Appearance of Quantum Mechanics

Wave-particle duality

Schrödinger equation

Born interpretation: normalization, quantization

Reading: Atkins, Ch. 8 (p. 249-260)

Wave-particle duality

	C.M.		Exp.
electromagnetic radiation	"wave"	$\rightarrow$	also "particle" characteristics
electron	"particle"	$\rightarrow$	also "wave" characteristics

(1) Particle characteristics of electromagnetic radiation

- spectrum: electromagnetic radiation of frequency ν possesses the energies of
  0, $h\nu$, $2h\nu$ $\rightarrow$ 0, 1, 2 particles, each particle having $h\nu$ energy: "**Photon**"

e.g., yellow light (560 nm) of 100 W lamp in 0.1 s (efficiency 100 %)
$\rightarrow$ number of photons: $N = E/h\nu = Pt/h(c/\lambda) = 2.8 \times 10^{20}$
(40 min $\rightarrow$ 1 mol photons)

- photoelectric effect: light energy = $nh\nu$ $\rightarrow$ particle-like collisions of light

(2) Wave characteristics of particles

- electron diffraction (Davisson & Germer Exp. (1925)): a characteristic property of waves

→ waves interfere constructively and destructively in different directions: wave-like property of electron, molecular hydrogen

de Broglie relation

- particle $\rightarrow$ wave-like
  wave $\rightarrow$ particle-like $\Rightarrow$ "wave-particle duality"

- 1924, Louis de Broglie (France) suggested that any particle travelling with a linear momentum p (=mv) should have a wavelength of

$$\lambda = h/p\text{: de Broglie relation}$$

- particle with high momentum $\rightarrow$ short wavelength

Macroscopic body: high momentum $\rightarrow$ wavelength are undetectably small: wave-like properties can not be observed

e.g., golf ball, 45 g, velocity 30 m/s $\rightarrow$ $\lambda = 4.9 \times 10^{-22}$ pm (no wave-like)

- wave-particle duality & quantized energy $\Rightarrow$ **new mechanics** needed

(cf. Classical mechanics treated particles and waves as entirely separate entities)

- wave in new mechanics replaces classical concept of trajectory: rather than travelling along a definite path, a particle is distributed through space like a wave $\Rightarrow$ "wavefunction" (Ψ, psi)

$$2\pi r = n\lambda = n(h/p) = n(h/mv)$$

$$mvr = n(h/2\pi) = n\hbar$$

Momentum is quantized $\rightarrow$ Bohr interpretation

If wave does not match $\rightarrow$ disappear!!

Schrödinger equation

- **Schrödinger equation** (1926): Austrian physicist

- He proposed an equation for finding the wavefunction of any system
- time-independent Schrödinger equation
  particle mass m moving in 1-dimensional with energy E

V(x): potential energy of the particle at point x
E: total energy
$\hbar$ (h-cross or h-bar) = $h/2\pi$ = 1.05457 x 10^{-34} Js

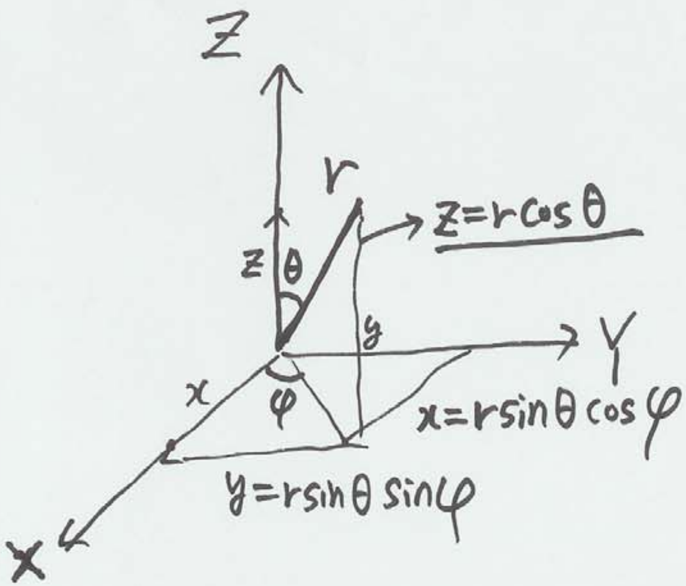
3-D

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad \nabla : \text{del}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

or in spherical symmetry

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Lambda^2 \qquad \Lambda : \text{lambda}$$



where

$$\Lambda^2 = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \cdot \frac{\partial}{\partial\theta}\right)$$

