Wave Mechanics

The complete state of a point particle of mass m is given by the complex function,

$$\psi(x,t)$$

called the wave function.

$\Rightarrow$ We will assume ψ is <u>normalized</u>, that is

$$\int_{-\infty}^{\infty} \psi^*(x,t)\,\psi(x,t)\,dx = 1$$

$\Rightarrow$ ψ can be constructed from any function $f(x,t)$ where the function is <u>square integrable</u>

$$\left| \int_{-\infty}^{\infty} f^* f \, dx \right| < \infty$$

The probability density ~~[illegible]~~ $\rho(x,t)$, the probability of finding the particle in the range $[x, x+dx]$ at time t is

$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

<u>Schrodinger Equation</u> The wave function evolves according to the Schrodinger equation (SE) -

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

where $V(x)$ is the classical potential energy.

$\Rightarrow$ Note, the equation is complex.

<u>Momentum</u> (p) - The average momentum of the particle is

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

<u>Momentum Operator</u> $(\hat{p})$ Inspection of the above suggests we identify

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

as a differential operator related to the momentum.

<u>Expectation Value of Any Classical Variable</u>

If $Q(x, p)$ is any classical quantity involving the position x and the momentum $p = m\dot{x}$, then the quantum expectation value of a measurement of that variable is

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \, Q(x, \hat{p}) \, \psi(x,t) \, dx$$

where we have made the replacement

$$p = m\dot{x} \longrightarrow \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Examples

Position $\quad Q = x \quad \Longrightarrow \quad \langle x \rangle = \int_{-\infty}^{\infty} \psi^* x \, \psi \, dx$

Momentum $\quad Q = p \quad \Longrightarrow \quad \langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \, \psi \, dx$

$$= \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi \, dx$$

Kinetic Energy $\quad Q = T = \frac{p^2}{2m} \Rightarrow \langle T \rangle = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hat{p}^2}{2m} \right) \psi \, dx$

$$= \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar^2}{-1} \frac{1}{2m} \frac{\partial^2}{\partial x^2} \right) \psi \, dx$$

$$= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^* \frac{\partial^2 \psi}{\partial x^2} \, dx$$

velocity $\quad Q = v \quad \Longrightarrow \quad$ Not fair, Q must be in terms of x and p.

$$Q = \frac{p}{m} = \frac{1}{m} \int \psi^* \hat{p} \, \psi \, dx$$

Probability Density of Momentum $\rho(p)$.

We have already argued that the distribution of position $\rho(x)$ and the distribution of momentum $\rho(p)$ are related.

Wave Function in Momentum Representation $\bar{\Psi}(p)$

$$\rho(p) = \bar{\Psi}^*(p)\,\bar{\Psi}(p)$$

$\Rightarrow$ Naturally $\bar{\Psi}$ must also be normalized

$$\int_{-\infty}^{\infty} \rho(p)\,dp = 1$$

$\Rightarrow$ Since the measured momentum must be something

Momentum Wave Function

$$\bar{\Psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ipx}{\hbar}}\,\Psi(x,t)\,dx$$

Relation to Fourier Transform

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ikx}\, dx$$

De Broglie $\qquad \lambda = \dfrac{h}{p}$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda} = \hbar k$$

where $\quad k = \dfrac{2\pi}{\lambda} \quad$ is the wave number

$$\phi\left(\frac{p}{\hbar}\right) = \frac{1}{\sqrt{2\pi}} \int \psi(x)\, e^{-px/\hbar}\, dx$$

A note about dimensionality,

$$1 = \int \psi^* \psi\, dx \implies [\psi] = \frac{1}{\sqrt{m}} = \frac{1}{\sqrt{\ell}}$$

$$1 = \int \Psi^* \Psi\, dp \implies [\Psi] = \frac{1}{\sqrt{p}}$$

hence the $\dfrac{1}{\sqrt{\hbar}}$ difference in the definitions.

A few properties of SE.

