

3. Schrödinger's Equation-II

Applications of Schrödinger's Equation

1. Introduction

Though, Schrödinger's equation has its limitations that we shall discuss later, the applications of Schrödinger's equation are many. For the present discussion we consider the following prominent applications of Schrödinger's equation: (i) the case of step potential; (ii) the case of potential barrier; (or analogous to infinitely deep potential well); and (iii) Sommerfeld's model of free electron gas. We would discuss other applications of Schrödinger's equation including its application to understand the 'Hydrogen atom' later in relevant spell of lectures.

2. Schrödinger's Equation and the Problem of Step Potential

The case of 'step potential' is a one-dimensional problem. To be precise it could be defined as a problem wherein an object or a particle is moving along X – axis and it suddenly finds an obstacle that we call a step barrier whose potential height is greater than the energy of the particle. We can picturize this problem schematically as follows:

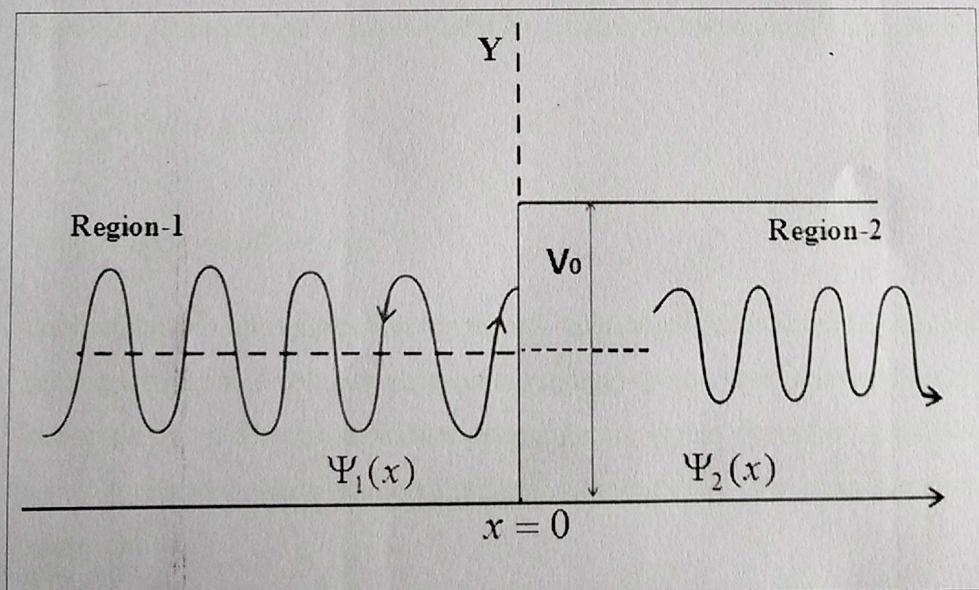


Fig. 3.1: A step potential barrier with potential height $V = V_0$.

Let's consider Schrödinger's equation for this one dimensional case in the region-I and II as:

$$\text{Region - I : } \frac{\partial \Psi_1(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \Psi_1(x) = 0; \quad (3.1)$$

$$\text{where, } \sqrt{\frac{8\pi^2 m}{h^2} E} = k_1 \text{ (let).} \quad (3.2)$$

$$\text{Region - II : } \frac{\partial \Psi_2(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V_0) \Psi_2(x) = 0; \quad (3.3)$$

$$\text{where, } \sqrt{\frac{8\pi^2 m}{h^2} (E - V_0)} = k_2 \text{ (let).} \quad (3.4)$$

Thus, Schrödinger's equation and its solution for the region-I are given as:

$$\frac{\partial \Psi_1(x)}{\partial x^2} + k_1^2 \Psi_1(x) = 0, \quad (3.5)$$

$$\text{with, } \Psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}; \quad (3.6)$$

here, the first term in this expression represents incident or the forward moving modes whereas the second term in this solution represents rebound or the back scattered modes.

Similarly, Schrödinger's equation and its solution for the region-II are given as:

$$\frac{\partial \Psi_2(x)}{\partial x^2} + k_2^2 \Psi_2(x) = 0, \quad (3.7)$$

$$\text{with, } \Psi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}; \quad (3.8)$$

the first term in this expression represents incident or the forward moving modes whereas the second term in this solution represents rebound or the back scattered modes. However, one can argue that if there is no further obstruction or barrier the state function need not have any term representing back scattered modes. Consequently, the state function in the region-II simplifies to:

$$\Psi_2(x) \cong A_2 e^{ik_2 x}. \quad (3.9)$$

In order to investigate that the particle remains in the region-I or transmits in the region-II we determine the probability of rebound or reflection R and the transmission T . In various descriptions R is referred as reflectance or coefficient of reflection and T is referred as transmittance or coefficient the transmission. To determine R and T , we discuss the Schrödinger's current in the two regions as follows:

$$\text{Region - I : } J_I = -\frac{i\hbar}{2m} \left(\Psi_1^* \nabla \Psi_1 - \nabla \Psi_1^* \Psi_1 \right) = -\frac{i\hbar}{2m} \left(\Psi_1^* \frac{\partial \Psi_1}{\partial x} - \frac{\partial \Psi_1^*}{\partial x} \Psi_1 \right); \quad (3.10)$$

and

$$\text{Region - II : } J_{II} = -\frac{i\hbar}{2m} \left(\Psi_2^* \nabla \Psi_2 - \nabla \Psi_2^* \Psi_2 \right) = -\frac{i\hbar}{2m} \left(\Psi_2^* \frac{\partial \Psi_2}{\partial x} - \frac{\partial \Psi_2^*}{\partial x} \Psi_2 \right). \quad (3.11)$$

