

CL14\_Q1. Define the terms reflection coefficient and transmission coefficient with respect to step potential.

**Ans:**

The classical reflection coefficient 'R' is defined as the ratio of intensity reflected to intensity incident. The classical transmission coefficient 'T' is the ratio of intensity transmitted to intensity incident.

Quantum mechanically, intensity is analogous to probability density. Quantum mechanical transmission and reflection coefficients are based on probability density flux.

$$R = \frac{\text{reflected flux}}{\text{incident flux}} ; \quad T = \frac{\text{transmitted flux}}{\text{incident flux}}$$

The reflection and transmission coefficients must sum to 1 in either classical or quantum mechanical regimes. I.e.  $R+T = 1$ , the flux incident has to be partially reflected and partially transmitted.

CL14\_Q2 A stream of particles of mass  $m$  and total energy  $E$  moves towards a potential step of height  $V_0$ , if the energy of the electrons is lesser than the step potential ( $E < V_0$ ) then by applying continuity conditions obtain the expression for reflection coefficient.

**Ans:**

By solving SWE in region 1 and 2 we get

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \text{ and } \psi_2 = De^{ik_2x}$$

Continuity condition

$$\text{at } x=0, \psi_1 = \psi_2 \quad A + B = D$$

$$\text{at } x=0, \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad (A - B)k_1 = Dk_2$$

$$\text{Reflection coefficient} = \frac{B*B v1}{A*A v1}$$

$$R = \frac{(k_1 - k_2)}{(k_1 + k_2)}$$

CL14\_Q3. The probability of reflection from a potential step is given by  $\frac{(k_2-k_1)^2}{(k_2+k_1)^2}$ , where the  $k$ 's are the wavenumbers in the two regions. If a 5 eV electron encounters a 2 eV potential step, what is the probability that it will be reflected?

Ans:

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \text{ where } k_1 = \frac{\sqrt{2mE}}{\hbar} \text{ and } k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$R = \frac{(\sqrt{3}-\sqrt{1})^2}{(\sqrt{3}+\sqrt{1})^2} = 0.0716$$

We know that  $R + T = 1$  therefore  $T = 0.928$

CL15\_Q1. Explain the term penetration depth?

**Ans:** It is the distance the particle penetrates into the classically forbidden region (region of negative K.E) where the wave function drops to  $1/e$

Penetration is given by  $\Delta x = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$ , Where  $V_0$  is the depth of the potential and E is the energy state of the wave function.

The penetration depth increases as the energy of the particle increases.

CL15\_Q2. A spherical dust particle of radius  $10^{-5} m$  and density  $10^4 \text{ Kg/m}^3$ , moving at a speed of  $10^{-2} \text{ m/s}$  encounters a step potential of height equal to twice the K.E of the particle. Estimate the penetration depth of the particle inside the step.

**Ans:** Mass of the particle is  $m = \frac{4}{3}\pi r^3 \rho = 4.2 \times 10^{-11} \text{ Kg}$

K.E of the particle before impinging the barrier  $E = \frac{1}{2}mv^2 = 2.1 \times 10^{-15} \text{ J}$

Given :  $V_0 = 2K.E = 2 \times 2.1 \times 10^{-15} \text{ J}$

$$\text{penetration depth} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} = 2.5 \times 10^{-22} \text{ m}$$

CL16\_Q1. What is a quantum mechanical tunnelling? Explain its significance.

**Ans:**

Quantum tunnelling or barrier tunnelling refers to the process of transmission through a potential barrier even when the energy of the particle is lesser than the barrier potential. This plays an essential role in several physical phenomena, such as the alpha decay and the nuclear fusion that occurs in main sequence stars like the Sun. It has important applications to modern devices such as the tunnel diode, quantum computing, and the scanning tunnelling microscope.

CL16\_Q2. Interpret the wave function and its nature in the three regions of the barrier potential?

