• Lecture 3

* Wave Function
(Born interpretation)

$\Psi(x)$: varies with time or $\Psi(r,t)$

for 1 particle system: $\Psi = \Psi(x,y,z,t)$
for 2 particle system: $\Psi = \Psi(x_1,y_1,z_1,x_2,y_2,z_2,t)$

wave function contains all info about the system

wave function $\longleftrightarrow$ classical trajectory
(quantum mechanics) (newtonian mechanics)

Probability density
$\hookrightarrow P(r) = |\Psi|^2 = \int \Psi^* \Psi \, d\tau$ — ①

① COPENHAGEN/BORN'S INTERPRETATION
The probability that a particle can be found at a point x at time t is given by ①

→ Psi can be represented as a linear combination of other Psis

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

	SYMBOL	OPERATOR	
Position	x	$\hat{X}$	$\times x$
	r	$\hat{R}$	$\times r$
Momentum	p_x	$\hat{P}_x$	$-i\hbar \frac{\partial}{\partial x}$
	p_x	$\hat{P}$	$-i\hbar\left(i\frac{\partial}{\partial x} + j\frac{\partial}{\partial x} + k\frac{\partial}{\partial x}\right)$
KE	T_x	$\hat{T}_x$	$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$
	T	$\hat{T}$	$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = \frac{-\hbar^2}{2m}\nabla^2$
PE	$V(x)$	$\hat{V}(x)$	$\times V(x)$
	$V(x,y,z)$	$\hat{V}(x,y,z)$	$\times V(x,y,z)$
Total Energy = KE + PE	E	$\hat{H}$	$\frac{-\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right) + V(x,y,z) = \frac{-\hbar^2}{2m}\nabla^2 + V(x,y,z)$

NOTE: Hermition matrix:
if $A = A^T$

③ $\hat{A}\Psi = a\Psi$ — ②

In any measurement of the observable associated with operator $\hat{A}$, the only values that will be observed are the eigenvalues 'a' which satisfy ②

$\hat{A}f(x) = kf(x)$
$f(x)$: eigenfunction of A with eigenvalue k

the eigenvalue gives the real observable

eg: e^{ikx} is an eigenfunction of the operator $\hat{P}_x = -i\hbar\frac{\partial}{\partial x}$

if I operate $\hat{P}_x$ on Ψ, i.e. $\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi$

and we get: $\#\Psi$
↳ some number

then # is eigenvalue
here $\Psi = e^{ikx}$

$-i\hbar\frac{\partial}{\partial x}e^{ikx} = -i^2\hbar k^2 e^{ikx} = \hbar k^2 e^{ikx}$

$k \equiv$ wave number
$\lambda \equiv$ wave length

: $k = \frac{2\pi}{\lambda}$

$P = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \hbar \cdot k$
($\hbar$ → reduced plank constant; k → wave number)

$\hbar = \frac{h}{2\pi}$

$P = \hbar \cdot k$

hence, Momentum space is also called K-space and we can swap between the two using a real number $\hbar$

$\Psi = e^{ikx}$ (momentum space → k; real space → x) time independent wave func
$\Psi = e^{i(kx-\omega t)}$ time dependent wave func

④ For a system in a state described by a normalized wave function Ψ, the avg or expectation value of the observable corresponding to A is given by

$$\langle A \rangle = \int \Psi A \Psi^* dz$$

⑤ SCHRODINGER EQUATION

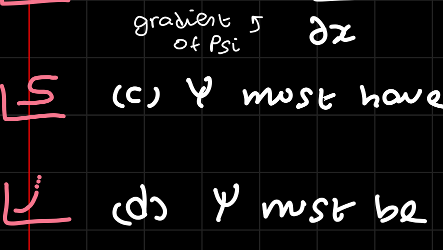
$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$ time dependent

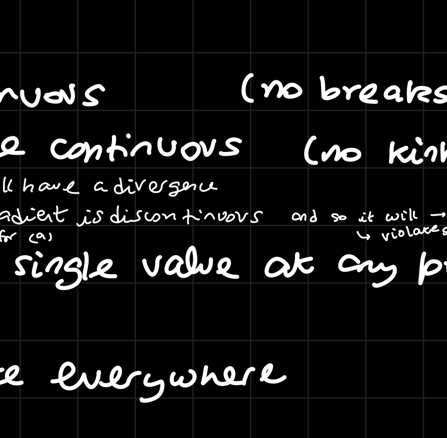
$E = \hat{H}\Psi$ time independent

$\tilde{H} \equiv$ Hamiltonian

$\hat{H} = \hat{T} + \hat{V} + V_{ext}$
(V_{ext} → external potential energy)

TE = KE = PE
total energy





* BORN'S Interpretation (CRITERIAS)

NOPE

(a) Ψ must be continuous (no breaks)

(b) $\nabla\Psi = \frac{\partial\Psi}{\partial x}$ must be continuous (no kinks)
gradient of Psi
we will have a divergence if gradient is discontinuous and so it will → ∞ ↳ violates (d)
same for (a)

(c) Ψ must have a single value at any pt. in space

(d) Ψ must be finite everywhere

(e) Ψ cannot be zero everywhere

Quantization of the wave function

These restrictions on Ψ ensures that only certain wavefunctions and only certain energies of system are allowed

$\therefore$ Quantization of $\Psi \Rightarrow$ Quantization of E

• Examples

① Particle moving in 1 dimension

Cases:
1. PE = 0 $\forall x$
2. PE = 0 for certain x
3. PE = ∞ $\forall x$

Case 1: PE ≡ zero

$\hat{H}\Psi = E\Psi$; $\hat{H} = \hat{T} + \hat{V}$ ($\hat{V}$ → zero) $\Rightarrow \hat{H} = \hat{T}$

$\hat{H}\Psi = E\hat{\Psi} \Rightarrow \hat{T}\Psi = E\Psi \Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right)\Psi = E\Psi$

$\hat{T} = \frac{\hat{P}^2}{2m}$; $\hat{P} = -i\hbar\frac{\partial}{\partial x}$; $\hat{P}^2 = -\hbar^2\frac{d^2}{dx^2}$

$\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

$\Psi = A\sin(kx) + B\cos(kx) = Ae^{ikx}$

$\frac{d^2\Psi}{dx^2} = -k^2(A\sin kx + B\cos kx) = -k^2\Psi$

Energy Dispersion Relation OR E-K Relation

$\boxed{E = \frac{k^2\hbar^2}{2m}}$ (E depends on k)
$E \propto k^2$

we know $p = k\hbar$

So, $E = \frac{p^2}{2m}$

Energy is a cont. function of momentum

$\therefore$ we can find out E from k-space

wave num → momentum → position
we can represent E in terms of x,y,z

if we have boundary condition like $\lim_{x\to 5}$, we are also restricting k