Eq. (3.10) upon simplification gives us:

$$J_I = \frac{\hbar k_1}{m} \left(A_1^* A_1 - B_1^* B_1 \right) = J_{I+} + J_{I-} \text{ (let)}; \quad (3.12)$$

where, we identify the forward moving current J_{I+} and reflected current J_{I-} as:

$$\left. \begin{aligned} J_{I+} &= \frac{\hbar k_1}{m} \left(A_1^* A_1 \right) = \frac{\hbar k_1}{m} |A|^2, \\ \text{and} \\ J_{I-} &= \frac{\hbar k_1}{m} \left(B_1^* B_1 \right) = \frac{\hbar k_1}{m} |B|^2. \end{aligned} \right\} \quad (3.13)$$

Similarly, Eq. (3.11) upon simplification gives us:

$$J_{II} = \frac{\hbar k_2}{m} \left(A_2^* A_2 \right) = J_{II+}; \quad (3.14)$$

Where, we note that the current in the region-II has only forward moving component J_{II+} .

We no deduce the probability of reflection R as:

$$R = \frac{J_{I-}}{J_{I+}} = \frac{|B_1|^2}{|A_1|^2}; \quad (3.15)$$

and similarly, the probability of transmission T as:

$$T = \frac{J_{II+}}{J_{I+}} = \frac{k_2 |A_2|^2}{k_1 |A_1|^2}; \quad (3.16)$$

with an overall condition that sum of the probabilities of reflection and transmission follows:

$$R + T = 1. \quad (3.17)$$

Thus, to determine R and T we need to know the ratio that is relation between B_1 and A_1 and between $v A_2$ and A_1 respectively. For this we ought to solve equations (3.8) and (3.9) analytically.

We argue that the state function in the region-II $\Psi_2(x)$ is continuity of the state function $\Psi_1(x)$ and therefore they must agree with each other at the junction $x = 0$ as:

$$\Psi_1(\text{at } x = 0) = \Psi_2(\text{at } x = 0). \quad (3.18)$$

This gives us

$$A_1 + B_1 = A_2. \quad (3.19)$$

Similarly, we argue that as the state function is differentiable too, the derivatives of the two state functions should also agree with each other at the junction $x = 0$ as:

$$\left. \frac{\partial \Psi_1}{\partial x} \right|_{\text{at } x=0} = \left. \frac{\partial \Psi_2}{\partial x} \right|_{\text{at } x=0}; \quad (3.20)$$

such that

$$ik_1 A_1 - ik_1 B_1 = ik_2 A_2. \quad (3.21)$$

Thus, by solving eq. (3.19) and (3.21) we get

$$\left. \begin{aligned} \frac{B_1}{A_1} &= \frac{k_1 - k_2}{k_1 + k_2}, \\ \text{and} \\ \frac{A_3}{A_1} &= \frac{2k_1}{k_1 + k_2}.. \end{aligned} \right\} \quad (3.22)$$

Hence, the transmission and the reflection probabilities are found as:

$$\left. \begin{aligned} R = \left| \frac{B_1}{A_1} \right|^2 &= \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2, \\ \text{and} \\ T = \frac{k_2}{k_1} \left| \frac{A_2}{A_1} \right|^2 &= \frac{2k_1 k_2}{|k_1 + k_2|^2}. \end{aligned} \right\} \quad (3.23)$$

One can easily verify that, $R + T = 1$.

3. Schrödinger's Equation and the Problem of Barrier Potential

The case of 'barrier potential' is also one-dimensional problem. It could be defined as a problem wherein an object or a particle is moving along X -axis and it suddenly finds an obstacle that rectangular barrier whose potential height is greater than the energy of the particle. We can picturize this problem schematically as follows:

