

Wave Functions

1 Time Independent Schrodinger Equation

In the last class, we "derived" time dependent Schroedinger equation

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

The wave function $\psi(x, t)$ depends on two variables (x, t) and the above equation is a **partial differential equation**. It contains **partial derivatives** of $\psi(x, t)$ with respect to both x and t . Note that, it is a first order differential equation in "t" and a second order differential equation in "x".

Initial Condition Theorem: To obtain a unique solution to a first order differential equation, we have to give one **initial condition**. To solve a second order differential equation, we have to give two **initial conditions**, as you know from solving Newton's second law.

Overall, ordinary differential equations, involving ordinary derivatives, are easy to solve compared to partial differential equations. So, we will attempt to convert the above partial differential equations into two separate equations: one involving derivatives with respect to t only and another involving derivatives with respect to x only. A standard technique to do this is to use **separation of variables**. We assume

$$\psi(x, t) = \phi(x)T(t),$$

that is, $\psi(x, t)$ can be written as a product of two functions: one of x alone and another of t alone. The assumption enables us to convert the partial derivatives of the original equation into ordinary derivatives, because each of the functions ϕ and T depend only on one variable.

Unique Solution Theorem: A given differential equation with specific initial conditions has a **unique solution**. If we find a solution to time dependent Schroedinger equation by some guess work and show that it satisfies the differential equation and the initial conditions, then **it is the solution**.

We substitute $\psi(x, t) = \phi(x)T(t)$ in time dependent Schroedinger equation. We then get

$$i\hbar\phi(x)\frac{dT(t)}{dt} = \left[-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) \right] T(t).$$

We divide both sides by $\psi(x, t) = \phi(x)T(t)$ to get

$$i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt} = \frac{1}{\phi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) \right].$$

The left-hand side is **purely a function of t** and the right-hand side is **purely a function of x** . The only way this equation can be satisfied is **both sides are equal to a constant!!!** We call this constant E . So, the time dependent Schroedinger equation splits into two **ordinary differential equations**

$$\begin{aligned} i\hbar\frac{1}{T(t)}\frac{dT(t)}{dt} &= E \\ \frac{1}{\phi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) \right] &= E. \end{aligned}$$

We re-write them as

$$\begin{aligned} i\hbar\frac{dT(t)}{dt} &= ET(t) \\ \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right] \phi(x) &= E\phi(x). \end{aligned}$$

Given our definition that $p = -i\hbar d/dx$, we see that the second equation can be written as

$$\begin{aligned} \left[\frac{p^2}{2m} + V(x) \right] \phi(x) &= E\phi(x) \\ H\phi(x) &= E\phi(x). \end{aligned}$$

The differential equation in x is called **Time independent Schroedinger equation**. The form of the equation is such that the action of the operator H on the function $\phi(x)$, gives a result which is a **number multiplied by $\phi(x)$** .

2 Energy Eigenfunctions

An equation of the form of time independent Schroedinger equation is called eigenfunction equation. A more exact statement is

The operator H has an energy eigenfunction $\phi(x)$ with energy eigenvalue E .

You have come across such eigenfunction form of differential equations before. The radio-active decay law equation

$$\frac{dN}{dt} = -\lambda N$$

is one such equation. It has the solution $N(t) = N(0)e^{-\lambda t}$. In this case, the real parameter λ can vary continuously and the exact solution needs one initial condition $N(0)$. A simple harmonic oscillator equation, which is of second order, is

$$\frac{d^2 X}{dt^2} = -\omega^2 X,$$

which has the solution $X(t) = A \cos(\omega t) + B \sin(\omega t)$. Here also ω^2 can be a continuous variable. To find the complete solution, we need two initial conditions: $X(0) = A$ and $\dot{X}(0) = B\omega$. **BUT**, the time independent Schroedinger equation will have solutions **only for some discrete values of E** .

The energy eigenvalues of time independent Schroedinger equation are QUANTIZED!!!

During the next few weeks, we will solve time independent Schroedinger equation for some simple potential functions.

The time differential equation has the simple solution

$$T(t) = T(0)e^{-iEt/\hbar},$$

which can be verified very easily. Hence, we can write

$$\psi(x, t) = \phi(x)T(t) = \phi(x)T(0)e^{-iEt/\hbar} \equiv \psi(x, 0)e^{-iEt/\hbar}.$$

If the wave function is an **energy eigenfunction**, then its time dependence is given by a simple phase factor $e^{-iEt/\hbar}$.

The above statement is NOT true for wave functions which are not energy eigenfunctions.

3 Probability Interpretation

We have discussed a lot about the wave function $\psi(x, t)$ and what equation it satisfies. I also mentioned that the Schroedinger equation for the wave function leads to energy quantization. But, **what is the physical significance** of the wave function? That was the question physicists asked Schroedinger, back in 1926. And, Schroedinger had no answer. Soon after, Max Born, who helped Heisenberg develop matrix mechanics, gave the probabilistic interpretation to wave function, that is widely accepted.

If a particle moving under the influence of a potential $V(x)$ has the wave function $\psi(x, t)$, then $|\psi(x, t)|^2 dx$ gives the probability of finding the particle in the region $x \pm dx/2$ at time t .

In three dimensions, the statement becomes: If a particle moving under the influence of a potential $V(\vec{r})$ has the wave function $\psi(\vec{r}, t)$, then $|\psi(\vec{r}, t)|^2 d^3r$ gives the probability of finding the particle in the small volume d^3r , surrounding the point with position vector \vec{r} , at time t .

This connection between the wave function and the probability means that **all the information about the particle is imbedded in the wave function**. I will make this statement more precise when we talk about operators in the next class.

We said that $|\psi(x, t)|^2 dx$ gives the probability of finding the particle in a specified region. But, the particle has to be somewhere. Which means that when we take sum of $|\psi(x, t)|^2 dx$ over all x , we should get 1. In the form an equation, we say

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

In mathematical language, **the wave function should be normalized**. A function can be normalized only if it is finite at every point and if it vanishes as $x \rightarrow \pm\infty$.

4 Constraints on Wave Functions

Both Schroedinger equation and the probabilistic interpretation impose certain important constraints on wave functions. In solving any quantum mechanical problem, we need to pay special attention to these constraints. Before we list the conditions, we define our quantum mechanical problem broadly. We consider only those potentials $V(x)$ which are finite for $-\infty < x < \infty$. The potential need not be smooth (or differentiable) or even continuous but it must be finite. We seek to find eigenfunctions of such potentials whose eigenvalues E are finite. We will not consider wavefunctions whose energy diverges. The constraints on energy eigenfunctions are

1. The probability of finding the particle in the region $x \pm dx/2$ has to be **unique**. Which means $\phi(x)$ has to be **single valued**.
2. Since E is finite, time independent Schroedinger equation implies that the second derivative $d^2\phi(x)/dx^2$ is finite for all x . This implies that the first derivative $d\phi(x)/dx$ also must exist. This, in turn, means that $\phi(x)$ must be **continuous** and **differentiable**.
3. The wave function must be finite for all x and must vanish as $x \rightarrow \pm\infty$.
4. The integral

$$\int_{-\infty}^{\infty} |\phi(x)|^2 dx,$$

must be finite. OR the wave function should be **normalizable**.