Schrödinger Equation

Now we move our consideration from a free particle to particle under a force. For such a particle the following equation would be valid.

$$E = \frac{p^2}{2m} + V$$

Multiply each side by ψ and replace relevant quantities by their operators, assuming one dimensional case initially.

$$E\psi = \frac{p^2\psi}{2m} + V\psi$$

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

In Three Dimensions

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

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

This is called Time dependent Schrödinger Equation

Wave Function

- A microscopic particle is described by a wave function, which contains all the information that we can have about the physical properties of the particle.
- The Schrödinger Equation gives the position and time dependence of the wave function.

The probability of finding the particle between x and $x+dx$ is given by

$$|\psi(x,t)|^2\, dx$$

The Probability

Imagine a very large number of separate identical particles described by the same wave function $\psi(x,t)$. If a measurement of position is done on all of them at a time t, the result would not be identical.

If the probability of finding particle between x_o and x_1 is 0.1, then in 10% of measurements the position would be found between x_o and x_1.

The Probability is Not

Defined over a measurement on a single particle. Suppose a measurement was made at a time t and the particle was found to be in the infinitesimal vicinity of x_o. If we make a measurement immediately afterwards, it will still be found there.

Experimental reproducibility is necessary.

At a time much later, the wave function may again evolve under Schrödinger Equation.

Measurements on different particles at the same time, may not yield the same result, however.

Various Approaches

- If a measurement was done and the particle was found at $x=x_o$, where was it just before?
  - Realistic: Indeterminacy could be different from ignorance. The particle was there only, but we were not knowing. Some additional information was needed to provide the complete description (hidden variable).

- Orthodox: The particle was not really there. Our method of measurement forced the particle to take a stand to be present there (Copenhagen interpretation).
- Agnostic: Refuse to Answer

Copenhagen interpretation is the accepted one.

See D.J. Griffiths: Introduction to QM.

Normalization

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

1. If ψ is a solution, $A\psi$ is also one.
2. The probability of finding the particle somewhere should be one. This in one-dimension would mean the following.

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

Normalization (*Cond.*)

In general, if $d\tau$ is the volume element in a given co-ordinate system

$$\int_{\substack{\text{entire}\\ \text{space}}} |\psi(x,t)|^2 \, d\tau = 1$$

$$d\tau \equiv dxdydz$$

$$d\tau \equiv r^2 dr \sin\theta d\theta d\phi$$

Normalization would determine the unknown constant, within a phase factor.

Normalization (*Cond.*)

- Square integrability puts a necessary condition on the wave function.
- The normalization is strictly not possible for a free wave, as the particle has equal probability of being found out over infinite space.

$$\int_{-\infty}^{+\infty} A^* e^{-i(kx-\omega t)} A e^{+i(kx-\omega t)} dx = 1$$

$$\Rightarrow \int_{-\infty}^{+\infty} |A|^2 \, dx = 1$$

Example

The wave function of a particle at $t=0$ is given by following.

$$\psi(x) = Ae^{-\frac{x^2}{a^2}}$$

Example *(cond.)*

A person performs a number of experiments on identical particles described by the same wave function at the same time and in 100 of them the particle was found to be in the infinitesimal vicinity of *x=2a*. In how many of the measurements, it would be found in the same infinitesimal vicinity of *x=a*?

Answer

$$P(x)dx = |\psi(x)|^2 dx$$

$$P(2a)dx = |A|^2 e^{-\frac{2(2a)^2}{a^2}} dx = |A|^2 e^{-8} dx$$

$$P(a)dx = |A|^2 e^{-\frac{2a^2}{a^2}} dx = |A|^2 e^{-2} dx$$

$$\frac{P(2a)dx}{P(a)dx} = \frac{e^{-8}}{e^{-2}} = \frac{100}{M}$$

$$M = 100e^{6} \approx 40{,}343$$

Expected Values

- In QM, normally there is a probability associated with the result obtained after measurement.
- Expected value (name somewhat misleading) is the average value that one would get after a very large number of measurements are made on identical systems, with same wave functions.

Expected Values*(Cond.)*

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) x \psi(x,t) dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t) x^2 \psi(x,t) dx$$

Expected Value *(Cond.)*

- There is an operator associated with every dynamical variable.
- The expected value of the variable expressed by operator $\hat{G}$ is defined as

$$\langle \hat{G} \rangle = \int_{\substack{\text{entire} \\ \text{space}}} \psi^*(x,t) \hat{G} \psi(x,t) d\tau$$

Expected Value *(Cond.)*

- The mean value of x- component of momentum and its square would thus be given by

$$\langle p_x \rangle = -i\hbar \int_{-\infty}^{+\infty} \psi^*(x,t) \frac{\partial \psi(x,t)}{\partial x} dx$$

$$\langle p_x^{\ 2} \rangle = -\hbar^2 \int_{-\infty}^{+\infty} \psi^*(x,t) \frac{\partial^2 \psi(x,t)}{\partial x^2} dx$$

Expected Value *(Cond.)*

- It can be shown that the expected value of momentum would always be real.
- The operators of the dynamical variables are always such that their expected value turns out to be real.