In general case, Schrödinger equation

$$\mathbf{H\Psi = E\Psi}$$

H: hamiltonian operator

Time-dependent Schrödinger equation

cf) Derive Schrödinger equation

plane wave: $f = A\sin\frac{2\pi}{\lambda}(x - vt) = A\sin 2\pi\left(\frac{x}{\lambda} - \nu t\right)$

$$\left(\begin{array}{l} \because v = \nu\lambda \\ \nu = \frac{1}{\tau} = \frac{v}{\lambda} \end{array}\right)$$

general differential equation of wave motion in 1-D

$$\frac{\partial^2 f}{\partial x^2} = -\frac{4\pi^2}{\lambda^2}f, \quad \frac{\partial^2 f}{\partial t^2} = -4\pi^2\nu^2 f$$

partial differential eq'n → can be simplified by the separation of variables technique (to separate x and t term)

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{\lambda^2\nu^2}\frac{\partial^2 f}{\partial t^2} = \frac{1}{v^2}\cdot\frac{\partial^2 f}{\partial t^2}$$

$$f = X(x)T(t)$$

$$\frac{\partial^2 f}{\partial x^2} = T(t)\frac{\partial^2 X(x)}{\partial x^2}, \quad \frac{\partial^2 f}{\partial t^2} = X(x)\cdot\frac{\partial^2 T(t)}{\partial t^2}$$

$$T(t)\frac{\partial^2 X(x)}{\partial x^2} = \frac{1}{v^2}X(x)\frac{\partial^2 T}{\partial t^2}$$

$$\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} = \frac{1}{v^2}\frac{1}{T(t)}\frac{\partial^2 T}{\partial t^2} = \boxed{-\frac{\omega^2}{v^2}}$$ separation constant

$$\frac{\partial^2 X(x)}{\partial x^2} + \frac{\omega^2}{v^2} X(x) = 0$$

$$\omega = 2\pi\nu = 2\pi\frac{v}{\lambda}, \quad \frac{\omega^2}{v^2} = \frac{4\pi^2}{v^2}\frac{v^2}{\lambda^2} = \frac{4\pi^2}{\lambda^2}$$ ← apply de Broglie relation

$$= \frac{4\pi^2}{(h/p)^2} = \frac{4\pi^2}{h^2}\cdot p^2 \quad \left(\leftarrow E = \frac{p^2}{2m} + V, \; p = \sqrt{2m(E-V)} \right)$$

$$= \frac{4\pi^2}{h^2}\cdot 2m(E-V)$$

time - independent

$$\frac{\partial^2 X}{\partial x^2} + \frac{4\pi^2}{h^2}\cdot 2m(E-V)X = 0 \xRightarrow{X \to \psi\text{로 바꿈}} \frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{h^2}\cdot 2m(E-V)\psi = 0$$

$$\therefore \underline{\underline{\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0}}$$

Born interpretation of the wavefunction

- "wavefunction" contains all the dynamic information about the system
- Max Born: interpretation of the wavefunction in terms of the location of the particle

cf: the wave theory of light: square of amplitude of electromagnetic wave = intensity: probability of finding a photon in the region

1-D

- if particle has Ψ at x, the probability of finding the particle between x and x + dx is proportional to $|\Psi|^2 dx$

$|\Psi|^2 dx = \Psi^*\Psi$ if Ψ is complex: $|\Psi|^2$ "probability density"

