PHYS-453

5- Solution of Schrödinger's equation

The solution of Schrödinger's equation-a

Newton's equation, **F**=*ma*, in classical mechanics is a second order differential equation with respect to time. Thus, to solve it you need to know both the initial position, **r**(0), and the initial velocity **v**(0).

Schrödinger's equation is first order with respect to time thus we need to know only the initial wavefunction $\psi(x,0)$ in order to solve it. The method we use for solving this equation is the so called *method of separation of variables*. In this method the solution has the form of a product of two separate functions, one of which depends only on position and the other only on time

The solution of Schrödinger's equation-b

The solution has the form:

$$\psi\left(x,t\right)=\psi\left(x\right)T\left(t\right)$$

Where we can show that $T\left(t\right)=e^{-iEt/\hbar}$ with E the energy of the particle. Thus the solution could get the form

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

The solution of Schrödinger's equation-c

The time independent wave function $\psi(x)$ is a solution of the so called **time independent Schroedinger equation**

$$\psi'' + \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi = 0$$

It is interesting to note that the solution of the time dependent part is always the same no matter the particular form of the potential V. Thus the solution of the Schroedinger equation is reduced to the solution of the time independent equation above.

Why separable solutions are desired?

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1. Because they are **stationary** states. That means:

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

The same happens for the expectation value of any dynamical variable. *Every expectation value is constant in time.*

$$\langle Q(x,p)\rangle = \int \psi^* Q\left(x, \frac{\hbar}{i}\frac{d}{dx}\right)\psi\, dx$$

Why separable solutions are desired? -a

2. They are states of **definite total energy**. Every measurement of the total energy is certain to return the value of *E*.

3. The general solution is a **linear combination** of separable solutions.

Why separable solutions are desired? -b

The time independent Schrödinger equation has physically accepted solutions (i.e. solutions that tend to zero at infinity) only if the energy E has a discrete set of eigenvalues (or eigenergies) E_1 , …, E_n , … with solutions (eigenfunctions) ψ_1 , …, ψ_n , … respectively.

$$\psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar} \qquad (n = 1, \ \ldots, \infty)$$

Solution of Schrödinger eq.

- Once we have found the separable solutions we can write the general solution, of the form

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

- The constants c_n are derived from the initial condition for the wave function $\Psi(x,0)$.

Solution of Schrödinger eq.

- The strategy is to solve the time independent Schroedinger equation and this gives you, in general, the infinite set of solutions $\psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$ each with each own associated energy and to write down the general linear combination of these solutions

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Solution of Schrödinger eq.

- To construct the final solution $\Psi(x,t)$ you simply tack onto each term its characteristic time dependence $e^{-iE_n t/\hbar}$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

- The separable solutions themselves,

$$\Psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar}$$

- are *stationary* states, in the sense that all probabilities and expectation values are independent of time, but this property is not shared by the general solution.