**Ans:**

The wave function in the first region is  $\psi_I(x) = Ae^{ik_I x} + Be^{-ik_I x}$ . It is oscillatory in nature

The wave function in the second region is  $\psi_{II}(x) = De^{-\alpha x}$ . It is exponentially decrease in nature

The wave function in the third region is  $\psi_{III}(x) = Ge^{ik_{III} x}$ . It is oscillatory in nature

**CL18\_Q1.** Show that the energy of an electron confined in a 1-D symmetric potential well of length 'L' and infinite depth is quantized. Is the electron trapped in a potential well allowed to take zero energy? If not, why?

**Answer**

The energy of the nth eigenstate is given by  $E_n = \frac{\hbar^2 n^2}{8mL^2}$  where  $n = 1, 2, 3, \dots$

$$\text{The Eigen values are } E_1 = \frac{\hbar^2}{8mL^2} \quad E_2 = \frac{\hbar^2 2^2}{8mL^2} \quad E_3 = \frac{\hbar^2 3^2}{8mL^2}$$

Thus, the energies are quantized with n being the quantum number. The quantization is imposed by the boundary conditions and the requirement of normalizability. All bound quantum states are in fact quantized.

For an electron trapped within a one dimensional potential well, when  $n = 0$ , the wave function is zero for all values of x, i.e., it is zero even within the potential well. This would mean that the electron is not present within the well. Therefore the state with  $n = 0$  is not allowed. As energy is proportional to  $n^2$ , the ground state energy cannot be zero since  $n = 0$  is not allowed

**CL18\_Q2.** Elaborate the concept of parity as applied to Eigen functions. When is it possible to describe the parity aspect of Eigen functions?

**Answer**

The parity of a function is determined by changing the sign of the variable. If the function remains unchanged, then it is defined as an even parity function and if the function changes sign then it is an odd parity function. If  $\psi(-x) = \psi(x)$ , then the function has an even parity and if  $\psi(-x) = -\psi(x)$ , then the function has an odd parity.

**CL18\_Q3.** Write the wave functions for the states  $n = 1$ ,  $n = 2$  and  $n = 3$ , for a particle in an infinite square well potential.

**Answer**

The eigen wave functions of the particle in box

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) \quad \text{for } n \text{ odd} \quad (\text{even parity})$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \text{for } n \text{ even} \quad (\text{odd parity})$$

The eigen wave functions of the particle in box in the first four states can be written as

$$\psi_1(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{1\pi}{a}x\right) \quad n = 1 \quad (\text{even parity})$$

$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right) \quad n = 2 \quad (\text{odd parity})$$

$$\psi_3(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{3\pi}{a}x\right) \quad n = 3 \quad (\text{even parity})$$

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**CL19\_Q1.** Find the least energy of an electron moving in a one-dimensional potential box (infinite height) of width 0.05 nm.

**Answer**

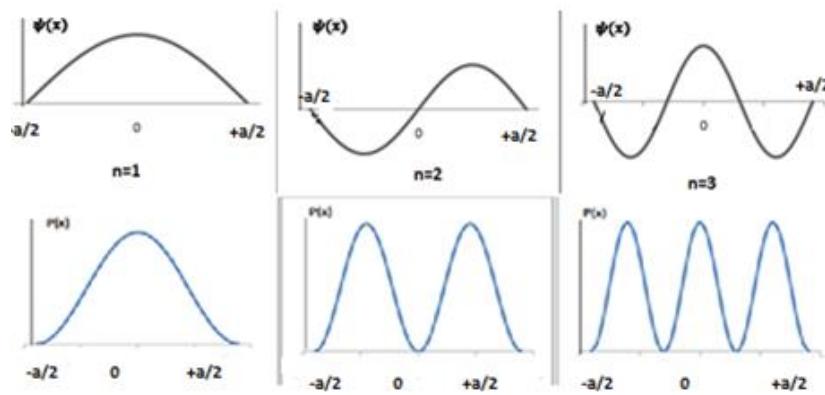
Eigen energy values for particle in a 1D potential box is given by  $E_n = \frac{\hbar^2 n^2}{8mL^2}$

For lowest state,  $n=1$

$$\text{Thus, } E_{\text{least}} = \frac{\hbar^2}{8mL^2} = 2.41 \times 10^{-17} \text{ J} = 151 \text{ eV}$$

**CL19\_Q2.** Plot the probability densities for the first three excited quantum states of an electron trapped in an infinite potential well of width L.