Ψ: probability amplitude

3-D

Ψ at r $\rightarrow$ probability of finding the particle in $d\tau = dxdydz \Rightarrow |\Psi|^2 d\tau$

$$-|\Psi|^2 > 0$$

(a) **Normalization**

Schrodinger equation $\rightarrow$ $N\Psi$: all probability of the particle must be 1
$\rightarrow$ possible to find “normalization constant” N

probability: $(N\Psi^*)(N\Psi)dx$
$\Rightarrow$ $N^2\int\Psi^*\Psi dx = 1 \Rightarrow N = 1/[\int\Psi^*\Psi dx]^{1/2}$

where the integral is over all the space (from $-\infty$ to $+\infty$)

We can find N and ‘normalize’ the wavefunction
$\rightarrow$ normalized wavefunction: $\int\Psi^*\Psi dx = 1$ or $\int\Psi^*\Psi d\tau = 1$

$d\tau = dxdydz$

in spherical polar coordinates, r, θ, ϕ

$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$

$d\tau = r^2\sin\theta\, dr\, d\theta\, d\phi$, $r: 0 \rightarrow \infty$, $\theta: 0 \rightarrow \pi$, $\phi: 0 \rightarrow 2\pi$

e.g. 8.4. (p.258) (e.g. 11.4)

Hydrogen atom , $\psi \propto e^{-r/a_0}$

$$\int \psi^* \psi \, d\tau = N^2 \left(\int_0^\infty r^2 e^{-2r/a_0} \cdot dr \right) \left(\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \right)$$

$$= N^2 \cdot \frac{1}{4} a_0^3 \cdot 2 \cdot 2\pi = \pi a_0^3 N^2 = 1$$

$$\therefore N = \left(\frac{1}{\pi a_0^3} \right)^{1/2}$$

$\therefore$ Normalized waveftn $\psi = \left(\frac{1}{\pi a_0^3} \right)^{1/2} \cdot e^{-r/a_0}$

(b) **Quantization**

$\int\Psi^*\Psi d\tau = 1 \Rightarrow$ severe restrictions on the acceptability of wavefunctions
(i) Ψ must not be infinite anywhere
if it were $\Rightarrow N\int\Psi^*\Psi = \infty = 1 \Rightarrow N\infty = 1 \Rightarrow N = 0$ (x)

cf: acceptable: infinite Ψ over infinitesimal since $\int\Psi^*\Psi$ is finite (infinitely high x infinetely narrow = finite area) e.g., a particle at a single, precise point

(ii) $|\Psi|^2 = \Psi^*\Psi$: probability of finding the particle $\Rightarrow$ wavefunction (Ψ) must be single-valued

(iii) Ψ: 2nd-order differential equation $\Rightarrow$ 2nd derivative should exist: Ψ should be continuous

1st derivative (slope) should also be continuous

$\therefore \Psi$ must be continuous, have a continuous slope, be single-valued, and be finite everywhere, cannot be zero everywhere (particle must be somewhere)

$\Rightarrow$ the energy of a particle is quantized (acceptable solutions of the Schrödinger equation for these severe restrictions at <u>only certain energies</u>)

Quantum Mechanical Principles

Reading: Atkins, ch. 8 (p. 260-272)