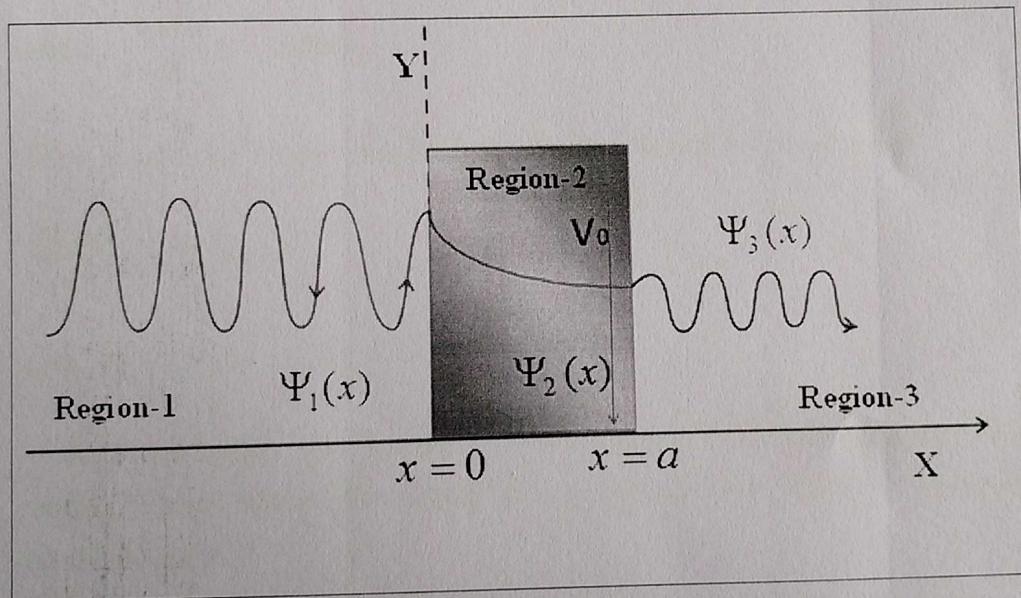


Fig. 3.2: Transmission through a barrier.

Let's consider Schrödinger's equation for this 1dimensional case in the regions-I, II and III as:

$$\text{Region - I: } \frac{\partial^2 \Psi_1(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \Psi_1(x) = 0; \quad (3.24)$$

$$\text{where, } \sqrt{\frac{8\pi^2 m}{h^2}} E = k_1 (\text{let}) . \quad (3.25)$$

$$\text{Region - II : } \frac{\partial \Psi_2(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V_0) \Psi_2(x) = 0 . \quad (3.26)$$

Now, if $V_0 > E$ in the region-II, we find that Schrödinger's equation suitably modifies to

$$\frac{\partial \Psi_2(x)}{\partial x^2} - \frac{8\pi^2 m}{h^2} (V_0 - E) \Psi_2(x) = 0 ; \quad (3.27)$$

$$\text{where, } \sqrt{\frac{8\pi^2 m}{h^2}} (V_0 - E) = k_2 (\text{let}) . \quad (3.28)$$

$$\text{Region - III : } \frac{\partial \Psi_3(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} E \Psi_3(x) = 0 ; \quad (3.29)$$

$$\text{where, } \sqrt{\frac{8\pi^2 m}{h^2}} E = k_1 (\text{let}) . \quad (3.30)$$

Thus, Schrödinger's equation and its solution for the region-I are given as:

$$\frac{\partial \Psi_1(x)}{\partial x^2} + k_1^2 \Psi_1(x) = 0 , \quad (3.31)$$

$$\text{with, } \Psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} ; \quad (3.32)$$

as discussed earlier, the first term in this expression represents incident or the forward moving modes whereas the second term in this solution represents rebound or the back scattered modes.

Similarly, Schrödinger's equation and its solution for the region-II are given as:

$$\frac{\partial \Psi_2(x)}{\partial x^2} - k_2^2 \Psi_2(x) = 0 , \quad (3.33)$$

$$\text{with, } \Psi_2(x) = A_2 e^{k_2 x} + B_2 e^{-k_2 x} . \quad (3.34)$$

Let us note that the solution of the Schrödinger's equation is real for the region-II.

Similarly, Schrödinger's equation and its solution for the region-III are given as:

$$\frac{\partial \Psi_3(x)}{\partial x^2} - k_1^2 \Psi_3(x) = 0, \quad (3.35)$$

$$\text{with, } \Psi_3(x) = A_3 e^{ik_1 x} + B_3 e^{-ik_1 x}. \quad (3.36)$$

We now argue that if there is no further obstruction or barrier the state function need not have any term representing back scattered modes in the region-III. So that the state function in the region-III simplifies to:

$$\Psi_3(x) \equiv A_3 e^{ik_1 x}. \quad (3.37)$$

Transmission and reflection probabilities could be given by:

$$\left. \begin{aligned} R &= \frac{J_{I-}}{J_{I+}} = \left| \frac{B_1}{A_1} \right|^2, \\ \text{and} \\ T &= \frac{J_{III+}}{J_{I+}} = \left| \frac{A_3}{A_1} \right|^2. \end{aligned} \right\} \quad (3.38)$$

In order to determine the transmission probability we ought to solve eq. (3.32), (3.34) and (3.37) and ascertain the information about the ratio $\frac{A_3}{A_1}$.