(1) Probability is conserved - If a particle exists at $t=0$, it exists at $t>0$.

$$\frac{d}{dt}\int \rho(x,t)\,dx = 0$$

(2) Probability is <u>Locally</u> conserved. There exists a probability current J s.t.

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

$\Rightarrow$ Compare to continuity equation for electric charge

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$$

$$\Rightarrow \quad J = \frac{i\hbar}{2m}\left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x}\right)$$

$\equiv$ Probability current

The change in the probability of finding the particle is the intrevol $[a, b]$ = the amount of probability that flowed in through a minus the amount that flowed out through b

$$\frac{d}{dt}\int_a^b \rho(x,t)\,dx = J(a,t) - J(b,t)$$

(3) Classical Mechanics in recovered –

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p\rangle$$

Proof Probability is locally conserved

$$\frac{\partial}{\partial t}\rho(x,t) = \frac{\partial}{\partial t}\psi^*\psi$$

$$= \psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}$$

SE

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right]$$

$$\frac{\partial \psi^*}{\partial t} = -\frac{1}{i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^*\right]$$

$$\Rightarrow \frac{\partial}{\partial t}(\psi^*\psi) = \frac{\psi^*}{i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right] - \frac{\psi}{i\hbar}\left[\frac{-\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^*\right]$$

$$= \left(\frac{1}{i\hbar}\right)\left(\frac{-\hbar^2}{2m}\right)\left[\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right]$$

$$\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} = \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t} \psi^* \psi = \frac{i\hbar}{2m} \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

Let $J = \frac{i\hbar}{2m}\left[\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x}\right]$

$$\frac{\partial}{\partial t} \psi^* \psi = \frac{\partial}{\partial t} \rho(x) = -\frac{\partial J}{\partial x}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

$\Longrightarrow$ Define J as a probability current and we have written a continuity equation for the probability.

Proof Probability is globally conserved

$$\frac{d}{dt}\int \rho(x,t)\,dx = \int \frac{\partial \rho}{\partial t}\,dx$$

$$= -\int_{-\infty}^{\infty} \frac{\partial J}{\partial x}\,dx = -J\Big|_{-\infty}^{\infty}$$

but $J = 0$ at $\infty, -\infty$ since $\psi \to 0$

(really comes out of square integrable).

Proof $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int \psi^* x\,\psi\,dx$$

$$= \int \frac{\partial}{\partial t}\left(\psi^* x\,\psi\right)dx$$

$$= \int x\,\frac{\partial\, \psi^*\psi}{\partial t}\,dx$$

$$\frac{d\langle x\rangle}{dt} = -\int x \frac{\partial J}{\partial x}\, dx$$

integration by parts

$$= -\int \frac{\partial(xJ)}{\partial x}\, dx + \int J\, dx$$

$$\boxed{\frac{\partial xJ}{\partial x} = J + x\frac{\partial J}{\partial x}}$$

$$\frac{d\langle x\rangle}{dt} = \underbrace{-\, xJ\Big|_{-\infty}^{\infty}}_{=0 \quad J=0 \text{ at } \infty} + \int J\, dx$$

$$\frac{d\langle x\rangle}{dt} = \int J\, dx = \frac{i\hbar}{2m}\int\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)dx$$

Integration by Parts

$$\frac{\partial\, \psi\psi^*}{\partial x} = \psi\frac{\partial\psi^*}{\partial x} + \psi^*\frac{\partial\psi}{\partial x}$$

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int \frac{\partial \psi\psi^*}{\partial x} - 2\psi^*\frac{\partial \psi}{\partial x}$$

$$= \underbrace{\frac{i\hbar}{2m}\,\psi\psi^*\Big|_{-\infty}^{\infty}}_{0 \quad \psi\to 0 \text{ at } \infty} + \frac{\hbar}{im}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}\,dx$$

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\int_{-\infty}^{\infty}\psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi\,dx$$

$$= \frac{1}{m}\langle p\rangle$$