- Information in wavefunction: probability density, eigenfunction &

eigenvalue, operator, expectation value

- The uncertainty principle

- Postulates of quantum mechanics

The information in a wavefunction

mass m particle, **free to move** parallel to x-axis with zero potential energy

(a) **The probability density**

if $B = 0$, $\Psi = Ae^{ikx}$

where is the particle? → Probability of finding the particle

$$|\Psi|^2 = (Ae^{ikx})^*(Ae^{ikx}) = (A^*e^{-ikx})(Ae^{ikx}) = |A|^2$$

equal probability of finding the particle

→ cannot predict where we will find the particle

same if $A = 0$, $|\Psi|^2 = |B|^2$

if A = B, $\Psi = A(e^{-ikx} + e^{ikx}) = 2A\cos kx$

$$|\Psi|^2 = 4|A|^2\cos^2 kx$$

(b) **eigenvalues and eigenfunctions**

total energy: $k^2 \hbar^2/2m = E = E_k + V(= 0) = E_k = p^2/2m$

$\Rightarrow p = k\hbar = (2\pi/\lambda)(h/2\pi) = h/\lambda$: de Broglie's law

k: wave vector ($= 2\pi/\lambda$), independent of A, B

Schrödinger equation

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

1-D, $H =$

H: Hamiltonian operator: carried out a mathematical operation on the function ψ

$\rightarrow$ correspondence between hamiltonian operator and energy

$\rightarrow$correspondence of operators and classical mechanical variables are fundamental to the quantum mechanics

cf. 19 century mathematician William Hamilton

Mathematical operation on the function ψ

(operator)(function) = (constant factor) x (same function)

$$\Omega\Psi = \omega\Psi$$

Ψ: **eigenfunction**
ω: **eigenvalue** of the operator Ω

e.g., $H\psi = E\psi$; eigenvalue is the energy, eigenfunction is wavefunction
$\Rightarrow$ "solve the Schrodinger equation" = "find the eigenvalues and eigenfunctions of the hamiltonian operator for the system"

e.g., show that e^{ax} is an eigenfunction of the operator d/dx, find eigenvalue

e^{ax2} ?

(operator)Ψ = (value of observable) x Ψ

observables: energy, momentum, dipole moment

(c) **operators**

Ω: operator ($\hat{\Omega}$ carat)

- Position operator: $\hat{x} = x \times \bigcirc$
- Momentum operator: $\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx} = -i\hbar\frac{d}{dx}$

$$\hat{p}_x \psi = p_x \psi, \quad \frac{\hbar}{i}\frac{d\psi}{dx} = p_x \psi$$

if $B=0$

$$\frac{\hbar}{i}\frac{d\psi}{dx} = \frac{\hbar}{i}A\frac{de^{ikx}}{dx} = \frac{\hbar}{i}\cdot A \times ike^{ikx} = k\hbar A e^{ikx} = k\hbar\psi$$

$p_x = +k\hbar$: $+x$-direction

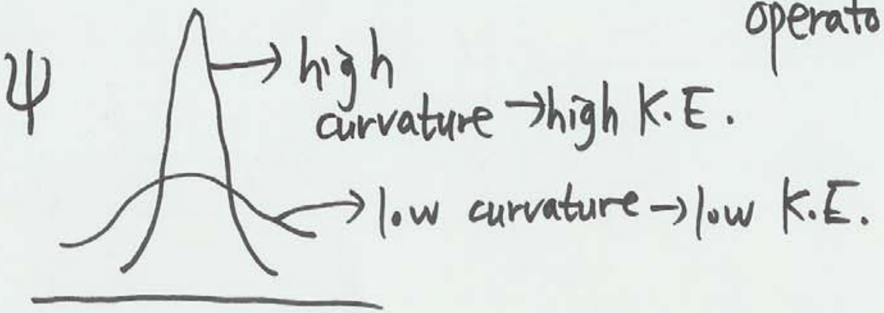
if $A=0$, $p_x = -k\hbar$: $-x$-direction

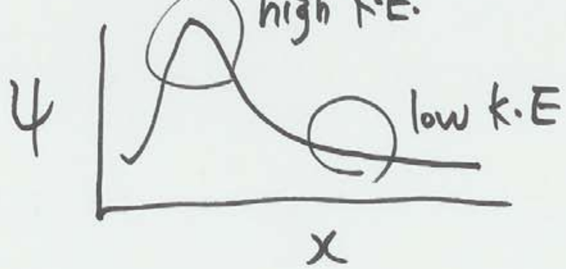
- $V = \frac{1}{2}kx^2 \Rightarrow \hat{V} = \frac{1}{2}kx^2 \times \bigcirc$
- $E_K = \frac{p_x^2}{2m} \Rightarrow \hat{E}_K = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

· Total energy $E = E_k + V \Rightarrow \hat{E} \equiv H = \hat{E}_k + \hat{V} = -\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2} + \hat{V}$

