College of Science
Department of Physics
Fourth Class
Lecture 10

Quantum Mechanics

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Lecture 10: Postulate 5 and the Schr*ö*edinger equation

Preparation

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Unit 5

Time Dependence and the Schröedinger Equation

5.1 Postulate 5 and the Schröedinger equation

The 5th postulate may be represented by the operator wave equation for time depended systems, which themselves are describable in terms of wave functions such as Ψ(x,y,z,t) . The eq. of motion in classical mechanic is

E = K.E + P.E

E =$\frac{p^2}{2m}$ $+V$ → $E\Psi = \frac{p^2}{2m}\Psi + V\Psi - - - - - - 1$

If $\Psi(x,t) = Ae^{i(px-Et)/\hbar}$

$\frac{\partial\Psi}{\partial x} = A\left(\frac{i}{\hbar}\right)p\ e^{i(px-Et)/\hbar} = \frac{i}{\hbar}\ p\ \Psi(x,t)$ ---------2

$\frac{\partial^2\Psi}{\partial x^2} = A\left(\frac{-p^2}{\hbar^2}\right)\ e^{i(px-Et)/\hbar} = \frac{-p^2}{\hbar^2}\ \Psi(x,t)$ ---------3

From eq.2 we can find $p\Psi = -i\hbar\frac{\partial\Psi}{\partial x}$

And from eq.3 we can find $p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2}$ ---------4

Also, we can take $\frac{\partial\Psi}{\partial t}$ to the wave function

$\frac{\partial\Psi}{\partial t} = -\frac{iE}{\hbar}\Psi$ → $E\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ -----------5

If we substitute eq.4&5 in eq.1, can find eq. of motion in quantum of mechanic.

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

When the Hamiltonian operator is $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$

$$\boxed{i\hbar\ \frac{\partial}{\partial t}\Psi(x,y,z,t) = \hat{H}\Psi(x,y,z,t)}$$

This called **Schr*ö*edinger** eq. contain time (time dependent Sch.eq.)

5.2 Separation of variables when the Hamiltonian is time independent

(i) If the Hamiltonian is independent of time and therefore does not operate on the time part of the solution. The time part of the solution is therefore the solution of a very simple differential equation. i.e V=V(x)

$\hat{H}\,\Psi(x) = E\,\Psi(x)$

$$\boxed{E\Psi(x) = -\frac{ħ^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} + V(x)}$$

Time indented **Schr*ö*edinger** eq.

(ii) The solution of **Schr*ö*edinger** eq. can be written as a product of space part and time part, i.e.

$$\Psi(x, y, z, t) = f(t)\Psi(x, y, z)$$

If Ĥ independent of time ($\hat{H} = -\frac{ħ^2}{2m}\nabla^2 + V$)

$\hat{H}\,\Psi(x,y,z,t) = E\,\Psi(x,y,z,t)$ --------------6

Where E is independent of time (the system in stationary states).

$\Psi(x,y,z,t) = \Psi(x,y,z)\, f(t)$

$\hat{H}\,\Psi(x,y,z,t) = iħ\,\Psi(x,y,z)\,\frac{\partial f(t)}{\partial t}$ ----------7

From eq.6 &7

$E\,\Psi(x,y,z)\, f(t) = iħ\,\Psi(x,y,z)\,\frac{\partial f(t)}{\partial t}$

$$-\frac{i}{ħ}E\,\partial t = \frac{\partial f(t)}{f(t)} \quad \rightarrow \int -\frac{i}{ħ}E\,\partial t = \int \frac{\partial f(t)}{f(t)}$$

$$-\frac{i}{ħ}\,Et = \ln f(t)$$

$$\boxed{f(t) = C\,e^{--\frac{i}{ħ}Et}}$$

Where E is an eigen value of Ĥ and C is another constant. Thus an overall wave function will be given by

$$\Psi(x,y,z,t) = Ce^{--\frac{i}{\hbar}Et}\Psi(x,y,z)$$

This may be interpreted physically as follows:

Suppose at time $t=t_o$ we measure the energy of a particle and discover that it is E, an eigen value corresponding to the stationary eigen state Ψ. If we when leave the system alone after making the measurement, it will continue to be described by the spatial eigen state Ψ, have a constant energy E, but will have an overall wave function $\Psi(x,y,z,t)$ which is time dependent. This time dependence will be oscillatory with angular frequency $\frac{E}{\hbar}$. The fact that the wave function of a particle varies with time does not necessarily mean that all its corresponding physical observable vary with time.

5.3 Mathematical properties of the wave functions and eigen functions

(a) For a particular time independent potential V(x) acceptable solutions of the Schröedinger equation exists only for the certain values of energy E_1, E_2,--------E_n (eigen values) corresponding to each eigen value an eigen function $\varphi_1(x), \varphi_2(x), ---- \varphi_n(x)$which is solution to the time independent Schröedinger equation for the potential V(x). For each eigen value there is also corresponding wave function $\Psi_1(x,y,z,t), \Psi_2(x,y,z,t)$----------,$\Psi_n(x,y,z,t)$ which is a solution to Schröedinger eq. for the potential .We saw that these functions are

$$e^{-\frac{iE_1t}{\hbar}}\varphi_1(x)\ ,\ e^{-\frac{iE_2t}{\hbar}}\varphi_2(x)\ ,\text{-----------------},\ e^{-\frac{iE_nt}{\hbar}}\varphi_n(x)$$

The index "n" which take on integer values from 1 to ∞ , and which is used to designate a particular eigen value and its corresponding eigen function is called the quantum number.

(b) Each of the wave function $\Psi_n(x,t)$ is a particular solution to the Schröedinger eq. for the potential V(x). Since Schröedinger eq. is linear in the wave functions, any linear combination of these functions is also a solution.

Let us check this for the simple case

$\Psi(x,t)=a_1\Psi_1(x,t) + a_2\Psi_2(x,t)$

Substituting this function into the Schröedinger eq.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)-i\hbar\frac{\partial\Psi(x,t)}{\partial t}=0$$

We have

$$-\frac{\hbar^2}{2m}(a_1\frac{\partial^2\Psi_1}{\partial x^2}+a_2\frac{\partial^2\Psi_2}{\partial x^2})+V(a_1\Psi_1+a_2\Psi_2)-i\hbar(a_1\frac{\partial\Psi_1}{\partial t}+a_2\frac{\partial\Psi_2}{\partial t}) \\ =0$$

Or

$$a_1\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1}{\partial x^2}+V\Psi_1-i\hbar\frac{\partial\Psi_1}{\partial t}\right]+a_2\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2}{\partial x^2}+V\Psi_2-i\hbar\frac{\partial\Psi_2}{\partial t}\right] \\ =0$$

Ψ1 &Ψ2 satisfy the Schröedinger eq. both brackets vanish.

This argument may be extended to show that the function

$$\Psi(x,t)=\sum_{n=1}^{\infty}a_n\Psi_n(x,t)$$

Is a solution to the Schröedinger where a_n are arbitrary constants.

(c) To calculate the probability density

$\Psi^*(x,t)\Psi(x,t)$ for the general case of a particle whose associated wave function is of the form

$$\Psi(x,t)=\sum_{n=1}^{\infty}a_n\Psi_n(x,t)$$

We write it

$$\Psi(x,t)=\sum_{n=1}^{\infty}a_n e^{-\frac{iE_nt}{\hbar}}\varphi_n(\text{x})$$

Substitute for $\Psi^*(x,t)\Psi(x,t)$ and integrate

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = \sum_n a_n^* a_n \int_{-\infty}^{\infty} \varphi_n^*(x)\varphi_n(x)dx$$
$$+\sum_l \sum_n a_l^* a_n\, e^{\frac{-i(E_n-E_l)t}{\hbar}} \int_{-\infty}^{\infty} \varphi_l^*(x)\varphi_n(x)dx$$