**Answer**



**CL21\_Q1. Compare the energy levels of the first three quantum states of identically sized finite and infinite potential wells.**

**Answer**

In the case of the finite potential well the energy of the particle can be written as

$$E_{\text{finite}} = \frac{h^2\pi^2n^2}{2m(\text{width of the well where } \psi \rightarrow 0)^2} = \frac{h^2\pi^2n^2}{2m(L+2\Delta x)^2}, \text{ where } n=1,2,3\dots$$

Hence the energy values are less than the energy values for the corresponding states of an infinite potential well of the width L.

Eigen energy values for an identical infinite well is given by  $E_n = \frac{h^2n^2}{8mL^2}$  where  $n = 1, 2, 3\dots$

First quantum state for  $n=1$ . Second state for  $n=2$  and third quantum state for  $n=4$ .

**CL21\_Q2. A particle trapped in a finite potential well. Sketch the Eigen functions for first three energy states.**

**Answer**

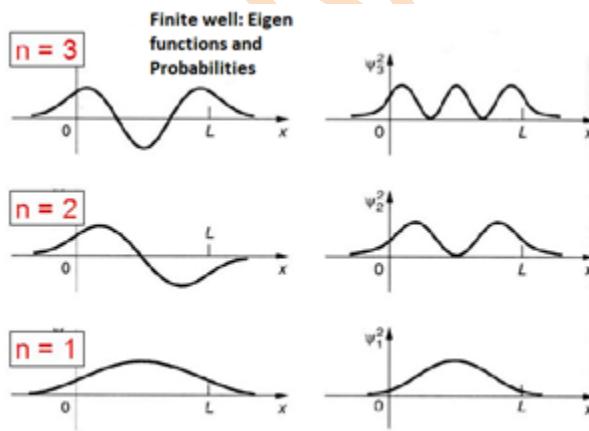


Image courtesy: adapted from slide share

**CL22\_Q1.** What is a linear harmonic oscillator? When can the oscillations become “anharmonic”?

**Answer**

Harmonic oscillator is one of the most fundamental systems in quantum mechanics which gives insight to a variety of problems such as the vibrational molecular spectroscopy as it describes the vibrations in molecules and their counterparts in solids, the phonons.

An oscillator that is not oscillating in harmonic motion, the oscillation becomes “anharmonic”.

**CL22\_Q2.** The lowest energy of the harmonic oscillator is non-zero. Explain why?

**Answer**

Eigen energy values of harmonic oscillator system is given by  $E_n = (n + \frac{1}{2})\hbar\omega$

This gives the allowed energy states as  $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \dots \dots$

Thus, the minimum energy state of the system is a non-zero  $\frac{1}{2}\hbar\omega$  where  $\omega$  is the fundamental frequency of vibration. The higher energy states are then equally spaced at  $\hbar\omega$ .

**CL22\_Q3.** What are the classical “turning points” of an oscillator?

**Answer**

Oscillator moves between positive and negative turning points  $\pm x_{\max}$  where the total energy  $E$  equals the potential energy  $\frac{1}{2} kx_{\max}^2$  while the kinetic energy is momentarily zero. When the oscillator moves past  $x=0$ , the kinetic energy reaches its maximum value while the potential energy equals zero.

