Schrödinger equation

(1925)

↳ governs the propagation of matter waves
wave equation governing the motion of particles with mass

(We can't derive Schröd. eq., as we can't derive Newton's laws of motion
Its validity lies in its agreement with experiments)

⇒ Wave equation for photons

$$\boxed{\frac{\partial^2 \mathcal{E}}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 \mathcal{E}}{\partial t^2}}$$

photon moves at the speed of light (c)

$$\mathcal{E}(x,t) = \mathcal{E}_0 \cos(kx-\omega t)$$

$$\underbrace{\frac{\partial^2 \mathcal{E}}{\partial x^2} = -k^2 \mathcal{E} \qquad \frac{\partial^2 \mathcal{E}}{\partial t^2} = -\omega^2 \mathcal{E}}$$

$$k^2 = \frac{\omega^2}{c^2} \Rightarrow \boxed{\omega = kc}$$

using $\omega = E/\hbar$ and $p = \hbar k$ $\longrightarrow$ $\boxed{E = pc}$

relation between E and p for photon (relativistic particle)

⇒ Schrödinger eq applies to $\boxed{\text{nonrelativistic}}$ problems
(Dirac eq to relativistic case)

Total energy of nonrelativistic particle: $E = \frac{p^2}{2m} + V$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V$$

linear in ω
quadratic in k^2 ⇒

$\boxed{\neq \text{ from photon } \omega^2 = k^2c^2}$

⇒ Schröd. eq. relates 1st time derivative to the 2nd space derivative and also involves the potential energy

The eq. also needs to be LINEAR in the wave function ⇒ ψ_1 is a solution, ψ_2 is a solution ⇒

⇒ any linear combination $\psi = a_1\psi_1 + a_2\psi_2$ is also a solution (interference can happen)

Schrödinger Equation in 1D

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

equation is <u>LINEAR</u> in $\Psi(x,t) \Rightarrow$ if Ψ_1 and Ψ_2 are two $\neq$ solutions for given V, any <u>arbitrary</u> <u>linear superposition</u> $a_1\Psi_1 + a_2\Psi_2$ is a solution

Example 5-2 (Eisberg)

$$\Psi = a_1\Psi_1 + a_2\Psi_2$$

$$a_1\underbrace{\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1}{\partial x^2} + V\Psi_1 - i\hbar\frac{\partial\Psi_1}{\partial t}\right)}_{(=0)} = -a_2\underbrace{\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2}{\partial x^2} + V\Psi_2 - i\hbar\frac{\partial\Psi_2}{\partial t}\right)}_{(=0)}$$

<u>free particle</u> : no net force acts on a free particle

$\hookrightarrow V(x,t) = V_0 \qquad \left(F = \frac{\partial V(x,t)}{\partial x} = 0\right)$

just $\cos(kx-\omega t)$ or $\sin(kx-\omega t)$ <u>don't</u> satisfy the eq.

$$\Psi(x,t) = A\,e^{i(kx-\omega t)} = A\left[\cos(kx-\omega t) + i\sin(kx-\omega t)\right]$$

constant

$$\frac{\partial\Psi}{\partial t} = -i\omega\Psi$$

$$\frac{\partial\Psi}{\partial x} = ikA \rightarrow \frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi$$

$$\frac{\hbar^2k^2}{2m}\Psi + V_0\Psi = \hbar\omega\Psi$$

$$\hookrightarrow \frac{\hbar^2k^2}{2m} + V_0 = \hbar\omega$$

$$\left(\frac{p^2}{2m} + V_0 = E\right)$$

- The wave function $\Psi(x,t)$ may be <u>COMPLEX</u> $\rightarrow$ it is a <u>computational</u> device

- $P(x,t)\,dx$: <u>probability</u> to find particle in the volume dx

$$P(x,t)\,dx = \Psi^*(x,t)\,\Psi(x,t)\,dx = |\Psi(x,t)|^2 dx$$

$\hookrightarrow$ has physical significance, is <u>REAL</u>

<u>Born's statistical</u> <u>interpretation</u>
(QM is intrinsically probabilistic)

