

Hamiltonian operator

If we consider potential term $V(\vec{r}, t)$ in study,
then total energy, $E = \frac{p^2}{2m} + V(\vec{r}, t)$

Then

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

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right) \psi(\vec{r}, t)$$

Then

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \quad (\text{Hamiltonian operator})$$

Position Probability

$$P(\vec{r}, t) = \psi^*(\vec{r}, t) \psi(\vec{r}, t)$$

Position probability density and its normalization condition ; $\int |\psi(\vec{r}, t)|^2 d\tau = 1$

Expectation value of dynamical variables

The average value of the measurements of the quantity performed on a very large number of independent identical systems represented by the wave function, ψ .

Thus expectation value of position is given by

$$\langle r \rangle = \int r P(\vec{r}, t) d\tau$$

$$= \int \psi^*(\vec{r}, t) r \psi(\vec{r}, t) d\tau$$

similarly, for 1-D

$$\langle x \rangle = \int \psi^* x \psi dx$$

$$\langle y \rangle = \int \psi^* y \psi dy$$

$$\langle z \rangle = \int \psi^* z \psi dz$$

The expectation value of any quantity is given by

$$\langle g(\vec{r}, t) \rangle = \int \psi^*(\vec{r}, t) g(\vec{r}, t) \psi(\vec{r}, t) d\vec{r}$$

similarly we can write

$$\langle E \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial t} \right) \psi d\vec{r}$$

$$\langle \vec{P} \rangle = \int \psi^* \left(-i\hbar \vec{\nabla} \right) \psi d\vec{r}$$

and its component

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

$$\langle P_y \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial y} dy \dots d\vec{r}$$

$$\text{and } \langle P_z \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial z} dz d\vec{r}$$