H ↓ hamiltonian operator

$-\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2}$ ↓ 2nd derivative ↓ curvature (곡률)

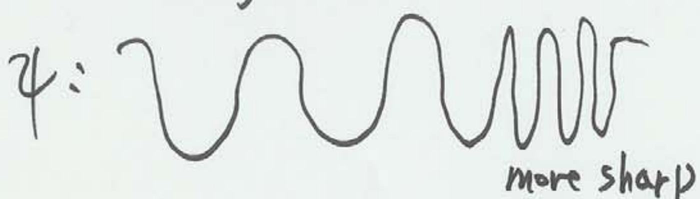




de Broglie relation ⇒

high linear momentum ⇒ short wavelength !

(high K.E.)



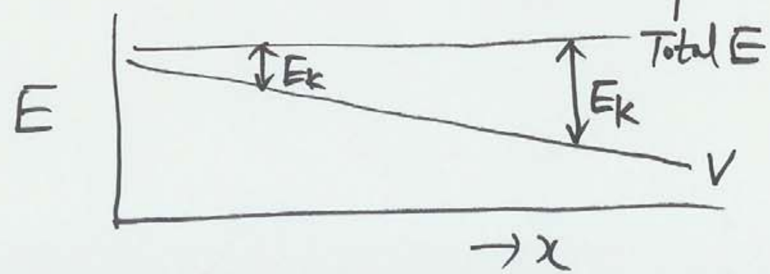


TABLE 4-1

Classical-Mechanical Observables and Their Corresponding Quantum-Mechanical Operators

Observable: *Name*	Observable: *Symbol*	Operator: *Symbol*	Operator: *Operation*
Position	x	$\hat{X}$	Multiply by x
	$\mathbf{r}$	$\hat{\mathbf{R}}$	Multiply by $\mathbf{r}$
Momentum	p_x	$\hat{P}_x$	$-i\hbar \dfrac{\partial}{\partial x}$
	$\mathbf{p}$	$\hat{\mathbf{P}}$	$-i\hbar\left(\mathbf{i}\dfrac{\partial}{\partial x} + \mathbf{j}\dfrac{\partial}{\partial y} + \mathbf{k}\dfrac{\partial}{\partial z}\right)$
Kinetic energy	K_x	$\hat{K}_x$	$-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$
	K	$\hat{K}$	$-\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right)$
Potential energy	$U(x)$	$U(\hat{x})$	Multiply by $U(x)$
	$U(x, y, z)$	$U(\hat{x}, \hat{y}, \hat{z})$	Multiply by $U(x, y, z)$
Total energy	E	$\hat{H}$	$-\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right) + U(x, y, z)$
Angular momentum	$l_x = yp_z - zp_y$	$\hat{L}_x$	$-i\hbar\left(y\dfrac{\partial}{\partial z} - z\dfrac{\partial}{\partial y}\right)$
	$l_y = zp_x - xp_z$	$\hat{L}_y$	$-i\hbar\left(z\dfrac{\partial}{\partial x} - x\dfrac{\partial}{\partial z}\right)$
	$l_z = xp_y - yp_x$	$\hat{L}_z$	$-i\hbar\left(x\dfrac{\partial}{\partial y} - y\dfrac{\partial}{\partial x}\right)$

$$l_x = -(\hbar/i)\{\sin\phi(\partial/\partial\theta) + \cot\theta\cos\phi(\partial/\partial\phi)\}$$
$$l_y = (\hbar/i)\{\cos\phi(\partial/\partial\theta) - \cot\theta\sin\phi(\partial/\partial\phi)\}$$
$$l_z = (\hbar/i)(\partial/\partial\phi).$$

(d) Superpositions and expectation values

if $A = B$

operate with $\hat{p}_x$

$$\frac{\hbar}{i}\frac{d\psi}{dx} = \frac{2\hbar}{i} A \frac{d\cos kx}{dx} = -\frac{2k\hbar}{i} A \sin kx$$

not an eigenvalue equation → no definite value

Actually definite value

∵ cosine waveftn = linear combination of $\underset{\text{definite}}{\underset{\downarrow}{e^{ikx}}}$ and $\underset{\text{definite}}{\underset{\downarrow}{e^{-ikx}}}$

