Optics + Spectroscopy — Lecture ⑪

Time-dependent S.E.

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = \hat{H}(\vec{r},t)\,\Psi(\vec{r},t)$$

$\Psi(\vec{r},t)$ ~ wavefunction, contains all the information we can know about the system

Time-independent Hamiltonian: $\hat{H} = \hat{H}(\vec{r})$

$$\Rightarrow i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = \hat{H}(\vec{r})\,\Psi(\vec{r},t)$$

try $\Psi(\vec{r},t) = \varphi(\vec{r})\,T(t)$

$$\Rightarrow i\hbar\, \varphi(\vec{r}) \frac{\partial T(t)}{\partial t} = \hat{H}(\vec{r})\,\varphi(\vec{r})\,T(t)$$

rearrange: $$\frac{i\hbar \frac{\partial T(t)}{\partial t}}{T(t)} = \frac{\hat{H}(\vec{r})\psi(\vec{r})}{\psi(\vec{r})}$$

no $\vec{r}$ dependence   not t dependence

~ both sides must be equal to a constant

$$\frac{i\hbar \frac{\partial T(t)}{\partial t}}{T(t)} = E = \frac{\hat{H}(\vec{r})\psi(\vec{r})}{\psi(\vec{r})}$$

$\psi(\vec{r})$s don't cancel b/c $\hat{H}$ is an operator (changes $\psi(\vec{r})$)

LHS: $$i\hbar \frac{\partial T(t)}{\partial t} = E\,T(t)$$

$$\Rightarrow \quad T(t) = e^{-iEt/\hbar}$$

RHS: $\hat{H}(r)\psi(\vec{r}) = E\psi(\vec{r})$

time-independent S.E. → ψ is an acceptable wavefunction if it satisfies this eqn.

Postulates of Q.M.

(i) every "observable" has a corresponding operator

~ construct operators using the following rules

$$x \rightarrow \hat{x}$$

$$p_x \rightarrow -i\hbar \frac{\partial}{\partial x}$$

eg. the operator for energy is the Hamiltonian $\hat{H}$

$$H = \frac{p^2}{2m} + V(x)$$

$$\Rightarrow \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x)$$ ← motion in 1-D

Postulate II: $\hat{A}\varphi_a = a\varphi_a$

~ measurement of "A" that yields the value "a" leaves the system in φ_a

~ a function is an eigenfunction of $\hat{A}$ if $\hat{A}\varphi_a = (\text{constant}) * \varphi_a$

$$\uparrow$$

eigenvalue $= a$

~ the wavefunction (which describes our system) is an eigenfunction of $\hat{H}$

Postulate III:

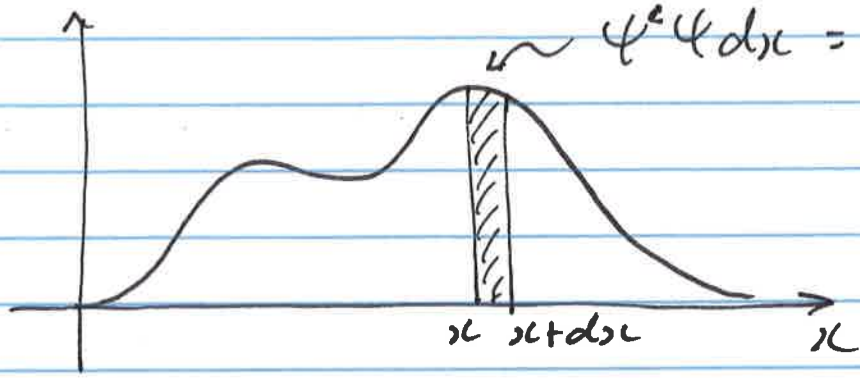
~ calculate "expectation values" of observables by

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(\vec{r})\, \hat{A}\, \psi(\vec{r})\, d\vec{r}$$

~ $\psi^*(\vec{r})\psi(\vec{r})d\vec{r}$ ~ prob'y of finding the particle b/w $\vec{r}$ + $\vec{r}+d\vec{r}$

~ more rigorously $\quad \psi^* \psi$ ~ prob^y density

1-D



~ $\psi^* \psi \, dx$ = prob^y of being b/w x and $x+dx$

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi \, dx$$

← averaging $\hat{A}$ over all values of x.

