Chapter Three
Simplified quantum systems

3.1 Introduction

The present and the following chapters deals with applications of the quantum mechanics rules mentioned in last chapter for different systems. Indeed, this analysis are set such that, the considered systems are gradually regarded from simple to complicate. In this chapter a simplified system that manely concrencs with a free particle are investigated.

3.2 Free particle

Free particle defined as that particle which moves free from a constraint force, which means it has not bound by an external force or equivalently moves in a region where its potential energy is vanished. However, such definition implies that this particle should have a constant velocity. Therefore, free particle that has zero potential energy ($V(x) = 0$) is the simplest system that can consider in quantum mechanics. Consequently, Schrödinger equation (2-10) for this system becomes;

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

Considering that, $k^2 = \frac{2mE}{\hbar^2}$, this equation can be written as follows;

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \qquad \text{…………..(3-1)}$$

Since equation (3-1) is a seconed order, linear and homogenous differential equation, its admits a special solution of the forms;

$$\psi(x) = e^{ikx} \qquad \text{…………..(3-2)}$$

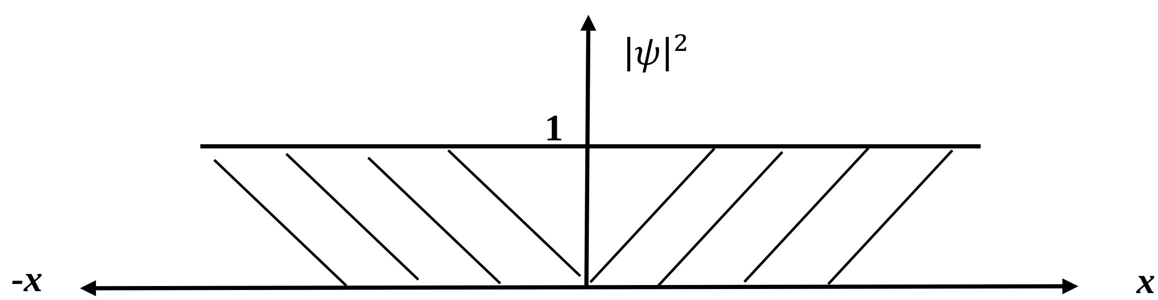
and;

$$\psi(x) = e^{-ikx} \qquad \text{.............(3-3)}$$

Equation (3-2) represent the wave function that describe the free particle that has momentum $\hbar k$ and energy $(\frac{\hbar^2 k^2}{2m})$ and moves along the positive direction of the *x*-axis. While equation (3-3) represent the wave function that describe the free particle that has a same momentum and energy and moves along the negative direction of the *x*-axis. The general solution of equation (3-1) is a linrear combination of the two solutions (3-2) and (3-3). i.e,

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{.............(3-4)}$$

Where, *A* and *B* are two arbitrary constants. The probability density for a free particle is similar at any point along the coordinate-x. i.e, $|\psi|^2 = \psi^*\psi = 1$, see the figure below. In other word, the wave function $\psi = e^{\mp ikx}$describe the situation in which we have a complete uncertinity about position. This is in agreement with the uncertainty principle because the wave function $\psi = e^{\mp ikx}$ describe a particle whose momentum is pricsely known ($p = \hbar k$), hence we exactly know that; $\Delta p = 0$ which require that $\Delta x = \infty$.



Example: By using the uncertainty Principle show that the variance in defining the position of a free particle is infinite.

Solution:

$$\Delta p \, \Delta x \geq \hbar$$

$\because \; p_x = \hbar k$ For free particle

$$\therefore \; \Delta p_x = 0$$

$$\therefore \; \Delta x \geq \frac{\hbar}{\Delta p} = \frac{\hbar}{\text{zero}} = \infty$$

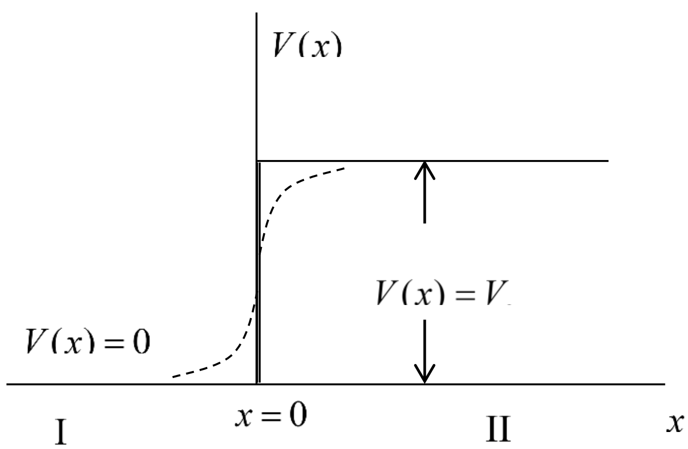
$$\therefore \; \Delta x = \infty$$

3-3 Potential step (barrier)