As discussed earlier we argue that the state function in the region-II $\Psi_2(x)$ is continuity of the state function $\Psi_1(x)$ and therefore they must agree with each other at the junction $x = 0$ as $\Psi_1(\text{at } x = 0) = \Psi_2(\text{at } x = 0)$, which results into

$$A_1 + B_1 = A_2 + B_2. \quad (3.39)$$

Similarly, if we argue that as the state function is differentiable too, the derivatives of the two state functions should also agree with each other at the junction $x = 0$ as

$$\left. \frac{\partial \Psi_1}{\partial x} \right|_{\text{at } x=0} = \left. \frac{\partial \Psi_2}{\partial x} \right|_{\text{at } x=0};$$

We get

$$ik_1 A_1 - ik_1 B_1 = k_2 A_2 - k_2 B_2;$$

Or,

$$A_1 - B_1 = -\frac{ik_2}{k_1} A_2 + \frac{ik_2}{k_1} k_2 B_2. \quad (3.40)$$

Also, one can argue that the state function in the region-III $\Psi_3(x)$ is continuity of the state function $\Psi_2(x)$ and therefore they must agree with each other at the junction $x = a$

as $\Psi_2(\text{at } x = a) = \Psi_3(\text{at } x = a)$, which results into

$$A_2 e^{k_2 a} + B_2 e^{-k_2 a} = A_3 e^{ik_1 a}. \quad (3.41)$$

And similarly, the derivatives of the two state functions $\Psi_2(x)$ and $\Psi_3(x)$ should also agree with each other at the junction $x = a$ as

$$\left. \frac{\partial \Psi_2}{\partial x} \right|_{\text{at } x=a} = \left. \frac{\partial \Psi_3}{\partial x} \right|_{\text{at } x=a}; \quad (3.42)$$

which gives us

$$k_2 A_2 e^{k_2 a} - k_2 B_2 e^{-k_2 a} = ik_1 A_3 e^{ik_1 a}. \quad (3.43)$$

Solving equations (3.39), (3.40), (3.41) and (3.43) would help us arriving at relevant probability of transmission.

When we solve (3.39) and (3.40) we get

$$\begin{aligned} A_1 &= \left(1 - \frac{ik_2}{k_1} \right) \frac{A_2}{2} + \left(1 + \frac{ik_2}{k_1} \right) \frac{B_2}{2}, \\ B_1 &= \left(1 + \frac{ik_2}{k_1} \right) \frac{A_2}{2} + \left(1 - \frac{ik_2}{k_1} \right) \frac{B_2}{2}. \end{aligned} \quad (3.44)$$

Now, if we solve (3.41) and (3.43), we get

$$\left. \begin{aligned} A_2 &= \left(1 + \frac{ik_1}{k_2} \right) \frac{A_3}{2} e^{ik_1 a} e^{-k_2 a}, \\ B_2 &= \left(1 - \frac{ik_1}{k_2} \right) \frac{A_3}{2} e^{ik_1 a} e^{+k_2 a}. \end{aligned} \right\} \quad (3.45)$$

By putting these values of A_2 and B_2 in the expressions of A_1 and B_1 in eq. (3.44) we get

$$A_1 = \left[\left(1 - \frac{ik_2}{k_1} \right) \left(1 + \frac{ik_1}{k_2} \right) e^{ik_1 a} e^{-k_2 a} + \left(1 + \frac{ik_2}{k_1} \right) \left(1 - \frac{ik_1}{k_2} \right) e^{ik_1 a} e^{+k_2 a} \right] \frac{A_3}{4}; \quad (3.46)$$

and,

$$B_1 = \left[\left(1 + \frac{ik_2}{k_1} \right) \left(1 + \frac{ik_1}{k_2} \right) e^{ik_1 a} e^{-k_2 a} + \left(1 - \frac{ik_2}{k_1} \right) \left(1 - \frac{ik_1}{k_2} \right) e^{ik_1 a} e^{+k_2 a} \right] \frac{A_3}{4}. \quad (3.47)$$

In order to know the transmission probability, we obtain an expression of $\frac{A_3}{A_1}$ from eq. (3.46)

as:

$$\frac{A_3}{A_1} = \frac{4e^{-ik_1 a}}{\left[\left(1 - \frac{ik_2}{k_1} \right) \left(1 + \frac{ik_1}{k_2} \right) e^{-k_2 a} + \left(1 + \frac{ik_2}{k_1} \right) \left(1 - \frac{ik_1}{k_2} \right) e^{+k_2 a} \right]}. \quad (3.46)$$

Similarly, know the reflection probability, we divide eq. (3.47) by eq. (3.46) and obtain an

expression of $\frac{B_1}{A_1}$. Eq. (3.46) upon simplification gives

$$\frac{A_3}{A_1} = \frac{4e^{ik_1 a} e^{-k_2 a}}{\left[\left\{ 2 - i \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \right\} e^{-2k_2 a} + \left\{ 2 + i \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \right\} \right]}; \quad (3.47)$$

Or, upon approximation

$$\frac{A_3}{A_1} \cong \frac{4e^{ik_1 a} e^{-k_2 a}}{\left[\left\{ 2 - i \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \right\} + \left\{ 2 + i \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \right\} \right]} \cong e^{ik_1 a} e^{-k_2 a}. \quad (3.48)$$

Hence, transmission probability implies:

$$T = \left| \frac{A_3}{A_1} \right|^2 \cong e^{-2k_2 a} = e^{-2\left(\sqrt{\frac{8\pi^2 m(V_0 - m)}{h^2}}\right)a} \quad (3.49)$$

Which decreases with passage in space, but, it is- *surely non-zero.*

3.1. The Case of α Decay and Tunnel Effect

Let us consider the phenomenon of emission of α particles from the nucleus of Uranium U_{92}^{238} atom. The potential height of the well of Nucleus is $\sim 26 \text{ MeV}$ i.e. α particle needs energy greater than or equal to 26 MeV . Whereas, the energy of the α particle in Uranium nucleus is only $\sim 4 - 6 \text{ eV}$. Logically, the α particle could never come out of the nucleus. But, emission of α particles from nucleus is a reality. This phenomenon could be understood only by means of "tunnel effect".