"expectation value" ~ value we expect to get

~ make a series of measurements, we get a distribution of values.

width: $\sigma = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

if ψ is an eigenfunction of $\hat{A}$

$$\hat{A} \psi = a \psi$$

$$\Rightarrow \quad \langle A \rangle = \int \psi^* \hat{A} \psi \, dx$$

$$= \int \psi^* a \psi \, dx$$

$$= a \underbrace{\int \psi^* \psi \, dx}_{=1}$$

$\sim$ prob^{ty} is normalized

$$\langle A^2 \rangle = \int \psi^* \hat{A}^2 \psi \, dx$$

$$= a \int \psi^* \hat{A} \psi \, dx$$

$$= a^2$$

$$\Rightarrow \quad \langle A^2 \rangle - \langle A \rangle^2 = 0$$

$\sim$ always get the same value of A.

Complete wavefunction for the time-independent Hamiltonian is:

$$\psi_n(\vec{r}, t) = A_n \varphi_n(\vec{r}) e^{-iE_n t/\hbar}$$

$$= A_n \varphi_n(\vec{r}) e^{-i\omega_n t}$$

~ in general, there is not just <u>one</u> solution to the S.E. (many times there is an infinite #!)

~ label the sol='s by a Q.N. "n"

<u>Time-independent problems</u>

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, dx$$

$$= \int A_n^* e^{i\omega_n t} \varphi_n^*(x) \hat{A} \varphi_n(x) A_n e^{-i\omega_n t} dx$$

$$= |A_n|^2 \int \varphi_n^*(x) \hat{A} \varphi_n(x) \, dx$$

$e^{-i\omega_n t}$ "phase factors" cancell, no time dependence

$|A_n|^2$ ~ normalization constant

require: $|A_n|^2 \int \varphi_n^*(x) \varphi_n(x) \, dx = 1$

Trivial Example: Free particle

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad (V(x) = 0)$$

$$\hat{H}\psi = E\psi$$

~ try $\psi(x) = Ae^{ikx}$

$$\frac{\partial \psi}{\partial x} = ikAe^{ikx}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 Ae^{ikx} = -k^2\psi$$

$$\Rightarrow \quad \hat{H}\psi = \frac{\hbar^2 k^2}{2m}\psi = E\psi$$

$\psi(x) = Ae^{ikx}$ works as an eigenfunction of $\hat{H}$

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

~ this wavefunction is also an eigenfunction of momentum

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{p}_x \psi = -i\hbar \frac{\partial A e^{ikx}}{\partial x} = \hbar k A e^{ikx}$$

$\psi = Ae^{ikx}$ ~ corresponds to a particle moving in the $+x$ direction w/ a momentum $= \hbar k$

Other functions that solve the S.E.

$$\psi = A\cos kx$$

$$\frac{\partial \psi}{\partial x} = -kA\sin kx \qquad \frac{\partial^2 \psi}{\partial x^2} = -k^2 A\cos kx$$
$$= -k^2 \psi$$

$$\Rightarrow \hat{H}\psi = \frac{\hbar^2 k^2}{2m}\psi \qquad \Rightarrow E = \frac{\hbar^2 k^2}{2m} \text{ as before}$$

However, now ψ is not an eigenfunction of $\hat{p}_x$

$$\hat{p}_x \psi = -i\hbar \frac{\partial}{\partial x} A\cos kx = i\hbar k A\sin kx$$

$$\Rightarrow \hat{p}_x \psi \neq (\text{constant}) \times \psi$$

~ now we need to calculate expectation values

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p}_x \psi \, dx$$

$$= -i\hbar |A|^2 \int_{-\infty}^{\infty} \cos kx \frac{\partial \cos kx}{\partial x} dx$$

$$= i\hbar |A|^2 \int_{-\infty}^{\infty} \cos kx \sin kx \, dx = 0$$

particle not stationary: $E_K = \frac{\hbar^2 k^2}{2m}$

$\psi(x) = A \cos kx$

know the K.E. & $\therefore$ the magnitude of the momentum $\left(\frac{|p|^2}{2m} = \frac{\hbar^2 k^2}{2m}\right)$ but we don't know the direction

~ see this more clearly by writing ψ as a superposition of e^{ikx} & e^{-ikx} wavefunctions.

$$\psi(x) = A \cos kx = A\left(e^{ikx} + e^{-ikx}\right)$$

sum of 2 wavefunctions, one corresponding to motion in $+x$, the other to motion in $-x$

Last point:

prob^{y} density $= \psi^* \psi$

$$= |A|^2 e^{ikx} \times e^{-ikx} = |A|^2$$

constant

~ equally likely to find the particle anywhere in space

~ no information about position

~ consistent w/ ψ being an eigenfunction of $\hat{p}_x$

~ well define (precise) momentum ($\hbar k$)

$\Delta x . \Delta p_x \geq \hbar/2$ ~ Heisenberg Uncertainty Principle.