Phys 4702 Intro QM II Fall 2024 17 Oct 2024

NOTE: Re $\langle \ell s j' m' | S_z | \ell s j m \rangle$

* HW #8 status

$[A,B]=0$

$\Rightarrow \langle a'|B|a\rangle = 0!$

* Office Hours Tomorrow (I have to leave after!)

Today: Discrete Translation Symmetry

Where we are going: Bloch's Theorem

$\Leftrightarrow$ Crystal Energy Bands / Gaps (HW!)

Recall: $T(\Delta x')|x'\rangle = |x'+\Delta x'\rangle$ [Easy to generalize to 2D or 3D!]

$\Leftrightarrow T(\Delta x') = \exp\left[-\frac{i p \Delta x'}{\hbar}\right]$

p = momentum (in x-direction); unitary operator

Detour: Eigenvalues of Unitary Operators

[Not Hermitian $\Rightarrow$ Not observable, OK, just go!]

$U|\lambda\rangle = \lambda|\lambda\rangle$ w/ $U^\dagger = U^{-1}$ i.e. $U^\dagger U = 1$

$\Leftrightarrow \langle\lambda|U^\dagger = \lambda^*\langle\lambda| \Rightarrow \left(\langle\lambda|U^\dagger\right)\left(U|\lambda\rangle\right) = \lambda^*\lambda\langle\lambda|\lambda\rangle$

But $U^\dagger U = 1 \Rightarrow \langle\lambda|U^\dagger U|\lambda\rangle = \langle\lambda|\lambda\rangle = |\lambda|^2\langle\lambda|\lambda\rangle$

i.e. $|\lambda|^2 = 1$ [Recall "positivity postulate" i.e. $\langle\lambda|\lambda\rangle > 0$]

$\Leftrightarrow$ Eigenvalue of unitary operator $\lambda = e^{i\alpha}$, $\alpha \in \mathbb{R}$

Note: Parity is a special case (Hermitian!)

$\Rightarrow$ Eigenvalues must be real $\Rightarrow$ Only ± 1

Discrete Translation...

$$T(a)|x'\rangle = |x'+a\rangle \quad \text{w/} \quad T(a) = \exp\left(-\frac{i}{\hbar}pa\right)$$

$$x\,T(a)|x'\rangle = x|x'+a\rangle = (x'+a)|x'+a\rangle$$

$$T^\dagger(a)\,x\,T(a)|x'\rangle = (x'+a)\,T^\dagger|x'+a\rangle$$

But $T^\dagger(a) = \exp\left(+\frac{i}{\hbar}pa\right) = \exp\left(-\frac{i}{\hbar}p(-a)\right)$

$= T(-a)$ [Of course! Inverse is reverse!]

$\Rightarrow$ $T^\dagger(a)\,x\,T(a)|x'\rangle = (x'+a)|x'\rangle = (x+a)|x'\rangle$

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i.e. $\underline{\underline{T^\dagger(a)\,x\,T(a) = x + a}}$ Makes sense! Good.

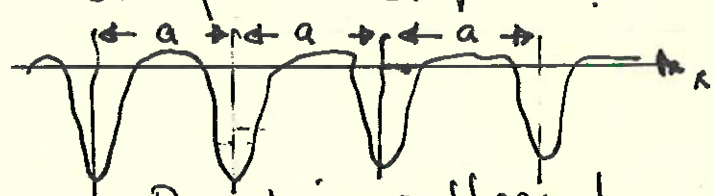
NOTE: $T^\dagger(a)\,F(p)\,T(a) = F(p)$ (i.e. $[T(a),p]=0$)

... Symmetry: Require $T^\dagger(a)\,H\,T(a) = H$

$\Rightarrow$ $[H,T(a)]=0$

$H = \frac{1}{2m}p^2 + V(x)$ $\longrightarrow$ Need "periodicity" i.e.

Symmetric!!



Repeating pattern!

i.e. $T^\dagger(a)V(x)T(a) = V(x+a) = V(x)$

$\Rightarrow$ $\underline{\underline{T^\dagger(a) H T(a) = H}}$ for $V(x)$ w/ period a

"Discrete Translation Symmetry"

<u>Eigenstates</u>

Translation symmetry $\Rightarrow$ $[H, T(a)] = 0$

"Simultaneous Eigenvalues for H and $T(a)$"

we know eigenvalues of $T(a)$ are $e^{i\alpha}$

$\Rightarrow$ How are these related to eigenvalues E of H?

Work in position space:

$$T(a)|\alpha\rangle = e^{i\alpha}|\alpha\rangle$$

$$\langle x|T(a)|\alpha\rangle = e^{i\alpha}\langle x|\alpha\rangle$$

$$\langle x-a|\alpha\rangle = e^{i\alpha}\langle x|\alpha\rangle$$

Define $\psi(x) \equiv \langle x|\alpha\rangle$

$\Rightarrow$ $\psi(x-a) = e^{i\alpha}\psi(x)$

<u>Convention</u>: $\alpha = -ka$ NOTE: $\hbar k$ has units of <u>momentum</u>.