Since the double sum contains only terms for which $l \neq n$, we apply the equation

$$\int_{-\infty}^{\infty} \varphi_l^*(x)\varphi_n(x)dx = \begin{cases} 1 & l = n \\ 0 & l \neq n \end{cases}$$

$(l \neq n)$ to each integral appearing in that double sum. We may also apply the same equation $l = n$ to each integral in the single sum. Then we obtain

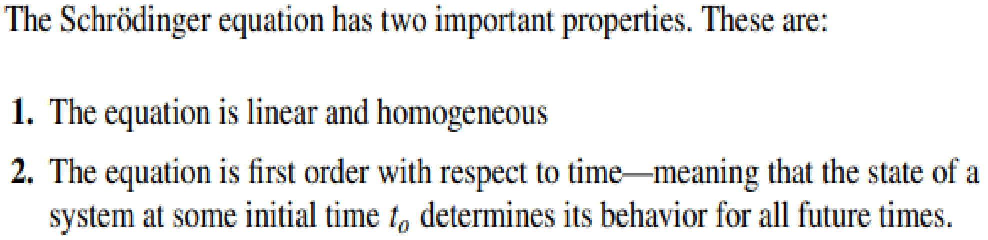
$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = \sum_{n=1}^{\infty} a_n^*\, a_n$$

Thus, normalization of the wave function is achieved if we have

$$\sum_{n=1}^{\infty} a_n^* a_n = 1$$

Since this condition does not involve time, we see that the wave function will always remain normalized.

The quantity $a_n^* a_n$ is equal to the probability that a single measurement of the observable will yield the value the (eigen value) i.e. It is equal to the prob. that the particle would find in the eigen state n.



The Schrödinger equation has two important properties. These are:

1. The equation is linear and homogeneous
2. The equation is first order with respect to time—meaning that the state of a system at some initial time t_0 determines its behavior for all future times.

EXAMPLE 1

Consider a particle trapped in a well with potential given by:

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$$

Show that $\psi(x,t) = A\sin(kx)\exp(iEt/\hbar)$ solves the Schrödinger equation provided that

$$E = \frac{\hbar^2 k^2}{2m}$$

SOLUTION

The potential is infinite at $x = 0$ and a, therefore the particle can never be found outside of this range. So we only need to consider the Schrödinger equation inside the well, where $V = 0$. With this condition the Schrödinger equation takes the form:

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

Setting $\Psi(x,t) = A\sin(kx)\exp(iEt/\hbar)$, we consider the left side of the Schrödinger equation first:

$$\begin{aligned} i\hbar\frac{\partial\psi(x,t)}{\partial t} &= i\hbar\frac{\partial}{\partial t}(A\sin(kx)\exp(-iEt/\hbar)) \\ &= i\hbar(-iE/\hbar)A\sin(kx)\exp(-iEt/\hbar) \\ &= E(A\sin(kx)\exp(-iEt/\hbar)) = E\psi \end{aligned}$$

Now consider the derivative with respect to x:

$$\frac{\partial}{\partial x}\psi = \frac{\partial}{\partial x}[A\sin(kx)\exp(-iEt/\hbar)] = kA\cos(kx)\exp(-iEt/\hbar)$$

$$\rightarrow -\frac{\hbar^2}{2m}\frac{\hbar^2\psi(x,t)}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}[kA\cos(kx)\exp(-iEt/\hbar)]$$

$$= -\frac{\hbar^2}{2m}[-k^2A\sin(kx)\exp(-iEt/\hbar)] = \frac{\hbar^2}{2m}k^2\psi$$

Using

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

we equate both terms, finding that:

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

And so we conclude that the Schrödinger equation is satisfied if

$$E = \frac{\hbar^2 k^2}{2m}$$