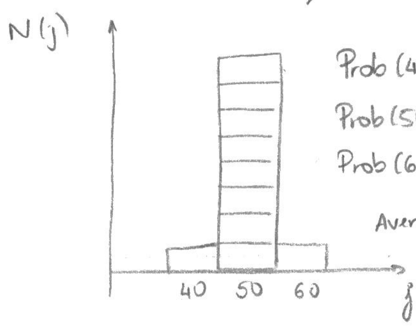
$P(x,t)$: probability density for finding particle at point x at time t

$\Psi(x,t)$: probability (density) amplitude

NOTES ON STATISTICS

in a room
$\left\{ \begin{array}{l} 1 \text{ person: } 40 \text{ years old} \\ 8 \text{ persons: } 50 \\ 1 \text{ person: } 60 \end{array} \right.$

total: $\boxed{10}$ average: $\dfrac{40 + 8\times 50 + 1\times 60}{10} = \boxed{50}$



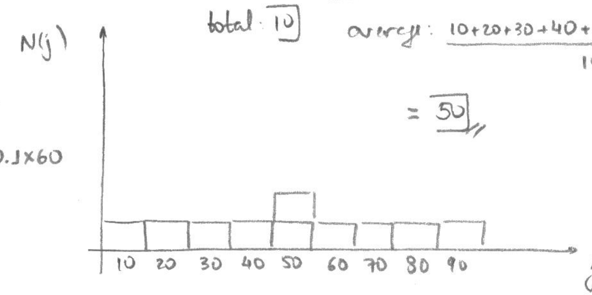
$\left. \begin{array}{l} \text{Prob}(40) = 1/10 \\ \text{Prob}(50) = 8/10 \\ \text{Prob}(60) = 1/10 \end{array} \right\}$ $\boxed{\text{Prob total} = 1}$

Average: $0.1\times 40 + 0.8\times 50 + 0.1\times 60$

another room
$\left\{ \begin{array}{l} 1 \text{ person: } 10 \\ \quad '' \quad : 20 \\ \quad '' \quad : 30 \\ \quad '' \quad : 40 \\ 2 \text{ persons: } 50 \\ 1 \text{ person: } 60 \\ 1 \quad '' \quad : 70 \\ \quad '' \quad 80 \\ \quad '' \quad 90 \end{array} \right.$

total: $\boxed{10}$ average: $\dfrac{10+20+30+40+2\times 50+60+70+80+90}{10}$

$= \boxed{50}$



more spread

↳ larger $\left\{ \begin{array}{l} \text{dispersion} \\ \text{standard deviation} \end{array} \right\}$ σ

variance

$$\sigma^2 \equiv \langle \underbrace{(j - \langle j \rangle)^2}_{\text{how much individuals deviate from average } \langle j \rangle} \rangle$$

$$\sigma^2 = \langle j^2 - 2j\langle j \rangle - \langle j \rangle^2 \rangle = \langle j^2 \rangle - 2\langle j \rangle \langle j \rangle - \langle j \rangle^2 = \boxed{\langle j^2 \rangle - \langle j \rangle^2}$$

Dispersion / standard deviation

$$\boxed{\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}}$$

uncertainty in x and p

$$\left\{ \begin{array}{l} \Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \end{array} \right.$$

- $\Psi(x,t)$: probability amplitude

- $\int_a^b |\Psi(x,t)|^2\, dx$: probability to find the particle between a and b at time t

$$\boxed{\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 1} \leftarrow \text{normalization condition}$$

→) wave function contains information about the behavior of the associated particle

Expectation Values

→) the most we can know about a particle position is the probability that a measurement will yield a value x

$$\langle x\rangle = \int_{-\infty}^{\infty} x\, P(x)\, dx = \int_{-\infty}^{\infty} x\, |\Psi(x,t)|^2\, dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\, x\, \Psi(x,t)\, dx$$

→) expectation value is the average of repeated measurements on a ensemble of identically prepared systems

(not the average of repeated measurements on one and the same system, because after a measurement we COLLAPSE the wave function)

$$\langle x^2\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, x^2\, \Psi(x,t)\, dx$$

any function $f(x)$

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, f(x)\, \Psi(x,t)\, dx$$

↳ how can we find $\langle p\rangle$? p is NOT function of x, because of the uncertainty princ.