**CL22\_Q4.** The eigen functions of a particle performing linear harmonic oscillations is given by

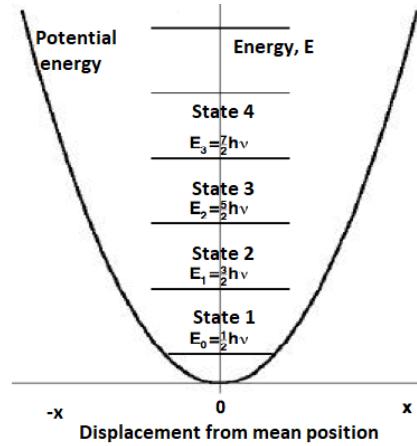
$\Psi(x) = [2n(\sqrt{\pi})n!]^{-1/2} \exp\left(-\frac{x^2}{2}\right) H_n(x)$  where  $H_n(x) = (-1)^n \exp(x^2) \frac{d^n}{dx^n} (\exp(-x^2))$ . Write down the mathematical expressions for the Eigen functions for the first four quantum states.

**Answer**

Eigen energy values of harmonic oscillator system is  $E_n = (n + \frac{1}{2})\hbar\omega$

This gives the allowed energy states as  $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \dots \dots$

Thus, the minimum energy state of the system is a non-zero  $\frac{1}{2}\hbar\omega$  where  $\omega$  is the fundamental frequency of vibration. The higher energy states are then equally spaced at  $\hbar\omega$ .



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**CL23\_Q1.** Electrons in hydrogen are described by four numbers,  $n$ ,  $l$ ,  $m$  and  $m_s$ . What restrictions (if any) are there on these four numbers?

**Answer**

The principal quantum number  $n$  is a positive integer,  $n=1,2,3,\dots$ . The integer  $l$  is a non-negative integer smaller than  $n$ , so  $l=0,1,2,\dots,n-1$ . The integer  $m$  is one of magnitude no greater than  $l$ , so  $m=-l, -l+1, -l+2, \dots, l$ . Finally,  $m_s$  takes on the values  $m_s = \pm \frac{1}{2}$

**CL23\_Q2.** In the analysis of Schrodinger's equation for a hydrogen atom using spherical polar coordinates, elaborate the azimuthal and polar. Also comment on the possible values of magnetic quantum number.

**Answer**

Azimuthal wave equation,  $\frac{d^2\Phi}{d\phi^2} + m_l^2\Phi = 0$

Polar wave equation,  $\frac{1}{\sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) + \left[ l(l+1) - \frac{m_l^2}{\sin^2\theta} \right] \Theta = 0$

$\Phi$ , the component of the complete wave function  $\psi$  must obey that it has a single value at a given point in space. The solution will satisfy this only when, magnetic quantum number  $m_l$  is zero or a positive or negative integer.

**CL20\_Q1. What is meant by the degeneracy of energy states in quantum systems?**

**Answer**

In quantum mechanics, for different combinations of quantum numbers, we may obtain the same energy value but the wave functions are different. Such quantum states having the same energy are called degenerate. Degeneracy state means two or more stationary states of the same quantum-mechanical system may have the same energy even though their wave functions are not the same.

Ex: In case of 2D, there are two allowed states for the same energy value of  $5Eo$ . This state is then doubly degenerate. Similarly, in case of 3D, there are three allowed states for the same energy value of  $6Eo$ . This state is then triply degenerate.

**CL20\_Q1. Give an example of a degenerate state in the case of a particle in a three dimensional box with infinite potential at the boundaries.**

**Answer**

For a different combination of quantum numbers, we may obtain the same energy value, but the wave functions are different. Such quantum states having the same energy are called degenerate. Here, the first excited state is degenerate since the same 'n' value is given by three sets (1,1,2), (1,2,1), and (2,1,1). The number of different states with a certain value of energy is known as the degree of degeneracy. Thus, the first excited state is threefold or triply degenerate.