We can understand the phenomenon of α particle emission schematically as follows:

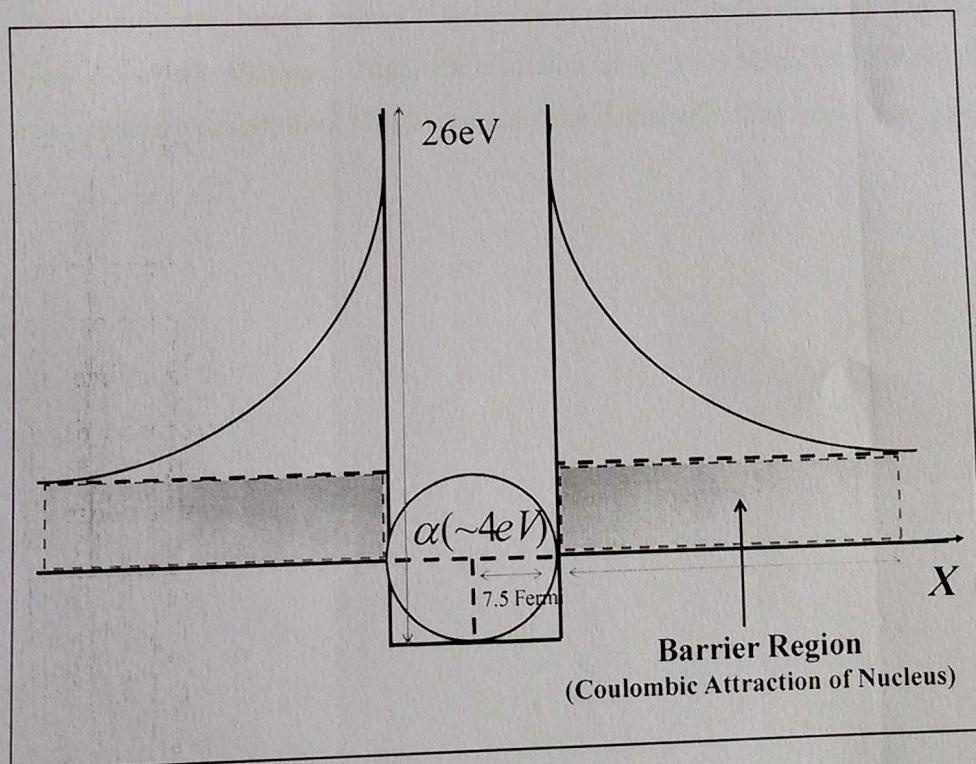


Fig. 3.3: Schematic representation of α particle emission from nucleus.

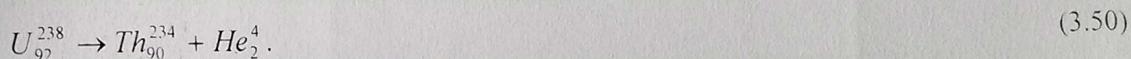
The quantum mechanical probability of transmission of Alpha particle through the nucleus is non-zero. This could not be explained by *Classical Mechanics*.

Remark: Let us understand that the barrier is not made of any hard stuff or bricks and boulders. In fact, this barrier is empty region! And yet, a particle finds it hard to penetrate this region. The barrier region is the region wherein coulombic attraction of the nucleus pulls the particle inward and does not let it escape.

The probability of transmission of α particle from the nucleus is given by the expression of transmittance of 'tunnel effect' as follows:

$$T = e^{-2\left(\sqrt{\frac{8\pi^2 m(V_0 - m)}{h^2}}\right)a}.$$

An example of α emission could be the decay of Uranium nucleus U_{92}^{238} as follows:



The size of the nucleus of Uranium is of the order- $R = 1.2 \times (238)^{1/3} \approx 7.5$ Fermi. Whereas, the extent of the barrier region that is extent to which the coulombic attraction prevails is manifold of this distance. Thus, the emission of α particle across this region requires an extra-ordinary description. This is precisely the tunnel effect that makes α emission possible.

4. Free Electron Gas Model for Solid Metals

Free electron gas model was introduced and developed by Drude and Lorentz in the year 1900.

Sömmersfeld made a significant contribution to the 'free electron gas model' that led to successful explanation of 'conductivity and mobility' of electrons and this finally led to the idea of Fermi energy and its application to the 'band theory of semiconductors'.

Free electron model is based on certain presumptions that we may call postulates too, are as follows:

- (i) The mutual repulsion amongst electrons is almost non-existent.
- (ii) Electrons vital for conduction (also valence electrons) are assumed to be free to move anywhere within the specimen with no change in their energy.
- (iii) The (electric) field potential representing the attractive interaction of ions is assumed to be completely uniform everywhere inside the crystal.