⇒ total waveftn is a <u>sperposition</u> of more than one waveftn !

$$\underset{}{\psi} = \underset{+\hbar k}{\psi_{\rightarrow}} + \underset{-\hbar k}{\psi_{\leftarrow}} \qquad \rightleftharpoons \text{ equal probability}$$

Generally any waveftn writtern as a linear combination of ~~wav~~ eigenftn of an operator

$$\psi = c_1\psi_1 + c_2\psi_2 + \cdots = \sum_k c_k \psi_k$$

$\Rightarrow$ 1. each eigenvalues to the ψ_k that contribute to the superposition will be found

2. probability $\propto |c_k|^2$ in the linear combination

3. average value $\rightarrow$ the expectation value $\langle \Omega \rangle$ of the operator $\hat{\Omega}$

- Expectation value of an operator $\hat{\Omega}$

$$\langle \Omega \rangle = \int \psi^* \hat{\Omega} \psi \, d\tau$$

, ψ should be normalized waveftn

more exactly,

$$\langle \Omega \rangle = \frac{\int \psi^* \hat{\Omega} \psi \, d\tau}{\int \psi^* \psi \, d\tau}$$

cf. C.M.(고전역학) 평균

$$\langle E \rangle = \frac{\int_0^\infty E(P(E))\, dE}{\int_0^\infty P(E)\, dE}$$

e.g.) Mean Kinetic energy of a particle in 1-D

$$\langle E_k \rangle = \int \psi^* \hat{E}_k \psi \, d\tau = -\frac{\hbar^2}{2m} \int \psi^* \frac{d^2\psi}{dx^2} \, d\tau$$

$$\langle r \rangle = \int \psi^* \hat{r} \psi \, d\tau$$

e.g.) If ψ is an eigenftn of $\hat{\Omega}$ with eigenvalue ω,
the expectation value of Ω is

$$\langle \Omega \rangle = \int \psi^* \hat{\Omega} \psi \, d\tau = \int \psi^* \omega \psi \, d\tau = \omega \underbrace{\int \psi^* \psi \, d\tau}_{\equiv 1} = \omega$$

If waveftn that is not an eigenftn of the operator $\Rightarrow$
can be written linear combination of eigenftns

e.g.) Consider sum of two eigenftns

$$\langle \Omega \rangle = \int (c_1\psi_1 + c_2\psi_2)^* \hat{\Omega} (c_1\psi_1 + c_2\psi_2) \, d\tau$$

$$= c_1^* c_1 \omega_1 \underbrace{\int \psi_1^* \psi_1 \, d\tau}_{\equiv 1} + c_2^* c_2 \omega_2 \underbrace{\int \psi_2^* \psi_2 \, d\tau}_{\equiv 1} +$$

$$+ C_1^* C_2 \omega_2^* \int \psi_1^* \psi_2 \, d\tau + C_2^* C_1 \omega_1 \int \psi_2^* \psi_1 \, d\tau$$

$\int \psi_1^* \psi_2 \, d\tau = 0$ (orthogonal) , $\int \psi_i^* \psi_j = 0$

↳ integral of the product is zero

$\psi_1, \psi_2 \rightarrow$ correspond to different energies

$\Rightarrow$ their product $= 0$

($\because$ different eigenvalues)

$$\therefore \langle \Omega \rangle = |C_1|^2 \omega_1 + |C_2|^2 \omega_2$$

$\langle p \rangle = \hbar k - \hbar k = 0$ equal propability ($\rightarrow, \leftarrow$)

Expectation value , $\langle p \rangle = \int 2A \cos kx \cdot \frac{\hbar}{i} \frac{d}{dx} (2A \cos kx) = \int 4A^2 i k \hbar \sin kx \cos kx$

$$= 2A^2 i k \hbar \int 2 \sin kx \cos kx = 2A^2 i k \hbar \int_{-\infty}^{\infty} \sin 2kx = \underline{\underline{0}}$$

