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

$$= \int_{-\infty}^{\infty} x \left[\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right] dx$$

From the Schödinge equation we get

$$\left.\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{i\hbar}{2m} \left(\frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) \\ \frac{\partial \psi^*}{\partial t} &= -\frac{i\hbar}{2m} \left(\frac{\partial^2}{\partial x^2} + V(x) \right) \psi^*(x). \end{aligned}\right\} \text{potential } V(x) \text{ is real}$$

Substituting we get

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} x \left[\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2} \psi \right]$$

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

Wave functions have property at $\psi \to 0$ at $x - \infty$

Using this property & doing integration by parts we get

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

$$= -\frac{i\hbar}{m}\int \psi^*\frac{\partial\psi}{\partial x}\,dx$$ {doing integration by parts in the 2nd terms

Note that $m\dfrac{d\langle x\rangle}{dt}$ has the dimension of momentum p.

Hence $m\dfrac{d\langle x\rangle}{dt}$ is the momentum expectation value $\langle p\rangle$

$$\Rightarrow \langle p\rangle = -i\hbar\int \psi^*\frac{\partial\psi}{\partial x}\,dx$$

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

$\hat{p} \equiv -i\hbar\dfrac{\partial}{\partial x}$ is called the momentum operator

The concept of "operator" is more general in quantum mechanics. For example, we define $\hat{x}$ as the position operator for position x

$$\langle x \rangle = \int \psi^* \hat{x} \psi \, dx = \int \psi^* x \psi \, dx$$

* In classical mechanics the kinetic energy is $T = p^2/2m$. In quantum mechanics the kinetic energy operator is

$$\hat{T} = \frac{\hat{p}^2}{2m}$$

$$\Rightarrow \langle T \rangle = \int \psi^* \left(\frac{\hat{p}^2}{2m} \right) \psi \, dx$$

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

* Total energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$

$$\langle E \rangle = \int \psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \psi \, dx$$

* Note that in the Schrödinger EoM

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

The operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ is called the Hamiltonian operator -

* Solution of Schrödinger Equation: Assume that $V(x)$ is independent of time. Then the wave function can be written as

$$\psi(x,t) = \phi(x) f(t) \quad \text{separation of variables}$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = \psi \frac{df}{dt} \quad \& \quad \frac{\partial^2 \psi}{\partial x^2} = \frac{d^2\psi}{dx^2} f$$

Schrödinger equation then becomes

$$i\hbar \frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} f + V\psi f$$

Dividing both sides by ψf we get

$$i\hbar \frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

The LHS is function of t only & RHS is function of x only. Hence both sides must be equal to a constant that we call E

$$\boxed{i\hbar \frac{1}{f}\frac{df}{dt} = E}$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

→ this is time-independent Schrödinger equation.

The solution for this equation is

$$f = e^{-iEt/\hbar}$$

* So the wave function can be written as

$$\psi(x,t) = \phi(x)\, e^{-iEt/\hbar}$$

$\Rightarrow |\psi|^2 = |\phi|^2 \rightarrow$ independent of time

Moreover, the time dependence drops out in all the expectation values — expectation values are constant in time. This type of wave functions are called the Stationary States.

* Note that in the time-independent schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

The left hand side is the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

Hence the constant E is the total energy.

So $\quad \hat{H}\psi = E\psi$

* Linar Superposition : The constant E is arbitrary. One can chose any value say $E_1, E_2, E_3 \cdots$ etc. For each of them the solutions are $\psi_1, \psi_2, \psi_3 \ldots$ etc. The general solution is superposition of all these solutions

$$\psi = \sum_{n=1}^{\infty} C_n \psi_n e^{-iE_n t/\hbar}$$

the coefficients $C_1, C_2, C_3 \ldots$ etc depend on initial conditions.

*