- one way is to use the wave function for momentum $\Psi(p,t)$ [Fourier transform $\Psi(x,t) \to \Psi(p,t)$]

- the other way is to use $p \to \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$\begin{cases} \dfrac{p^2}{2m} + V_0 = E & \xleftarrow[\text{particle}]{\text{free}} \quad \Psi(x,t) = A e^{i(kx-\omega t)} \\ \\ -\dfrac{\hbar^2}{2m}\dfrac{\partial^2 \Psi}{\partial x^2} + V_0 \Psi = i\hbar \dfrac{\partial \Psi}{\partial t} \end{cases}$$

HW

5.24, Prob. 1.9 (Griffiths), Prob. 1.17 (Griffiths)

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}$$

$$\int_{-\infty}^{\infty} x e^{-\alpha x^2} dx = 0$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

$$\boxed{p \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}}$$ momentum operator

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

no forces act on the particle

Example 5-9 (Eisberg) Consider a particle of mass m which can move freely along the x axis anywhere from $x = -a/2$ to $x = a/2$, but which is strictly prohibited from being found outside this region. The particle bounces back and forth between the walls at $x = \pm a/2$ of a one-dimensional box.

The wavefunction for the lowest energy state of this particle is

$$\Psi(x,t) = \begin{cases} A \cos \dfrac{\pi x}{a}\, e^{-iEt/\hbar} & -a/2 < x < a/2 \\ \\ 0 & x \leq -a/2 \text{ or } x \geq a/2 \end{cases}$$

a) Show that $\Psi(x,t)$ is a solution to the Schrödinger eq. and determine E

b) Determine the value of the constant A so that the probability to find the particle somewhere in x is 1

c) Evaluate $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$

d) Show that $\Delta x \Delta p$ is consistent with the uncertainty principle

no forces act on the particle $\Rightarrow$ V = const
↳ can choose V = 0

a) $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \cancel{V\psi} = i\hbar\frac{\partial\psi}{\partial t}$

$\psi = A\cos\frac{\pi x}{a}\, e^{-iEt/\hbar}$

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

$$\frac{\partial\psi}{\partial x} = -\frac{\pi}{a}A\sin\frac{\pi x}{a}\, e^{-iEt/\hbar} \longrightarrow \frac{\partial^2\psi}{\partial x^2} = -\left(\frac{\pi}{a}\right)^2\psi$$

to satisfy Schröd eq $\Rightarrow$ $\boxed{+\frac{\hbar^2}{2m}\frac{\pi^2}{a^2} = E}$

$\cos(2y) = \cos^2 y - \sin^2 y = 2\cos^2 y - 1$
↳ $\cos^2 y = \frac{1+\cos 2y}{2}$

b) $\int_{-\infty}^{\infty}|\psi|^2\,dx = 1 \Rightarrow \int_{-a/2}^{a/2} A^2\cos^2\left(\frac{\pi x}{a}\right)dx = 1$

$$A^2\left[\underbrace{\int_{-a/2}^{a/2}\frac{dx}{2}}_{a/2} + \underbrace{\int_{-a/2}^{a/2}\frac{1}{2}\cos\left(\frac{2\pi x}{a}\right)dx}_{y=\frac{2\pi x}{a} \quad dx=\frac{a}{2\pi}dy}\right] = A^2\left[\frac{a}{2} - \cancel{\frac{a}{4\pi}\sin y\Big|_{-\pi}^{\pi}}\right] = A^2\frac{a}{2}$$

$$\frac{1}{2}\int_{-\pi}^{\pi}\frac{a}{2\pi}\cos y\,dy$$

↳ $\boxed{A = \sqrt{2/a}}$

EVEN function : $f(x) = f(-x)$
Examples: x^2, $\cos x$

ODD function : $-f(x) = f(-x)$
Examples : x, x^3, $\sin x$

c) $\langle x\rangle = \int_{-a/2}^{a/2}\frac{2}{a}\underbrace{\cos^2\frac{\pi x}{a}}_{\text{even}}\underbrace{x}_{\text{odd}}\,dx = 0$

$$\langle x^2\rangle = \frac{2}{a}\int_{-a/2}^{a/2}\cos^2\left(\frac{\pi x}{a}\right)x^2\,dx = \frac{1}{a}\left[\int_{-a/2}^{a/2}x^2\,dx + \int_{-a/2}^{a/2}\cos\left(\frac{2\pi x}{a}\right)x^2\,dx\right]$$

