Schroedinger Equation

Note: From now on all our massive particles will move with **non-relativistic** speeds.

1 Schroedinger's Big Idea

Till now, we have studied the early quantum ideas. These were a series of random ideas, loosely connected to one another by the Planck's constant $\hbar$. In 1925, Heisenberg developed the first version of quantum mechanics based on the concept of **non-commuting observables**. He presented these quantities using matrices and obtained the energy levels of hydrogen atom (the same problem solved by Bohr earlier). Matrices were quite unfamiliar to physicists at that time and this formalism was not used much. In 1926, quite independently, Schroedinger developed a **differential equation** obeyed by a curious object called ψ. Using this equation, he also solved the problem of hydrogen atom and got the correct energy levels. Physicists were more familiar with differential equations and Schroedinger equation was used to solve a number of problems in physics, such as emission of a photon by an excited atom, electrical conductivity of solids, alpha decay etc. Initially there was a lot of confusion as to why two different and unrelated techniques work equally well. In a year or so, Schroedinger showed the mathematical equivalence of his **wave mechanics** and Heisenberg's **matrix mechanics**.

As mentioned before, physicists find it more convenient to use differential equations (having grown up solving Newton's second law and Maxwell's equations, both of which are differential equations). So almost all quantum mechanical calculations are done using Schroedinger equation. All textbooks discuss only Schroedinger equation. Only consolation Heisenberg had is that he got his Nobel prize one year earlier.

deBroglie said that a matter particle should have a wavelength. But what is "waving" is never mentioned. Whereas in all the classical waves, there is a physical, observable quantity that is varying with both space and time. For waves on a string, it is the displacement from the equilibrium position. Same is true for sound waves and water waves. For electromagnetic waves, the electric and magnetic fields vary sinusoidally in space and in time. But what is the quantity that "waves" in a quantum wave. deBrogile had no idea.

Schroedinger also had no idea of what it is. But he gave it a name. He called it a **wave function** and represented it by the Greek letter $\psi(x,t)$. Having done that, he asked the question that one usually asks in Newtonian mechanics: How does this object change with time? What is the differential equation which governs its **time evolution**? By some inspired guess work, he came up with the answer. The picture he built up could explain Planck hypothesis, Einstein's photon hypothesis and deBroglie hypothesis. His hydrogen atom differs from Bohr atom in some important details but they both have the feature that **angular momentum is quantized**.

2 Heuristic Development of Schroedinger Equation

Let us attempt a "derivation" of Schroedinger equation. To keep the algebra simple, we will limit ourselves to motion of a point particle of mass m in one dimension. Its energy and momentum are related by

$$E = \frac{p^2}{2m}.$$

Planck said $E = \hbar\omega$ and deBroglie said $p = \hbar k$. So for a quantum free particle, the above equation can be re-written as

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}.$$

Classically, we represent a wave of a given wave number k as $Ae^{i(kx-\omega t)}$, where A is the amplitude of the wave. The frequency is the product of the speed of the wave and the wave number $\omega = vk$. To keep things extremely simple, we take $\psi(x,t)$ to be a wave a single k. That is, we take $\psi(x,t) = Ae^{i(kx-\omega t)}$. It is easy to see that

$$\begin{aligned}\frac{\partial^2\psi(x,t)}{\partial x^2} &= -k^2\psi(x,t)\\ \frac{\partial\psi(x,t)}{\partial t} &= -i\omega\psi(x,t).\end{aligned}$$

Let us consider the partial differential equation

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

Substituting $\psi(x,t) = Ae^{i(kx-\omega t)}$ in the above equation, we get

$$\hbar\omega\psi = \frac{\hbar^2 k^2}{2m}\psi,$$

which is the energy momentum relation for a quantum free particle. The above partial differential equation is the **Schroedinger equation** for a free particle with **wave function** $\psi(x,t)$.