Let's here try to find the energy and wave function for a particle moves in a potential varies as follows;

$$V(x) = \begin{cases} zero, & x < 0 \qquad region\ I \\ V_o & x \geq 0 \qquad region\ II \end{cases}$$

Or graphically;



It should be mention that, the step potential argued above is an approximated case for the dashed curve in the last figure, where free electrons in metals suffer from. However, the reason behind such an approximation is to get simplifying the mathematical procedure. Here we will investigate the cases where the energy of the incident particle is less and greater than the potential step respectively.

a) $E < V_\circ$

In sense of classical mechanics, this region considered to forbidden for the particle to be in because it has a kinetic energy less than the potential of the step. Anyway, the situation is differs in quantum mechanics, as we shall see. Schrodinger equation (2-10) can be written as follows;

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V(\hat{x})\right)\psi = 0 \qquad \text{…………..(3-5)}$$

i)Region-I.

For this region Schrodinger equation (3-5) becomes;

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{…………..(3-6)}$$

Where $k^2 = \frac{2mE}{\hbar^2}$. The general solution of the such equation is given by;

$$\psi_1(x) = \overrightarrow{Ae^{ikx}} + \overleftarrow{Be^{-ikx}} \qquad \text{…………..(3-7)}$$

Where Ae^{ikx} is the wave function for the incident particle and Be^{-ikx} is its counterpart for the reflected one.

ii)Region-II

Schrödinger equation (3-5) for this region converts to;

$$\frac{d^2\psi_2}{dx^2} - \alpha^2\psi_2 = 0 \qquad \text{…………..(3-8)}$$

Where $\alpha^2 = \frac{2m}{\hbar^2}(V_\circ - E)$. The general solution for this equation is;

$$\psi_2(x) = Ce^{-\alpha x} + De^{+\alpha x} \qquad \text{…………..(3-9)}$$

The second term in the last equation must be neglegted due to tow reasons, the first one is the finite condition and second one is that there is no reason make the penetrated particle to rfleted back. Hence, equation (3-9) becomes;

$$\psi_2(x) = Ce^{-\alpha x} \qquad \text{…………..(3-10)}$$

The fact that ψ_2 not equal to zero means that there is a certain probability for the particle to be exsist in this region, altough it being forbidden region in sense of classical mechanics. Furthermore, this probability get rise decreases as the particle going deeply in this region. In order to find the constants A, B, C we must start applying the continuity condition for the wave function and its first drifitive at x = 0 as follows;

1. $\psi_1(x=0)=\psi_2(x=0)$
2. $\left.\frac{d\psi_1}{dx}\right|_{x=0}=\left.\frac{d\psi_2}{dx}\right|_{x=0}$

Therefore, from the first condition we have;

$$A+B=C$$

Howevere from the second one get;

$$ik(A-B)=-\alpha\ C$$

This leads to;

H.W $C=\left(\frac{2ik}{ik-\alpha}\right)A \quad , \quad B=\left(\frac{ik+\alpha}{ik-\alpha}\right)A$

So equations (3-7) and (3-10) becomes;

$$\psi_1(x)=\frac{A}{ik-\alpha}\left\{(ik-\alpha)\ e^{ikx}+(ik+\alpha)\ e^{-ikx}\right\} \qquad \text{.............(3-11)}$$

$$\psi_2(x)=\frac{2ikA}{ik-\alpha}\ e^{-\alpha x} \qquad \text{.............(3-12)}$$

If we consider that $|A|^2$ is the intensity of the incident wave function then $|B|^2$ is the intensity of the reflected wave function, which is given as;

$$|B|^2=B^*\cdot B=\left(\frac{-ik+\alpha}{-ik-\alpha}\right)\cdot\left(\frac{ik+\alpha}{ik-\alpha}\right)\cdot A^*\cdot A$$

$$|B|^2 = B^* \cdot B = \left(\frac{-ik+\alpha}{-ik-\alpha}\right)\cdot\left(\frac{-(-ik-\alpha)}{-(-ik+\alpha)}\right)\cdot A^* \cdot A$$