$y = \frac{2\pi x}{a}$ $\qquad dx = \frac{a}{2\pi}dy$

$$\int_{-a/2}^{a/2} \cos\left(\frac{2\pi x}{a}\right) x^2\, dx = \frac{a}{2\pi}\,\frac{a^2}{4\pi^2} \overbrace{\underbrace{\int_{-\pi}^{\pi} \cos y\; y^2\, dy}}^{-4\pi}$$

$u = y^2 \qquad dv = \cos y\, dy$

$du = 2y\, dy \qquad v = \sin y$

$$\cancel{y^2 \sin y}\Big|_{-\pi}^{\pi} - 2\underbrace{\int_{-\pi}^{\pi} y \sin y\, dy}$$

$u = y \qquad dv = \sin y\, dy$

$du = dy \qquad v = -\cos y$

$$\underbrace{-y\cos y\Big|_{-\pi}^{\pi}}_{+\pi + (\pi) = 2\pi} + \underbrace{\cancel{\int_{-\pi}^{\pi} \cos y\, dy}}_{\sin y|_{-\pi}^{\pi}}$$

$$\langle x^2 \rangle = \frac{1}{a}\left[\frac{(a/2)^3}{3} - \frac{(-a/2)^3}{3} - \frac{a^3}{2\cancel{8}\pi^{\cancel{3}2}}\cancel{4\pi}\right] = \frac{a^2}{12} - \frac{a^2}{2\pi^2} = \boxed{\frac{a^2}{2\pi^2}\left(\frac{\pi^2}{6} - 1\right)} = 0.033a^2$$

$$\langle p \rangle = \frac{2}{a}\int_{-a/2}^{a/2} \cos\frac{\pi x}{a} \underbrace{\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\cos\frac{\pi x}{a}\right)}_{-\frac{\hbar}{i}\frac{\pi}{a}\sin\frac{\pi x}{a}} dx = -\frac{2\hbar\pi}{i a^2}\int_{-a/2}^{a/2} \underset{\text{even}}{\cos\frac{\pi x}{a}}\ \underset{\text{odd}}{\sin\frac{\pi x}{a}}\, dx = 0$$

$$\langle p^2 \rangle = \frac{2}{a}\int_{-a/2}^{a/2} (-\hbar^2) \cos\frac{\pi x}{a}\ \underbrace{\frac{\partial^2 \cos \pi x/a}{\partial x^2}}\ dx = \frac{2}{a}\hbar^2\frac{\pi^2}{a^2}\underbrace{\int_{-a/2}^{a/2} \cos^2\left(\frac{\pi x}{a}\right) dx}$$

$$-\frac{\pi}{a}\frac{\partial}{\partial x}\sin\frac{\pi x}{a}$$

$$-\left(\frac{\pi}{a}\right)^2 \cos\frac{\pi x}{a}$$

$$\underbrace{\int_{-a/2}^{a/2} \frac{dx}{2}}_{\frac{a}{2}} + \underbrace{\int_{-a/2}^{a/2} \cos\left(\frac{2\pi x}{a}\right) dx}$$

$y = \frac{2\pi x}{a}$

$dx = \frac{a\, dy}{2\pi}$

$$\int_{-\pi}^{\pi} \cos y\, dy = \cancel{-\sin y\Big|_{-\pi}^{\pi}} = 0$$

$$\langle p^2 \rangle = \frac{\cancel{2}\hbar^2\pi^2}{a^{\cancel{3}2}}\frac{\cancel{a}}{\cancel{2}} \longrightarrow \boxed{\langle p^2 \rangle = \left(\frac{\hbar\pi}{a}\right)^2}$$

d) $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = 0.18\, a$

$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\langle p^2\rangle} = \frac{\hbar\pi}{a}$

$\Delta x\, \Delta p = 0.18\, \cancel{a}\, \frac{\hbar\pi}{\cancel{a}} = \boxed{0.57\,\hbar}$ which is consistent with the lower limit $\hbar/2$ set by the uncertainty principle