Lecture : 4

16/01/25

$\hat{H} = \hat{T} + \hat{V}$ ⟶ $\hat{H}\Psi = \hat{T}\Psi + \hat{V}\Psi = E\Psi$

hamiltonian operator : associated the overall energy of the system

1d motion $= -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right) + V(x)\Psi = E\Psi$

V(x) depends on the physical state of the particle
① free particle: $V(x) = 0 \; \forall x$
② harmonic oscillation: $V(x) = \frac{1}{2}kx^2$

Note: if there is Coulomb potential btw the particle, the Potential Energy → $V(x) \propto \frac{1}{x}$

NOTE 2: Kinetic energy is defined for individual objects and anything that moves has KE. Any object at rest has KE = 0
Generally: $KE = \frac{1}{2}mv^2$

NOTE 3: Potential Energy
~ stored energy
~ energy due to position
gravitational potential = mgh

NOTE 4: Elastic PE: $U = \frac{1}{2}kx^2$
k: spring constant : N/m
x: how much the spring been stretched : m

NOTE 5: wave particle duality principle:
momentum of photon → $p = \frac{h}{\lambda}$ (p: momentum; h: plank's constant; λ: de broglie's wavelength)

→ when can an object that appears as particle behave as wave ?
↳ when the dimension (r) over which the change of potential energy V(r) of a particle becomes smaller as compared to its wavelength, its wave nature reveals.

Heisenberg's Uncertainity Principle

$\Delta p \Delta x \geq \hbar$ # note: $\hbar = \frac{h}{2\pi}$

both momentum and position cannot be precisely determined at the same time

$\Delta E \Delta t \geq \hbar$ # another form of the uncertainity principle
(ΔE: energy of the particle; Δt: the time instant the particle had that Energy)

Using this version, Energy cannot be zero
minimum Energy ≡ ZPE → Zero Point Energy ≠ 0

Wave Function Ψ

describes the quantum state of an isolated system of one or more particles.
There exists only one wave function containing info for an entire system

$\Psi(x) \,/\, \Psi(r,t)$

Probability Density : $P(r) = |\Psi|^2 = \int \Psi^* \Psi \, d\tau$
↓
probability that a particle can be found at a point x in time t

- POSTULATES OF QUANTUM MECHANICS

① The state of a quantum mechanical system is completely specified by a wave function $\psi(r,t)$ that depends on the particle's position 'r' and time 't'

$$\psi(x_1, y_1, z_1, \ldots, x_i, y_i, z_i, t)$$

$$P(r) = |\psi|^2 = \int \psi^* \psi \, d\tau$$

the probability that the particle can be found at point x at time t

$$\Rightarrow P(r) \geq 0$$

$$\Rightarrow \int_{\text{all space}} \psi^* \psi \, d\tau = 1$$

② To every physical property observable in classical mechanics, there corresponds a linear, hermitian operator in quantum mechanics

OBSERVABLE		OPERATOR	
Position	x	$\hat{X}$	multiply by x
	r	$\hat{R}$	multiply by r
Momentum	p_x	$\hat{P}_x$	$-i\hbar \frac{\partial}{\partial x}$
	p	$\hat{P}$	$-i\hbar\left(i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + k\frac{\partial}{\partial z}\right)$
Kinetic Energy	T_x	$\hat{T}_x$	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
	T	$\hat{T}$	$\frac{-\hbar^2}{2m}\underbrace{\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)}_{\nabla^2}$
Potential Energy	$V(x)$	$\hat{V}(\hat{x})$	multiply by $V(x)$
	$V(x,y,z)$	$\hat{V}(\hat{x},\hat{y},\hat{z})$	multiply by $V(x,y,z)$
Total Energy	E	$\hat{H}$	$\frac{-\hbar^2}{2m}\nabla^2 + V(x,y,z)$
Angular Momentum	L_x	$\hat{L}_x$	$-i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$
	L_y	$\hat{L}_y$	$-i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$
	L_z	$\hat{L}_z$	$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

③