Chapter Two
Elementary Properties of Quantum Mechanics

2-1 Introduction

The failure of classical mechanics to describe the path of the atomic particle due to the uncertainty in defining its position has investigated in previous chapter. So how one can describe the motion of the atomic particle. According to De Broglie’s hypothesis and Einstein's interpretation of the Photoelectric Effect, one can say that each moving object is associates with a matter field. For example, the electron in the atom does not move far and does not approach a very short distance from the nucleus. Strictly spiking, it is confined in a small region in the atom’s space whose dimension of order 10^{-9} m, and so the associated matter field can be expressed in terms of a standing wave (the wave that is restricted in a limited region such as the wave in a wire that is bound from its two terminals). These waves are localize in this region with varying amplitude at each different point and zero outside this region. The amplitude of this matter field called the wave function.

2-2 Wave function and its interpretation

According to the last section, the wave function may define to be the amplitude of the matter field that associates with a moving particle and denoted byΨ. Wave function has a considerable importance in quantum mechanics due to the uncertainty in defining the position, and so any dynamical variable, for the atomic particle. Therefore, we needs a tool by means these dynamical variables could be determined. The tool that request this requirement is the wave function which is, in general, a complex function space (x,y,z) and time (t) and written as $\Psi(\vec{r},t)$. However, one intend that it contain a complete description of the behavior of a particle, such as an electron.

It is well known that the intensity of a wave function is proportional to the square of its own amplitude. Consequently, the intensity of the matter given by;

$$\Psi^*(x)\Psi(x) = |\Psi(x)|^2$$

The physical meaning of the last formula is that, the intensity of matter field represent the number of particle per unit length when the wave function describe more than one particle. However, when the wave function describe only one particle the intensity of the matter field represent the probability density. Probability density defined to be the probability for finding the particle per unit length at a point x, i.e.

$$P_d = |\Psi(x)|^2 \qquad \text{………..(2-1)}$$

In three dimensions;

$$P_d = |\Psi(x,y,z)|^2$$

Therefore, the probability for finding a particle (electron for example) within the volume V in atom space is;

$$P_V = \int_V |\Psi(\vec{r})|^2\, dx\, dy\, dz = \int_V |\Psi(\vec{r})|^2\, d\tau$$

Since the electron is always in the space of atoms, when the integration above is extends for all of the atom space the probability become certainty. i.e.

$$P_t = \int_V |\Psi(\vec{r})|^2\, d\tau = 1 \qquad \text{…………(2-2)}$$

Last equation called ***normalization condition*** and a wave function satisfies such formula called ***normalized*** wave function.

It is important to mention that the wave function must be;

i- **Finite** function. i.e. satisfy the normalization condition. Strictly speaking, when x goes to infinity the wave function $\Psi(x)$must be goes to zero.

ii- **Contentious** function and so its derivatives.

iii- **Single-valued** function. i.e. there is only one value for $\Psi(x)$ for each value of x.

2-3 Mathematical interpretation of wave function

Since the matter field associated with a moving particle can be expressed by standing waves, the wave function can be formulated as follows;

$$.\Psi(x,t) = \Psi(x)e^{i(\frac{2\pi}{\lambda}x-\omega t)}$$

Keeping in mind that; $k=\frac{2\pi}{\lambda}$ and $p = \hbar k$ and E=$\hbar\omega$ so;

$$\Psi(x,t) = \Psi_o e^{\frac{i}{\hbar}(p_x x - Et)} \qquad \text{…………(2-3a)}$$

In three dimensions;

$$\Psi(\vec{r},t) = \Psi_o e^{\frac{i}{\hbar}(\vec{p}.\vec{r} - Et)} \qquad \text{…………(2-3b)}$$

2.4 Derivation of Schrödinger wave equation

Schrödinger's equation in quantum mechanics has a same impact of Newton's second law in classical mechanics. However, this equation describe the physical situation of a microscopic system.

2.4.1 Time Dependent Schrödinger Equation (T.D.S.E)

In order to derive the T.D.S.E one have to starts by differentiate equation (2-3b) with respect to (x) as follows;

$$\frac{\partial\psi(x,t)}{\partial x}=\frac{\partial}{\partial x}(\psi_\circ e^{\frac{i}{\hbar}(p_x x-Et)})=\psi_\circ e^{\frac{i}{\hbar}(p_x x-Et)}(\frac{i}{\hbar}p_x)$$

So;

$$\frac{\partial\psi(x,t)}{\partial x}=\frac{i}{\hbar}p_x\psi(x,t)$$

By multiple both sides of the last equation by $-i\hbar$, one get

$$-i\hbar\frac{\partial\psi(x,t)}{\partial x}=p_x\psi(x,t) \qquad \text{…………(2-4)}$$

When equation (2-4) is differentiate with respect to (x), the following expression can be obtained;

$$-\hbar^2\frac{\partial^2\psi(x,t)}{\partial x^2}=p_x^2\psi(x,t) \qquad \text{…………(2-5)}$$

Now differentiate equation (2-4) with respect to (t), one get;

$$\frac{\partial\psi(x,t)}{\partial t}=\frac{\partial}{\partial t}(\psi_\circ e^{\frac{i}{\hbar}(p_x x-Et)})=\psi_\circ e^{\frac{i}{\hbar}(p_x x-Et)}(-\frac{i}{\hbar}E)$$

Or,

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

Multiple both sides of last equation by $-i\hbar$ one get;

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=E\psi(x,t) \qquad \text{…………(2-6)}$$

Since, $E=T+V$ or; $E=\frac{P^2}{2m}+V(x)$ so the multiplication of both sides of last formula by $\psi(x,t)$ leads to;

$$E\psi(x,t)=\frac{P^2\psi(x,t)}{2m}+V(x)\psi(x,t) \qquad \text{...........(2-7)}$$

Substituting (2-5) and (2-6) into (2-7) gives:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t) \qquad \text{...........(2-8)}$$

Equation (2-8) called time dependent Schrödinger equation, which take the following form in three dimensions;

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

2.4.2 Time Independent Schrödinger Equation (T.I.S.E)

To find a time-independent Schrödinger equation, the general form of standing waves represented by equation (2-3b) can written as follows;

$$\psi(x,t)=\psi_\circ e^{\frac{i}{\hbar}(p_x x-Et)} \quad \text{.....(2-9)} \qquad \psi(x,t)=e^{\frac{-i}{\hbar}Et}\psi(x)==\psi(t)\,\psi(x)$$

By substituted equation (2-9) in (2-8) we get :

$$i\hbar\cdot(\frac{-i}{\hbar})E\psi(x)\,e^{-\frac{i}{\hbar}Et}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\,e^{-\frac{i}{\hbar}Et}+V(x)\,\psi(x)\,e^{-\frac{i}{\hbar}Et}$$

Or;

$$[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)]\,\psi(x)=E\psi(x) \qquad \text{...........(2-10)}$$

Last equation called T.I.S.E which in three dimensions becomes;

$$\nabla^2\psi(r)+\frac{2m}{\hbar^2}[E-V(r)]\cdot\psi(r)=0$$