As an approximation, potential energy is neglected and the total energy of conduction electrons is thus assumed to be kinetic energy only.

- (iv) The potential energy of an electron inside the metal must be lower than that of an electron outside the metal as the conduction electrons are not free to move outside of the metal at room temperature.

Remark: In a simple free electron gas model the interior of metals comprises of a gas of electrons often within a region represented by 'box comprising of potential energy with depth V_0 (say).'

4.1. Sömmersfeld's Estimation of Density of States

It incorporates application of Schrödinger's equation to the particle in a cubical box. Sömmersfeld applied the result of energy eigen-values as found in case of particle in a cubical box to approximate the number of electronic states in a soup of electrons in atom of target material. That is to say, Sömmersfeld estimated density of electronic states in an abstract space. To be more precise, Sömmersfeld estimated number of electronic states per unit energy,

per unit volume in for the given electron-gas as follows. The energy eigen-values of the particle in a cubical box with side ' a ' are given by the expression:

$$E = \frac{n^2 h^2}{8ma^2} \quad (3.51)$$

Where,

$$n_x^2 + n_y^2 + n_z^2 = n^2 \quad (3.52)$$

This is equation of a sphere in n -space i.e. an abstract number space spanned by parameters n_x, n_y , and n_z . Let us consider a sphere in the n -space as follows:

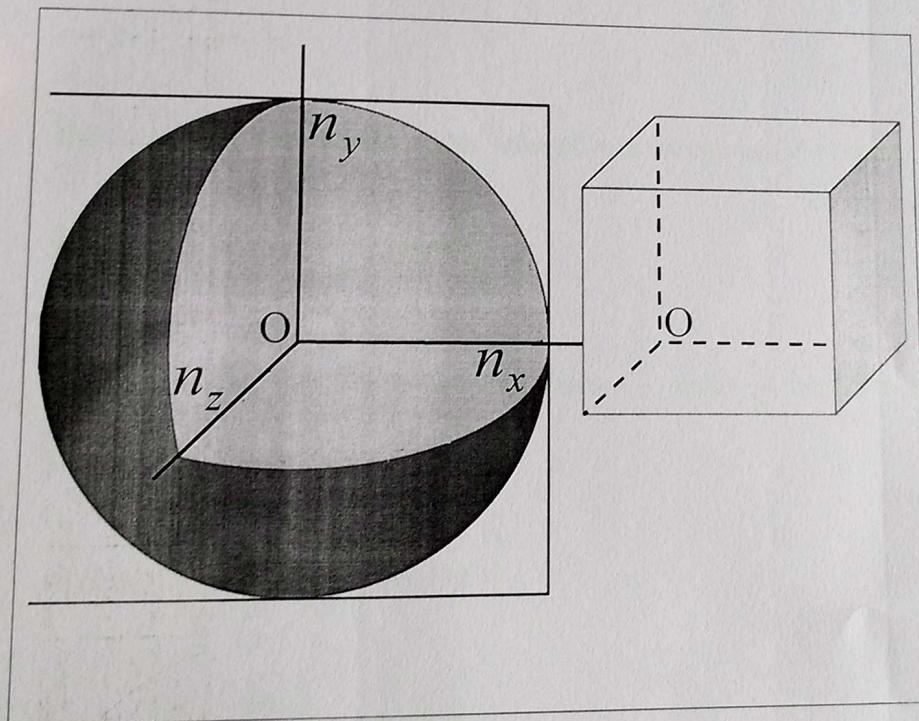


Fig. 3.4: Sömmerfeld's model of octant of a sphere in n -space by a cube.

The space created by the cut out octant of the sphere is replaced by a cube with side equal to radius of the sphere such that the corner O of the cube coincide with the centre O of the sphere and the three orthogonal sides with corner at O coincide maximally with the three flat surfaces of the left over sphere.

The volume of a sphere in n -space could be given as:

$$Vol.(= N) = \frac{4}{3} \pi n^3. \quad (3.53)$$

This is volume of a sphere in the notional sense, otherwise, it is a unitless (dimensionless) quantity in the physical sense. Thus, it is just a number, which we say, represents number of states.

Thus, to estimate the number of states in a region equivalent to octant of this sphere, we ought to consider one-eighth of this volume i.e. $\frac{1}{8} \left(\frac{4}{3} \pi n^3 \right)$.

