |n-1\rangle & |n\rangle & |n+1\rangle & \dots \end{matrix} \\ \begin{matrix} \langle n-1| \\ \langle n| \\ \langle n+1| \\ \vdots \end{matrix} & \begin{bmatrix} E_0' & -A & & & 0 \\ -A & E_0' & -A & & \\ & -A & E_0' & -A & \\ 0 & & -A & E_0' & \ddots \end{bmatrix} \end{array}$$

Since $\tau(a)|n\rangle = |n+1\rangle$, then

$$|\phi\rangle = \sum_{n=-\infty}^{+\infty} e^{in\phi}|n\rangle$$ is still an eigenstate of $\tau(a)$

$\left(\tau(a)|\phi\rangle = e^{-i\phi}|\phi\rangle\right)$

What about $H|\phi\rangle$?

$$H|\phi\rangle = \sum_{n=-\infty}^{+\infty} e^{in\phi}\left(E_0'|n\rangle - A|\underbrace{n+1}_{n'}\rangle - A|\underbrace{n-1}_{n''}\rangle\right)$$

$$= E_0' \sum_{n=-\infty}^{+\infty} e^{in\phi}|n\rangle - A\sum_{n'=-\infty}^{+\infty} e^{i(n'-1)\phi}|n'\rangle - A\sum_{n''=-\infty}^{+\infty} e^{i(n''+1)\phi}|n''\rangle$$

$$= \left(E_0' - Ae^{-i\phi} - Ae^{i\phi}\right)|\phi\rangle$$

$$= \left(E_0' - 2A\cos\phi\right)|\phi\rangle$$

$\Rightarrow$ $|\phi\rangle$ is an eigenstate of H with eigenenergy $E_\phi = E_0' - 2A\cos\phi$

note 1: the tight binding limit was not essential. $|\phi\rangle$ remains a eigenstate of H even with ~~cont~~ longer range couplings.

note 2: The energy spectrum is no longer discrete but continuous

$E_\phi = E(\phi) = E_0' - 2A\cos\phi$ ~~with $\phi \in [-\pi, \pi]$~~

what sort of state is $|\phi\rangle$?

By analogy $|\phi\rangle$ is some kind of momentum state:

$\tau(a)|p\rangle = e^{-i\frac{pa}{\hbar}}|p\rangle$ and $\tau(a)|\phi\rangle = e^{-i\phi}|\phi\rangle$

$\langle x|p\rangle = \dfrac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}$

this suggests $|p\rangle \stackrel{?}{\doteq} |\phi\rangle$

$$\frac{pa}{\hbar} \stackrel{?}{\doteq} \phi \qquad \left(p = \hbar k \text{ so } ka \stackrel{?}{\doteq} \phi\right)$$

but, we note that $\tau(a)\,|p + \frac{2\pi\hbar}{a}j\rangle = e^{-i\left(p+\frac{2\pi\hbar}{a}j\right)a/\hbar}\,|p+\frac{2\pi\hbar}{a}j\rangle$

$(j = 0, \pm 1, \pm 2, \dots)$

$$= e^{-ipa/\hbar}\,|p + \frac{2\pi}{a}j\rangle$$

A better guess is $|\phi\rangle = \sum_{j=-\infty}^{+\infty} c_j\,|p + \frac{2\pi\hbar}{a}j\rangle$

$$\Rightarrow \langle x|\phi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\sum_{j=-\infty}^{+\infty} c_j\, e^{i\left(p+\frac{\hbar 2\pi}{a}j\right)x/\hbar}$$

$$= \frac{e^{i\overset{k}{\frac{p}{\hbar}}x}}{\sqrt{2\pi\hbar}}\sum_{j=-\infty}^{+\infty} c_j\left(e^{i\frac{2\pi x}{a}}\right)^j$$

~~define~~ $b = \frac{2\pi}{a}$ (units of momentum) reciprocal lattice unit vector

$$\Rightarrow \langle x|\phi\rangle = e^{ikx}\underbrace{\sum_{j=-\infty}^{+\infty}\frac{c_j}{\sqrt{2\pi\hbar}}\,e^{i\frac{2\pi}{a}xj}}_{\text{Fourier series for a function of spatial period } a}$$

Fourier series for a function of ~~plane~~ spatial period $\underline{a}$.

$u_\phi(x) \to u_k(x)$ since $k = \frac{\phi}{a}$

We thus get the <u>Bloch Theorem</u>:

$$\boxed{\psi_k(x) = \langle x|\phi\rangle = e^{ikx}\,u_k(x)}$$

$\Rightarrow$ $\psi_k(x) = \langle x|\phi\rangle = e^{ikx}u_k(x)$, where $u_k(x)$ is a function of period $\underline{a}$, is an eigenstate of H and $\tau(a)$.

($u_k(x)$ determined by $V(x)$ specifics.)

$\psi_k(x)$ is essentially a plane wave with a spatially modulated amplitude.

Stopped here