Lecture M3L04

PH101: Physics 1

Module 3: Introduction to Quantum Mechanics

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The time-independent Schrodinger equation

Basis states of the Hamiltonian: In the Schrodinger equation we encountered an expression $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)$. This is called the Hamiltonian operator or Hamiltonian for short. It acts on functions of x (and possibly t) and gives other functions as the end result. We denote the Hamiltonian by the symbol H.

$$H=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)$$

Consider the case when the potential energy is independent of time i.e. we write V(x) instead of V(x,t). Just as in rigid bodies, the moment of inertia matrix $\mathbf{I}$ had specific directions $e_1, e_2\ and\ e_3$ so that $\mathbf{I}\ e_j=I_j\ e_j$ called eigenvectors, we could also ask if there are special functions $\varphi_j(x)$ that have the eigenvector property.

$$H\varphi_j(x)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\varphi_j(x)=E_j\ \varphi_j(x)$$

The time-independent Schrodinger equation

Then the functions $\varphi_j(x)$ would be analogous to finding the "principal directions" of the Hamiltonian. Just as in rigid bodies the three directions $e_1, e_2\, and\, e_3$ were linearly independent and any other vector may be expressed as a linear combination of these directions viz. $\mathrm{v} = \sum_j c_j\, e_j$ here too we may write for any function $\psi(x,t)$,

$$\psi(x,t) = \sum_j c_j(t)\, \varphi_j(x)$$

Specifically we want $\psi(x,t)$ to obey Schrodinger's equation.

This means,

$$i\,\hbar\frac{\partial}{\partial t}\psi(x,t)=\sum_j i\,\hbar\,\frac{d}{dt}c_j(t)\varphi_j(x)$$

$$and\ \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\psi(x,t)=\sum_j E_j c_j(t)\,\varphi_j(x)$$

gives us

$$i\,\hbar\,\frac{d}{dt}c_j(t)=\ E_j c_j(t)\ \ which\ means\ \ c_j(t)\ =\ \ e^{-\frac{i}{\hbar}E_j\,t}\ \ c_j(0)$$

If we assume that $c_j(0)$ = 0 for all j except one special j = n where $c_n(0)$ = 1 then we obtain a stationary state.

$$\psi(x,t) = e^{-\frac{i}{\hbar}E_n\, t}\ \varphi_n(x)$$

This has the property that the probability density $|\psi(x,t)|^2$ is independent of time. It also means all expectation values are independent of time.

$$< A > = \int dx\ \psi^*(x,t)\ A\ \psi(x,t)\ = \int dx\ \varphi_n^*(x)\ A\ \varphi_n(x)$$

Practical Quantum Mechanics

Q. A stationary state of a quantum particle has an eigen function described by,

$$\varphi_0(x) \begin{cases} \sqrt{\dfrac{2}{L}}\,\sin\left(\dfrac{\pi\, x}{L}\right)\ ; & 0 < x < L \\ 0\ ; & \text{otherwise} \end{cases}$$

a) Find the expectation value of the position.

$$< x > = \int_0^L \varphi_0(x)\, x\, \varphi_0(x)\ dx = \frac{L}{2}$$

b) Find the expectation value of the momentum.

$$< p > = \int_0^L \varphi_0(x)(-i\,\hbar\frac{\partial}{\partial x})\,\varphi_0(x)\ dx = 0$$

This is because the waves are moving in both directions.

c) Find the expectation value of the kinetic energy.

$$< KE > = \frac{1}{2m}\int_0^L \varphi_0(x)\left(-i\,\hbar\frac{\partial}{\partial x}\right)^2 \varphi_0(x)\ dx = \frac{\hbar^2\,\pi^2}{2m\,L^2}$$

d) Find the probability that the particle is between 0 and L/4

probability = $\int_0^{L/4} \varphi_0(x)\ \varphi_0(x)\ dx\ = \frac{\pi-2}{(4\ \pi)} = 0.09$

e) Estimate the size of the deviation of the position of the particle from its expected value.

Deviation from expected value = $x - \frac{L}{2}$

But is as likely for the particle to be to the left of $x = \frac{L}{2}$ as it is to the right of this value.

We want to know how far in absolute terms it can be found far away from $x = \frac{L}{2}$. For this we can do one of two things. We could calculate the average of $|x - \frac{L}{2}|$. This means we could say,

$$\Delta x = \int_0^L \varphi_0(x)\, |x - \frac{L}{2}|\, \varphi_0(x)\ dx$$

which is possible but the absolute value is a mathematically clumsy operation since we have to take into account the cases $x > \frac{L}{2}$ and $x < \frac{L}{2}$ separately while performing the above integral [do it as a homework].

What is usually done is to find the average of the square of $x - \frac{L}{2}$ and then we get a quantity whose units is [length]^2 but represents the deviation from the average value. To get a quantity with units of length we simply take the square root at the end. This is called RMS value.

$$(\Delta x)^2 = \int_0^L \varphi_0(x) \left(x - \frac{L}{2}\right)^2 \varphi_0(x)\ dx$$

In the present example we may evaluate this to get, Δx **= 0.18 L**. Hence the quantum particle is most likely to be found between 0.5 L - 0.18 L and 0.5 L + 0.18 L.

Next natural question is how likely is most likely? The probability that the particle is found between 0.5 L - 0.18 L and 0.5 L + 0.18 L is,

$$\text{probability} = \int_{0.5\ \mathrm{L} - 0.18\ \mathrm{L}}^{0.5\ \mathrm{L} + 0.18\ \mathrm{L}} \varphi_0(x)\ \varphi_0(x)\ dx = 0.65$$

or 65% probability. If you want a higher probability choose, the interval to be $\frac{L}{2} - 2\ \Delta x\ \ and\ \ \frac{L}{2} + 2\ \Delta x$. The probability that the particle is in this interval now is much higher.

$$\text{probability} = \int_{0.5\ \mathrm{L} - 0.36\ \mathrm{L}}^{0.5\ \mathrm{L} + 0.36\ \mathrm{L}} \varphi_0(x)\ \varphi_0(x)\ dx = 0.97$$

or 97% probability.

e) Estimate the size of the deviation of the momentum of the particle from its expected value.

This is easier to do since the expected value of momentum is zero.

$$(\Delta p)^2 = \int_0^L \varphi_0(x) \left(-i\,\hbar \frac{\partial}{\partial x} - 0\right)^2 \varphi_0(x)\; dx = < p^2 > = 2m < KE > = \frac{\hbar^2 \pi^2}{L^2}$$

or $\boldsymbol{\Delta p} = \frac{\hbar\, \boldsymbol{\pi}}{\boldsymbol{L}}$ Combining with the earlier result namely, $\boldsymbol{\Delta x}$ **= 0.18 L** we conclude that

$$\Delta \boldsymbol{x}\, \Delta \boldsymbol{p} = \mathbf{0.565}\, \hbar > \hbar\mathbf{/2}$$

which is consistent with **Heisenberg's uncertainty principle.**