Where, value of n could be substituted from eq. (3.51) as:

$$n = 2\sqrt{2} \left(\frac{a}{h} \right) (mE)^{\frac{1}{2}}. \quad (3.54)$$

Therefore, upon substitution of this value of n in the expression of number of states, we get

$$N(E) = \frac{1}{8} \left(\frac{4}{3} \pi \left(16\sqrt{2} \left(\frac{a}{h} \right)^3 (mE)^{\frac{3}{2}} \right) \right). \quad (3.55)$$

Since, an electron can live in two spin states $+\frac{1}{2}$ and $-\frac{1}{2}$, we double the number of states $N(E)$ as:

$$N(E) = 2 \left(\frac{1}{8} \right) \frac{64\sqrt{2}}{3} \pi \left(\frac{a}{h} \right)^3 (m)^{\frac{3}{2}} (E)^{\frac{3}{2}}. \quad (3.56)$$

$$g(E) = \frac{N(E)}{a^3} = \frac{16\sqrt{2}}{3h^3} \pi (m)^{\frac{3}{2}} (E)^{\frac{3}{2}}. \quad (3.57)$$

But, this function represents only number of states that correspond to energy E . We thus, first estimate the number of states in the energy range $E + dE$.

We now differentiate this expression with respect to energy E and reparametrize as:

$$Z = \frac{dg(E)}{dE} \left(= \frac{1}{a^3} \frac{dN(E)}{dE} \right) = \frac{8\sqrt{2}}{h^3} \pi (m)^{\frac{3}{2}} (E)^{\frac{1}{2}}. \quad (3.58)$$

This function represents number of electronic states per unit energy per unit volume and truly qualifies to be a function representing density of states. This is with the reason that later we can estimate number of states corresponding to any energy and in any energy range. We can also write the expression in (3.58) as:

$$Z = CE^{\frac{1}{2}} ; \text{ where, } C = \frac{8\sqrt{2}}{h^3} \pi(m)^{\frac{3}{2}}. \quad (3.59)$$

This expression in the eq. (3.59) is geometrically a parabola as depicted in fig. 3.5.

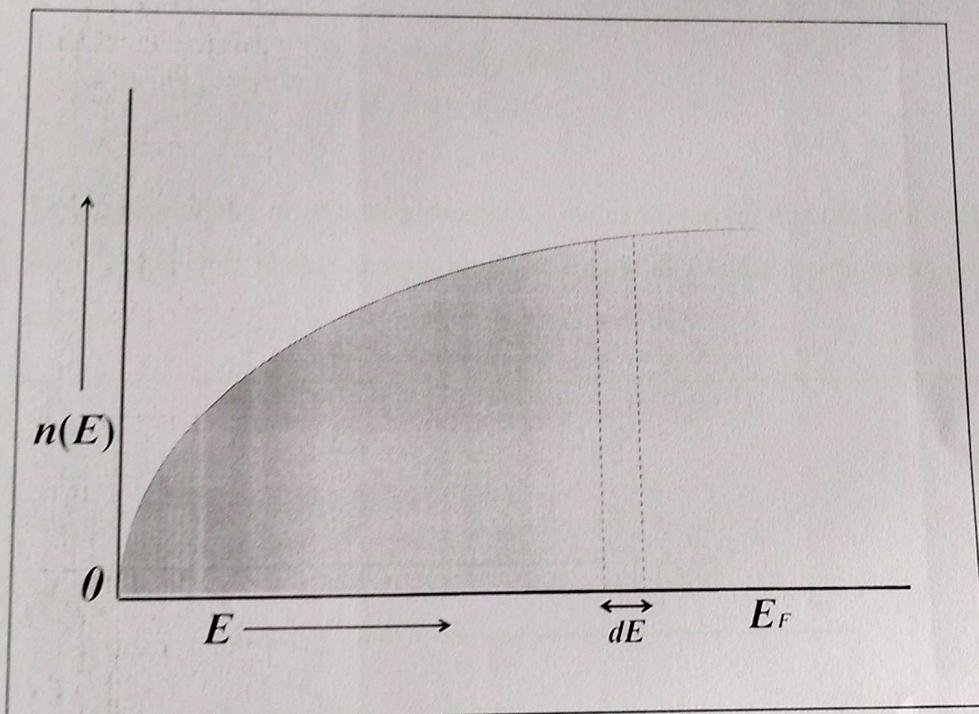


Fig. 3.5: The number of states as function of energy depicting Fermi energy level.

We now briefly discuss the idea of Fermi energy distribution function and accommodate it in the Sömmersfeld's estimation of density of (electronic) states as it imperative for all those particles that obey 'Pauli's exclusion principle' and hence 'Fermi-Dirac Statistics.'

4.2. Fermi energy distribution function

Let us consider the particle distribution function with energy, called the Fermi distribution function or Fermi-Dirac distribution function meant for those particles that obey Fermi-Dirac Statistics *i.e.* particles that obey Pauli's exclusion principle.

$$f(E) = \frac{1}{e^{\left(\frac{E-E_F}{kT}\right)} + 1}. \quad (3.60)$$

We briefly analyze this Fermi distribution function. Let us examine this distribution function in the limit when $T \approx 0$;

$$f(E) = \frac{1}{e^{\left(\frac{E-E_F}{kT}\right)} + 1} = \begin{cases} 1, & \text{if } E \ll E_F; \text{and} \\ 0, & \text{if } E \gg E_F. \end{cases} \quad (3.61)$$

This is like behavior of a step-function. One can interpret this result as follows: All states are filled below the Fermi energy level, whereas, above the Fermi energy level all states are empty.