Another property of eigenftn : "orthogonality"

→ eigenftns corresponding to different eigenvalues of the same operator are orthogonal → only to 'Hermitian operators'

The uncertainty principle

if $\Psi = Ae^{ikx}$, $p_x = +k\hbar$: travelling to the right, but we cannot predict the position of the particle ($|\Psi|^2 = |A|^2$)

if the momentum is specified precisely, it is impossible to predict the location of the particle

Heisenberg uncertainty principle

“It is impossible to specify simultaneously, with arbitrary precision, both the momentum and the position of a particle”

if we know a definite location, Ψ must be large there and zero everywhere else. To do so, an infinite number of linear combinations of wavefunctions is needed

$\rightarrow$ perfect localization $\rightarrow$ lost all information about its momentum; completely unpredictable quantitatively,

$$\Delta p \Delta q \geq \tfrac{1}{2}\hbar$$

(and $\Delta t \Delta E \geq \tfrac{1}{2}\hbar$)

Δp: uncertainty in position along that axis
Δq: uncertainty in the linear momentum parallel to the axis q

if $\Delta q = 0$ (exact position) $\rightarrow \Delta p = \infty$
$\Delta p = 0 \rightarrow \Delta q = \infty$

e.g., 1g particle, speed 1×10^{-6} m/s, minimum position uncertainty?

Electron in $2a_0$

General uncertainty principle: the Heisenberg uncertainty principle applies to any pair of observables called "**complementary observables**"

e.g., position & momentum

C.M.: position & momentum of a particle could be specified simultaneously with arbitrary precision
Q.M.: position and momentum are complementary

The postulates of quantum mechanics (1-D)

(1) Physical state of a particle at time t is fully described by a wavefunction $\Psi(x,t)$

(2) $\Psi(x,t)$, $\partial\Psi(x,t)/\partial x$, $\partial^2\Psi(x,t)/\partial x^2$ must be continuous, finite and single valued for all values of x

(3) Any quantity that is physically observable can be represented by a Hermitian operator. Hermitian operator is a linear operator F that satisfies

(4)

Ψ_i: eigenfunction of F with eigenvalue f_i

(5) average or expectation value <F>

(6) Quantum mechanical operator is constructed by the classical expression of x, p_x, t, E and converting the expression to an operator by means of following rules,

Classical variable	Q.M. operator	(operation) Expression for operator
x	$\hat{x}$	x
p_x	$\hat{p}_x$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
t	$\hat{t}$	t
E	$\hat{E}$	$-\frac{\hbar}{i}\frac{\partial}{\partial t}$

(7) $\Psi(x,t)$ is a solution of time-dependent Schrödinger equation

$$\hat{H}(x,t)\,\psi(x,t) = \frac{i\hbar\,\partial\psi(x,t)}{\partial t}$$

where, $\hat{H}$: Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

<u>Operator</u>: fundamental in Q.M.

(1) commute → in Q.M., many operators <u>do not commute</u>
cf: uncertainty principle

$$[\hat{A}, \hat{B}] = \hat{A}\cdot\hat{B} - \hat{B}\cdot\hat{A}$$

When $[\hat{A}, \hat{B}] = 0$ "Commute"

e.g.). $f(x) = x^2$, operator $\frac{d}{dx}$

$$\frac{d}{dx} f(x) = \frac{d}{dx} x^2 = 2x$$

· $\hat{O}_2 = \frac{d}{dx}$, $\hat{O}_1 = x$, $f(x) = x^2$

Then $\hat{O}_1 \hat{O}_2 f(x) = x \cdot \frac{d}{dx} x^2 = 2x$
$\hat{O}_2 \hat{O}_1 f(x) \quad \frac{d}{dx} \cdot x \cdot x^2 = 3x^2$
$\Rightarrow \hat{O}_2 \hat{O}_1 \neq \hat{O}_1 \hat{O}_2$
"do not commute"