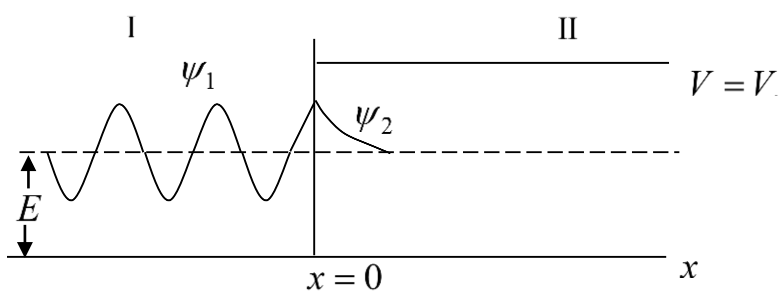
$$|B|^2 = |A|^2$$

Therefore, the intensity of the incident wave function is equal to the intensity of the reflected one. The physical meaning of this result is that all of the incident particles that reach the potential barrier (potential step) when $E < V_\circ$ are reflected back including those that penetrate the region II. Anyway, the using of Euler's theorem can leads to rewrite equation (3-11) to be as follows;

$$\psi_1(x) = \frac{2ikA}{ik-\alpha}(\cos kx - \frac{\alpha}{k}\sin kx) \qquad \text{.............(3-13)}$$

$$\psi_2(x) = \frac{2ikA}{ik-\alpha}\, e^{-\alpha x} \qquad \text{.............(3-12)}$$

By neglect the constant $\frac{2ik}{ik-\alpha}$, the last two equations can be drawn as follows.



Now as the value of potential step $V_\circ$ increases the value of α increases too and so for very high values of $V_\circ$, the last two equations becomes;

$$\psi_1(x) = 2iA\, sinkx \approx sinkx \qquad \text{.............(3-14)}$$

$$\psi_1(x) = 0 \qquad \text{.............(3-15)}$$

Indeed, this mean that no particle can be penetrate region-II for this case and hence all of the incident particle being reflects back at x=0.

b) $E > V_\circ$

For such a case the results of classical physics include that all of the incident particle are going through the region-II. But a result of Q.M. shows different outcomes as the following section reveals.

i) Region-I

Schrodinger equation in this region takes the following form;

$$\frac{d^2\psi_1(x)}{dx^2} + k^2\psi_1(x) = 0 \qquad \text{………….(3-16)}$$

Where k is expressed as; $k^2 = \frac{2mE}{\hbar^2}$, and the solution of equation (3-16) is given by;

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{………….(3-17)}$$

The presence of the second term in the last formula refers to there some particles are reflects back at x=0.

ii) Region-II

Schrödinger equation in this region must take the form;

$$\frac{d^2\psi_2}{dx^2} + k'^2\psi_2 = 0 \qquad \text{………….(3-18)}$$

Where $k'^2 = \frac{2m}{\hbar^2}(E - V_\circ)$, and the solution for this equation given by;

$$\psi_2(x) = Ce^{ik'x} + De^{-ik'x} \qquad \text{………….(3-19)}$$

The second term must be neglected because there are no reason makes the particle to reflecting back towards the negative part of x-axis. Therefore;

$$\psi_2(x) = Ce^{ik'x} \qquad \text{………….(3-20)}$$

In order to evaluates the constants A, B and C we have to making use continuity condition for the wave function and its derivatives at x=0 as shown below.

1. $\psi_1(x=0) = \psi_2(x=0)$, this leads to; $A + B = C$

2. $\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$, this leads to; $k(A-B) = k'C$

Consequently, from the two conditions we get;

H.W: $C = \left(\frac{2k}{k'+k}\right)A$, $B = \left(\frac{k'-k}{k'+k}\right)A$

Example: Determine the reflection and transmission coefficients of the potential step for the case $E > V_\circ$.

Solution:

Let us define the following quantities; $v = \frac{p}{m} = \hbar k/m$ is the particle velocity in the region-I. $|A|^2$is the intensity of the incident beam of particle (or intensity of the incident particles, i.e. the number or particles per unit volume). $v|A|^2$ is the flux of the incident beam (the number of particles that passes from unit area per unit time). $\acute{v} = \frac{\acute{p}}{m} = \hbar\acute{k}/m$ is the velocity of the particles in region-II, $|B|^2$ is the intensity of the reflected beam of particle, $\acute{v}|B|^2$ is the flux of the reflected beam and $\acute{v}|C|^2$ is the flux of the transmitted beam.

Therefore, the reflection and transmission coefficients can be set up such that;

$$R = \frac{v|B|^2}{v|A|^2} = \left(\frac{k-\acute{k}}{k+\acute{k}}\right)^2 \qquad \text{.............(3-21)}$$

$$T = \frac{\acute{v}|C|^2}{v|A|^2} = \frac{4k\acute{k}}{\left(k+\acute{k}\right)^2} \qquad \text{.............(3-22)}$$

H.W: Show that the law of conservation of mass is satisfied for the above example. i.e. *R*+*T*=1.