$\Rightarrow$ $\psi(x-a) = e^{-ika}\psi(x)$

Now write $\psi(x) = e^{ikx}u(x)$ for some $u(x)$

$\Rightarrow$ $e^{ik(x-a)}u(x-a) = e^{-ika}e^{ikx}u(x)$

$$u(x-a) = u(x)$$

i.e. $\psi(x) = e^{ikx} u(x)$ w/ $u(x+a) = u(x)$ "Periodic"

"Bloch's theorem"

... Now explore the energy eigenvalues!

NOTE: e^{ikx} looks like a free particle wave of $p = \hbar k$

NOTE: $\psi(x+a) = e^{ik(x+a)} u(x+a)$
$= e^{ika} e^{ikx} u(x) = e^{ika} \psi(x)$

Another way to state Bloch's thm

$\Rightarrow |\psi(x+a)|^2 = |\psi(x)|^2$ Makes sense!

Energy Eigenvalues

Substitute $\psi(x) = e^{ikx} u(x)$ into Schrödinger Eqn.

$\Rightarrow$ Expect to find $E = E(k)$.

What can we say about the values of k?

First consider "infinite" periodicity as $N \sim 10^{23}$ sites that wrap around start to end.

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i.e. $\psi(x+Na) = \psi(x) \Rightarrow \exp(Nika) = 1$

$\Rightarrow k = \frac{2\pi}{Na} n \qquad n = 0, \pm 1, \pm 2, \ldots$

But N is very large!

$\Rightarrow$ Take k to be a continuous variable.

For specific problem need to know $V(x)$!

Homework: Periodic δ-functions

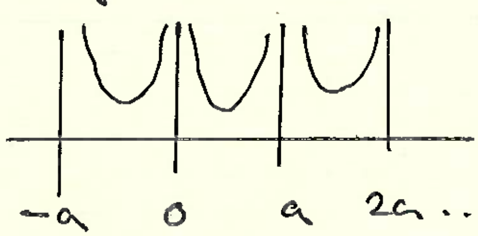
$$V(x) = \frac{\hbar^2}{2m}\lambda \sum_{n=-\infty}^{\infty} \delta(x-na)$$

wave function is just "free particle" for $0<x<a$

[the problem guides you $\Rightarrow$ "Energy Bands"

General Considerations

1) Infinite Barrier : Completely localized state $|n\rangle$



$H|n\rangle = \underline{E_0|n\rangle \text{ for all } n}$ (Ground states)

"Infinite Degeneracy"

But $T(a)|n\rangle = |n+1\rangle \Rightarrow |n\rangle$ not eigenstates of $T(a)$!

Try the linear combination

$$|\theta\rangle \equiv \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \qquad \text{Still } H|\theta\rangle = E_0|\theta\rangle$$

$$\text{But } T(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle$$

$$= e^{-i\theta}|\theta\rangle \qquad \text{Simultaneous Eigenstates!}$$

NOTE: (2) $\langle n-1|H|n\rangle = \int dx \, \underbrace{\langle n-1|x\rangle}_{\psi_{n-1}^*(x)} \underbrace{\langle x|H|n\rangle}_{\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + V(x)\psi_n(x)\right]}$

(1) $\langle x-a|\theta\rangle = e^{-i\theta}\langle x|\theta\rangle$

i.e. $\underline{\theta \equiv \alpha = ka}$.

$= 0$ (NO OVERLAP DUE TO INFINITE BARRIER)

2) Finite (But "high") Barrier $\Rightarrow$ $\langle n-1|H|n\rangle \neq 0$

"Off Diagonal elements" so must diagonalize for energy eigenvalues!

Write Diagonal elements as $\langle n|H|n\rangle \equiv E_0$

Assume $\langle n'|H|n\rangle = 0$ unless $n' = n \pm 1$

"Tight Binding Approximation"

Put $\langle n\pm 1|H|n\rangle \equiv -\Delta$

Also $\langle n\pm 1|n\rangle = \int dx \, \langle n\pm 1|x\rangle\langle x|n\rangle \simeq 0$

$\Rightarrow H|n\rangle = E_0|n\rangle - \Delta|n-1\rangle - \Delta|n+1\rangle$ $\left[= \sum_{m=-\infty}^{\infty} |m\rangle\langle m|H|n\rangle \right]$

But is $|\theta\rangle$ still an energy eigenstate?

$$H|\theta\rangle = H\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}\left[E_0|n\rangle - \Delta|n-1\rangle - \Delta|n+1\rangle\right]$$

$$= \sum_{n=-\infty}^{\infty} e^{in\theta} E_0|n\rangle - \sum_{n=-\infty}^{\infty} \Delta\left[e^{i(n+1)\theta} + e^{i(n-1)\theta}\right]|n\rangle$$

$$= \left[E_0 - \Delta\left(e^{i\theta} + e^{-i\theta}\right)\right] \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$$

$\Rightarrow H|\theta\rangle = (E_0 - 2\Delta\cos\theta)|\theta\rangle$ yes! Eigenstate!

$$E = E_0 - 2\Delta\cos\theta = E_0 - 2\Delta\underline{\cos(ka)}$$

Between -1 and 1

i.e. "Energy Band" ω $E_0 - 2\Delta \leq E \leq E_0 + 2\Delta$

[Remember: this is a specific example]