Schrodinger Eq.

Motivation (not derivation):

$E = \hbar\omega = hf \qquad (\hbar = h/2\pi,\ \omega = 2\pi f,\ k = 2\pi/\lambda)$

$p = \hbar k = \frac{h}{\lambda}$

$E = \frac{p^2}{2m} + V$ or $E = \frac{p^2}{2m}$ (free particle)

Consider a plane wave, $e^{i(kx-\omega t)} = \psi(x,t)$

$E = \hbar\omega = i\hbar \frac{\partial}{\partial t}\psi$

partial deriv.

$p = \hbar k = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi \rightarrow \frac{p^2}{2m} = +\frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$

$E = \frac{p^2}{2m}$: $\quad i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$

$E = \frac{p^2}{2m} + V$: $\quad i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi \qquad (1D)$

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \qquad (3D)$$

Interpretation of ψ:

$|\psi(x,t)|^2 dx$ is the probability of finding a particle between x & $x+dx$ at time t.

$P(x,t) = |\psi(x,t)|^2$ = probability density

$$\int_{-\infty}^{+\infty} P(x,t)\,dx = 1 = \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx$$

Continuity equation: (1D)

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

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

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

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

$$= \frac{\hbar}{2mi}\left(\frac{\partial^2 \psi^*}{\partial x^2}\psi - \frac{\partial^2 \psi}{\partial x^2}\psi^*\right)$$

$$= \frac{\hbar}{2mi}\frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right)$$

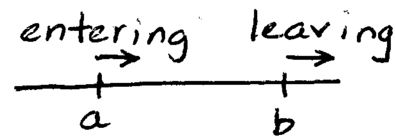
$$\rightarrow \frac{\partial P}{\partial t} + \frac{\partial}{\partial x}\frac{\hbar}{2mi}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi^*\frac{\partial \psi}{\partial x}\right) = 0$$

or $$\frac{\partial P(x,t)}{\partial t} + \frac{\partial}{\partial x} j(x,t) = 0$$

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) = \text{probability current density}$$

$$\frac{\partial}{\partial t}\int_a^b dx\, P(x,t) = -\int_a^b dx \frac{\partial}{\partial x} j(x,t)$$

$$= j(a,t) - j(b,t)$$



In 3D,

$$\vec{j}(r,t) = \frac{\hbar}{2mi}\left[\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right].$$

Expectation values: (probability interpretation)

$$\langle x \rangle = \int dx\, |\psi(x,t)|^2 x$$

$$\langle x^2 \rangle = \int dx\, |\psi(x,t)|^2 x^2$$

$$\langle f(x) \rangle = \int dx\, |\psi(x,t)|^2 f(x) = \int dx\, \psi^*(x,t) f(x) \psi(x,t)$$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = m \frac{d}{dt} \int dx\, \psi^*(x,t) \quad x \quad \psi(x,t)$$

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

$$\frac{\partial \psi^*}{\partial t} = \frac{\hbar}{2mi} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*$$

$$\frac{\partial \psi}{\partial t} = \frac{-\hbar}{2mi} \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$\rightarrow \langle p \rangle = \frac{\hbar}{2i} \int dx \left(\frac{\partial^2 \psi^*}{\partial x^2} x \psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2} \right)$$

Integrate by parts assume ψ vanishes at $\pm\infty$:

$$\langle p \rangle = \frac{\hbar}{2i} \int dx \left(-\frac{\partial \psi^*}{\partial x} \psi - \cancel{\frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x}} + \cancel{\frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x}} + \psi^* \frac{\partial \psi}{\partial x} \right)$$

and again $$= \frac{\hbar}{2i} \int dx \left(\psi^* \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial \psi}{\partial x} \right)$$

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

$p = \frac{\hbar}{i} \frac{\partial}{\partial x} =$ momentum operator. In 3D $\vec{p} = \frac{\hbar}{i} \vec{\nabla}$.