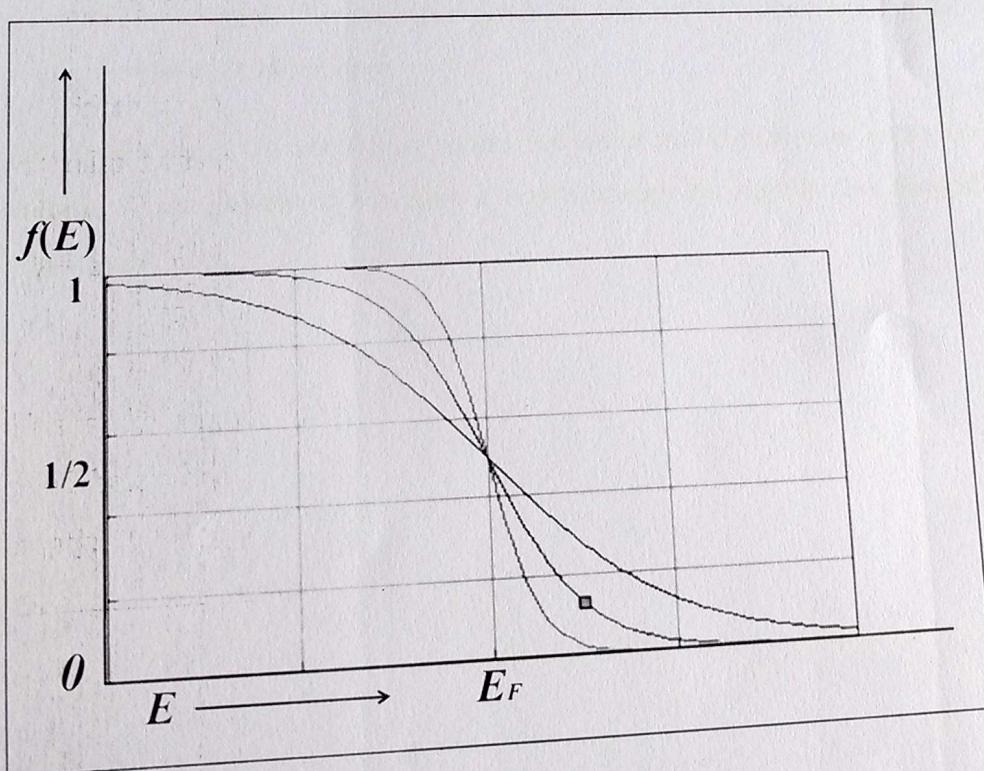


Fig. 3.6: Fermi energy distribution function as function of energy.
Also, when the temperature is $T \neq 0$, and significantly high; and if $E = E_F$,

$$f(E_F) = \frac{1}{e^{\frac{E_F}{kT}} + 1} = \frac{1}{2}. \quad (3.62)$$

We thus evaluate the number (density) of states in the limit $0 \leq E \leq E_F$ as follows:

$$n_F = \left(\frac{8\sqrt{2}}{h^3} \pi m^{\frac{3}{2}} \right) \int_0^{E_F} dE f(E) E^{\frac{1}{2}} = \left(\frac{8\sqrt{2}}{h^3} \pi m^{\frac{3}{2}} \right) \int_0^{E_F} dE E^{\frac{1}{2}} \left(\frac{1}{e^{\left(\frac{E-E_F}{kT}\right)} + 1} \right). \quad (3.63)$$

Sömmersfeld estimated density of electronic states that proved to be very useful. This has been successfully applied to determine electrical conductivity and mobility and also to describe band theory and semi-conductor Physics.

Remarks:

- (i) One might wonder how precisely an octant of a sphere can be represented by a cubical box comprising of electrons? Frankly speaking, it does very well. The reason could be given as: When box containing electrons is situated in a central potential with the centre of the potential at one corner of the box, all electrons would be confined in a region like octant of the sphere within the box such that electrons tend to live within a region that at most extends up to the radius of the sphere.
- (ii) In this case, the density of states estimated would represent upper limit as the actual volume of the octant of the sphere would always be slightly less than the volume of the equivalent cube.

Exercises

Multiple choice questions:

1. Work function is the (energy) gap between
 - (a) Conduction band minimum and Fermi level
 - (b) Valence band maximum and Fermi level
 - (c) Vacuum and Fermi level
 - (d) Vacuum and conduction band minimum
- 2.

Descriptive questions

3. What is Fermi sphere?
4. What is conductor of electricity? Describe on the basis of Fermi surface?
5. Imagine the nucleus of an atom to be a cube with side ~ 1.5 Fermi . Can we determine the binding energy of a neutron with this fact? How? Analyze the remarkable proximity of this result with the realistic case.
6. Calculate Fermi energy for Iron, assuming that each Iron atom contributes one electron to the electron gas. You are given density of Iron $\rho_{Fe} = 8.94 \times 10^3$ kg/m³ and its' atomic mass number $A_{Fe} = 56$ amu .
7. For Iron, Fermi energy is 11.1 eV and the its electron density is $n_e = 17 \times 10^{28}$ per m³. Find the electron density of a metal for which Fermi energy is 14.3 eV and identify the atom.

Suggested Readings

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