We argued in previous classes that a finite wave packet is a superposition of an infinite number of waves of different wave numbers and wave speeds. Let us consider such a superposition

$$\psi(x,t) = \int A(k) e^{i(kx-\omega(k)t)} dk.$$

Substituting this in Schroedinger equation, we get

$$\int [\hbar\omega(k)] A(k) e^{i(kx-\omega(k)t)} dk = \int \left[\frac{\hbar^2 k^2}{2m}\right] A(k) e^{i(kx-\omega(k)t)} dk.$$

This can be re-written as

$$\int \left[\hbar\omega(k) - \frac{\hbar^2 k^2}{2m}\right] A(k) e^{i(kx-\omega(k)t)} dk = 0.$$

It can be shown that the LHS is zero **only if** the quantity in the square brackets is zero. That is, if

$$\hbar\omega(k) = \frac{\hbar^2 k^2}{2m}.$$

If we construct a wave packet such that each component wave of this packet satisfies the free particle energy-momentum relation, then the wave packet satisfies free particle Schroedinger equation.

This concept can be extended to particles moving under the influence of a force also. We will assume that the force is such that it can be written as $F = -dV(x)/dx$. Then the energy of the particle is given by

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

and the corresponding Schroedinger equation is

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

It is left as an exercise for you to show that the wave packet

$$\psi(x,t) = \int A(k) e^{i(kx-\omega(k)t)} dk.$$

satisfies the above Schroedinger equation if each component wave of the packet satisfied the energy momentum relation

$$\hbar\omega(k) = \frac{\hbar^2 k^2}{2m} + V(x).$$

In constructing a wave packet, we said "Just superpose a set of sinusoidal waves of different wave numbers and wave speeds". Here we are being more restrictive. We demand that all the waves which make up the wave packet should satisfy the **energy-momentum relation**, $E = p^2/(2m) + V(x)$, that is satisfied by the particle in question. Thus, given a potential $V(x)$, only the appropriate special waves will be allowed to be the part of the wave packet.

Consider, for example, a light pulse. Since it is of finite duration, it will have a range frequencies given by $\Delta\omega = 1/\Delta t$. But all the waves in this frequency range MUST satisfy the energy momentum relation $E = pc$, which means all the waves travel with speed of light and hence the whole pulse travels with the speed of light.

3 Operator Language

You all know about functions. A function f takes the number x as input and gives the number $f(x)$ as output. You can think of it along the following way. f "operates" on a number "x" and converts into the number "$f(x)$".

We extend this concept further. We consider an "**Operator**", which acts on a function f_1 and converts into a different function f_2. One very common operator, you have come across is the **differential operator** d/dx. When d/dx acts on x^2, it gives out $2x$. When it acts on $\sin x$, it gives out $\cos x$.

We now rephrase Schroedinger equation using the above operator language. We think of E as an operator and identify it with $i\hbar\partial/\partial t$. Similarly, we think of momentum as another operator and identify it with $-i\hbar\partial/\partial x$. With these identifications, the energy-momentum relation

$$[E]\psi(x,t) = \left[\frac{p^2}{2m} + V(x)\right]\psi(x,t)$$

automatically becomes the Schroedinger equation

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

Newtonian mechanics was further refined by later mathematicians who developed two related styles of mechanics called **Lagrangian Mechanics** and **Hamiltonian Mechanics**. In the latter, an operator called **Hamiltonian** is introduced which is defined to be

$$H = \frac{p^2}{2m} + V(x).$$

In Hamilton Mechanics point of view, the Hamiltonian guides the time evolution of any dynamical variable. Schroedinger borrowed this concept, modified it and wrote the original Schroedinger equation as

$$\left[i\hbar\frac{\partial}{\partial t}\right]\psi(x,t) = [H]\psi(x,t),$$

(where I put operators in square brackets, to emphasize their nature as operators). Identifying $p = -i\hbar\partial/\partial x$ in the above form of the Hamiltonian, we get the Schroedinger in its usal form.