S. S. College. Jehanabad (Magadh University)

Department : Physics

Subject : Quantum Mechanics

Class : B.Sc(H) Physics Part III

Topic: Time independent Schrodinger equation.

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Time independent Schrodinger equation

There are many Physical Problems in which the potential energy of the particle doesnot depend on time ; $V = V(\vec{r})$ — (1)

In such cases, $\psi(\vec{r},t) = \psi(\vec{r})\,\phi(t)$

Then schrodinger equation becomes

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

dividing both side by $\psi(\vec{r})\,\phi(t)$, we get

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = \frac{1}{\psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) \quad \text{— (2)}$$

Thus each side must depend upon a constant 'E' such that,

$$E\phi = i\hbar\frac{d\phi}{dt}$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \quad \text{(3)}$$

$$\phi(t) = \exp\left(-\frac{iEt}{\hbar}\right) \quad \text{— (4)}$$

$$\psi(\vec{r},t) = \psi(\vec{r})\exp\left(-\frac{iEt}{\hbar}\right)$$

$$\boxed{H\psi(\vec{r}) = E\,\psi(\vec{r})}$$

where H is the Hamiltonian operator,

$$H = \frac{-\hbar^2 \nabla^2}{2m} + V(\vec{r})$$

The operator H acting on the function $\psi(\vec{r})$ gives back the function multiplied by the constant, E.

$$\boxed{H\psi = E\psi}$$

eigen function

eigen value

eigenvalue equation

Degeneracy

- Sometimes it happens that more than one linearly independent eigenfunctions correspond to the same eigenvalue. This type of eigen values are called degenerate.
- If $\psi_1, \psi_2 \ldots \psi_n$ are linearly independent eigen functions corresponding to eigen value E, then $\psi = c_1\psi_1 + c_2\psi_2 + \ldots + c_n\psi_n$ is also eigen function corresponding to E.

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Important properties

1.) Stationary states

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

$$= \psi^*(\vec{r})\, e^{iEt/\hbar}\, \psi(\vec{r})\, e^{-iEt/\hbar}$$

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

These states are called stationary states. This name is further justified by the fact that expectation value of the total energy operator in a state;

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

$$= \int \psi^*(\vec{r},t)\, e^{iEt/\hbar} H\, \psi(\vec{r})\, e^{-iEt/\hbar}\, d\vec{r}$$

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

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

$$= E$$

2.) orthogonality of eigen functions.

let ψ_K and ψ_n be eigen functions such that

$$H\psi_K = E_K \psi_K \quad -(1)$$

$$H\psi_n = E_n \psi_n \quad -(2)$$

Taking complex conjugate

$$(H\psi_n)^* = E_n \psi_n^* \quad -(3)$$

Premultiplying eq ① by ψ_n^* and postmultiply eq ③ by ψ_k given

$$\psi_n^* (H\psi_k) = E_k \psi_n^* \psi_k \quad — (4)$$

$$(H\psi_n)^* \psi_k = E_n \psi_n^* \psi_k \quad — (5)$$

substracting eq (5) − (4)

$$(E_n - E_k) \int \psi_n^* \psi_k \, d\vec{r} = \int [\psi_n^* (H\psi_k) - (H\psi_n)^* \psi_k] d\vec{r}$$

$$(E_n - E_k) \int \psi_n^* \psi_k \, d\vec{r} = 0$$

since, $E_k \neq E_n$

$$\int \psi_n^* \psi_k \, d\vec{r} = 0$$

This shows that eigen function are orthogonal.

In general

$$\int \psi_k^* \psi_n \, d\vec{r} = \delta_{kn} = \begin{cases} 0, & k \neq n \\ 1, & k = n \end{cases}$$

3:) Parity

The one dimensional schrodinger equation is

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

Replacing x by $-x$, we get

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

Case 1 If eigen value is non degenerate then $\psi(x)$ and $\psi(-x)$ can be written as

$$\psi(-x) = c\,\psi(x)$$

Changing the sign of x in this equation, we get

$$\psi(x) = c\,\psi(-x)$$

Combining these two equations,

$$\psi(x) = c^2\,\psi(x)$$

$$c^2 = 1$$

$$c = \pm 1$$

Therefore $\psi(-x) = \pm\,\psi(x)$

even Parity

$$\psi(-x) = \psi(x)$$

odd Parity

$$\psi(-x) = -\psi(x)$$

4) Continuity and Boundary Conditions

1.) The second order schrodinger equation wave function must have single-valued, finite and continous at every point in space.

2.) The wave functions are bounded at large distances in all directions.

3.) If there is an infinite potential step at a surface then the wave function at the surface is zero and the component of the gradient of the wave function normal to the surface is not determined.

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