**CL20\_Q3. Calculate the Eigen value of the electron in the lowest energy level, confined in a 2D potential box of 0.1 nm side.**

**Answer**

For the lowest energy level,  $n_x = n_y = 1$

$$\begin{aligned} \text{The energy of the electron in (11) state is, } E_{11} &= \frac{\hbar^2}{8mL^2} (1^2 + 1^2) \\ &= \frac{2\hbar^2}{8mL^2} \\ &= 75.4 \text{ eV} \end{aligned}$$

**CL26\_Q1.** Explain the concept of Fermi factor and discuss its temperature dependence.

### Answer

Under thermal equilibrium the free electrons occupy various energy levels in accordance with a statistical rule known as Fermi – Dirac statistics. Fermi – Dirac statistics enables the evaluation of probability of finding electron in energy levels over a certain range of energy values. The evaluation is done with the help of a quantity called Fermi factor  $F_d$  given by:

$$F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$$

#### Effect of temperature on Fermi factor

- If  $E < E_f$  then for  $E - E_f$  is negative, then the Fermi factor  $F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)} + 1\right)}$ .

At 0K this becomes  $F_d = \frac{1}{(e^{-(\infty)}+1)} = 1$ .

This implies that at 0K all electron states below the Fermi level are filled states.

- If  $E > E_f$  then for  $E - E_f$  is positive, then the Fermi factor  $F_d = \frac{1}{\left(e^{\left(\frac{\Delta E}{k_B T}\right)} + 1\right)}$ .

At 0K this becomes  $F_d = \frac{1}{(e^{(\infty)}+1)} = 0$ .

This implies that at 0K all electron states above the Fermi level are empty states.

- For  $T > 0$  and  $E = E_f$  the Fermi factor  $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)} = \frac{1}{e^0 + 1} = \frac{1}{2} = 0.5$ .

This gives a probability of occupation of 50% for the Fermi energy.

**CL26\_Q2.** Show that the probability of occupancy of an energy level  $\Delta E$  below the Fermi leve is the same as that of the probability of non-occupancy of an energy level  $\Delta E$  above the Fermi level.

### Answer

The Fermi distribution function is

$$F(E) = \frac{1}{1 + e^{\left(\frac{E-E_f}{k_B T}\right)}}$$

For  $E-E_f = -\Delta E$ ,  $F(E) = x$

$$\therefore x = \frac{1}{1 + e^{\left(\frac{-\Delta E}{k_B T}\right)}}$$

For  $E-E_f = \Delta E$ ,

$$F(E + \Delta E) = \frac{1}{1 + e^{\left(\frac{\Delta E}{k_B T}\right)}}$$

$F(E+\Delta E)$  is the probability of occupancy of energy level  $\Delta E$  above the Fermi level. Therefore the probability of non-occupancy of energy level  $\Delta E$  above the Fermi level is

$$\begin{aligned} 1 - F(E + \Delta E) &= 1 - F(E + \Delta E) = \frac{1}{1 + e^{\left(\frac{\Delta E}{k_B T}\right)}} \\ &= \frac{1 + e^{\left(\frac{\Delta E}{k_B T}\right)} - 1}{1 + e^{\left(\frac{\Delta E}{k_B T}\right)}} \\ &= \frac{e^{\left(\frac{\Delta E}{k_B T}\right)}}{1 + e^{\left(\frac{\Delta E}{k_B T}\right)}} \end{aligned}$$

$$= \frac{1}{1 + e^{\left(\frac{-\Delta E}{k_B T}\right)}}$$

(dividing numerator and denominator by  $e^{\left(\frac{\Delta E}{k_B T}\right)}$ )

$$1 - F(E + \Delta E) = x$$

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**CL25\_Q1.** Mention the postulates of quantum free electron theory of metals.

**Answer**

1. The valence electrons in the metal are arranged in discrete energy states following Pauli's exclusion principle. Only electrons close to the Fermi level participate in the conduction process
2. The occupation probability of the electron states is described by the Fermi Dirac distribution function applicable to fermions.
3. The conduction electrons in a metal move in an array of positive ions, colliding with the ionic centers and other electrons resulting in the resistance of the material.
4. The electrostatic interactions, namely the electron – electron interaction and the electron – ion interactions are negligible.
5. The electrons undergo random scattering due to the vibrating ionic centers, giving rise to resistance to flow of electrons.