(2) linear operation → Q.M: deal with linear operators

$$\hat{O}[c_1 f_1(x) + c_2 f_2(x)] = c_1 \hat{O} f_1(x) + c_2 \hat{O} f_2(x)$$

e.g.) i) $\frac{d}{dx}$? : $\frac{d}{dx}[c_1 f_1(x) + c_2 f_2(x)] = c_1 \frac{df_1(x)}{dx} + c_2 \frac{df_2(x)}{dx}$ "linear"

ii) SQR (square)

$$SQR[c_1 f_1(x) + c_2 f_2(x)] = c_1^2 f_1(x)^2 + c_2^2 f_2(x)^2 + 2c_1 c_2 f_1(x) f_2(x)$$

$$\neq c_1 f_1^2(x) + c_2 f_2^2(x)$$ "not linear"

(3) Hermitian operator: Q.M. operators must be hermitian operators: Operators generally are complex quantities but certainly the eigenvalues must be real quantities (experimental measurement)

if $\langle F \rangle$ is to be real, $\langle F \rangle = \langle F \rangle^*$ ← complex conjugate

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

Then $\hat{F}$: "Hermitian operator"

⇒ expectation value is real

e.g.) $i = \frac{d}{dx}$, $\int_{-\infty}^{\infty} f^* \frac{d}{dx} f \, dx = f \cdot f^* \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f \cdot \frac{df^*}{dx} dx$

$$\Rightarrow \int_{-\infty}^{\infty} f^* \frac{d}{dx} f \, dx = -\int_{-\infty}^{\infty} f \frac{d}{dx} f^* \, dx$$ "not Hermitian"

$\hat{p} : -i\hbar \frac{d}{dx}$ "Hermitian"

- More general definition of a Hermitian operator

$$\int_{-\infty}^{\infty}\psi_1^*\hat{F}\psi_2\,dx = \int_{-\infty}^{\infty}\psi_2\hat{F}^*\psi_1^*\,dx$$

유도) let $\psi \Rightarrow f$ or g

$$\int f^*\hat{A}f\,dx = \int f\hat{A}^*f^*\,dx\ ,\quad \int g^*\hat{A}g\,dx = \int g\hat{A}^*g^*\,dx$$

now let $\psi = c_1 f + c_2 g$

$$\int (c_1^*f^* + c_2^*g^*)\hat{A}(c_1 f + c_2 g)\,dx = \int (c_1 f + c_2 g)\hat{A}^*(c_1^*f^* + c_2^*g^*)\,dx$$

$$c_1^*c_2\int f^*\hat{A}g\,dx + c_2^*c_1\int g^*\hat{A}f\,dx = c_1c_2^*\int f\hat{A}^*g^*\,dx + c_1^*c_2\int g\hat{A}^*f^*\,dx$$

$$c_1^*c_2\int \underbrace{(f^*\hat{A}g - g\hat{A}^*f^*)}_{=0}\,dx = c_1c_2^*\int \underbrace{(f\hat{A}^*g^* - g^*\hat{A}f)}_{=0}\,dx$$

$\because$ if $z = x + iy$ (complex) $\Rightarrow z = x + iy = z^* = x - iy$

$\Rightarrow y$ must be $-y \Rightarrow y = 0$

(4) orthogonal: the eigenfunctions of hermitian operators are orthogonal

$\int \psi_i^* \psi_i \, d\tau = 1$ Normalized

$\int \psi_i^* \psi_j \, d\tau = 0$ Orthogonal

$$\Rightarrow \int \psi_i^* \psi_j \, d\tau = \delta_{ij}, \quad \delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}$$

$\downarrow$

Knonecker delta

Summary

(1) The Schrödinger equation is the equation for the wavefunction of a particle
(2) The Schrödinger equation can be formulated as an eigenvalue problem
(3) C.M. quantities are represented by linear operators in Q.M.
(4) Wavefunctions have a probabilistic interpretation
(5) Wavefunctions are normalized
(6) Average value, expectation is given by