**CL25\_Q2.** Explain the distribution of electrons at 0K based on the quantum theory.

**Answer**

We know that for a metal containing N atoms there will be N allowed energy levels in each band. As per the Pauli's exclusion principle, each energy level can accommodate a maximum of two electrons, one with spin up and the other one with spin down. When the filling up of the energy levels is undertaken, the universal rule is that, any system which is free tends to go to the state of lowest energy. Thus, a pair of electrons- one with spin up and the other with spin down occupy the lowest level. The next pair of electrons occupy the next higher level, and so on. In this way when all the electrons are accommodated in the permitted

energy levels, we see that all the energy levels in all the bands below the valence band will be completely filled. The valence band for a metal, however, will be partially filled i.e. below a particular filled energy level all the energy levels are completely filled and the ones above it will remain completely vacant. This is the picture when there is no external energy supply for the electrons, such as thermal energy or electrical energy, i.e. at the temperature of absolute zero, and when the metal is not under the influence of any external field.

**CL25\_Q3.** Describe the Matthiessen's rule. Discuss how temperature and impurities affect the resistivity of metals?

**Answer**

Matthiessen's rule states that the total resistivity of a metal is the sum of the ideal resistivity due to phonon scattering, which is temperature dependent and the residual resistivity due to scattering by impurities which is temperature independent.

With increase in temperature, the lattice vibrations also increase and the resistivity due to scattering of electrons by lattice vibrations also increases. The impurities in a metal act as scattering centers for electrons. Thus the electrons in an impure metal are scattered by impurity atoms and contribute to the resistivity even at absolute zero temperature.

**CL28\_Q1.** Explain Fermi level and Fermi energy.

**Answer**

The energy corresponding to the highest occupied level in the valence band at 0 K is called Fermi energy. The corresponding energy level is called the Fermi level. At 0 K all the energy levels above the Fermi level are empty and all those below the Fermi level are completely filled.

**CL28\_Q2.** Obtain an expression for Fermi energy using the concept of density of states.

**Answer**

The upper most occupied energy state at 0K is then termed as the Fermi energy of the metal. Thus, at 0K all the states below the Fermi energy are filled and all the states about the Fermi energy are empty.

We know that the density of states is given by

$$g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

The density of occupied states  $N(E) = g(E) * F_d$  when evaluated for all levels from 0 to  $E_f$ , should result in the total count of free electrons in the metal, ie.,

The total free electronic concentration  $n = \int_0^{E_f} N(E) dE = \int_0^{E_f} g(E) * F_d dE$ .

We know that  $F_d$  has to be 1 for all energy levels below  $E_f$  at 0K and hence

$$n = \int_0^{E_f} N(E) dE = \int_0^{E_f} g(E) dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE = \frac{\pi}{3} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

The Fermi energy can be estimated if the concentration of free electrons is known and can be evaluated as

$$E_f = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{\hbar^2}{8m}\right) n^{2/3}$$

**CL 28 \_Q3.** Using the expression of density of states, show that average energy of electrons in a metal at 0K is  $\frac{3}{5} E_F$

Answer

Since the distribution of electrons in the different energy states shows a non-linear variation, the average energy of the electron is not the simple average of the electron's max and min energy. From the graph of  $N(E)$  vs  $E$  we observe that  $N(E)$  states have energy  $E$  which implies that the total energy of all electrons in filled states upto  $E_f$  should be the summation of all  $N(E)*E$

The average energy of the electron =  $\frac{\text{total energy of all electrons in different energy states}}{\text{total number of electrons}}$

$$\frac{\int_0^{E_f} g(E) * E * F_d dE}{\int_0^{E_f} g(E) * F_d dE} = \frac{\frac{\pi}{2} \left(\frac{8m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE * E}{\frac{\pi}{2} \left(\frac{8m}{\hbar^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE}$$

This on integration gives the average energy  $E = \frac{3}{5} E_f$