Chapter 1
FROM THE ATOM TO THE SOLID STATE

1.1 The Atom

Electronics owes its name to the electron. The electron is one of many fundamental particles. It has certain properties; mass, charge and spin (rotation about its own axis). This electron may exist in one of two conditions, either as free or confined (attached to an atom for example). The atom is the building block of the universe. It consists of a small nucleus whose diameter is in the order of 10^{-15}m surrounded by a number of electrons. No one has seen an electron, but its size is estimated to be in the order of 10^{-19}m.

The nucleus consists of mainly positively charged protons and neutral neutrons. The mass of a proton or that for a neutron is 1836 times that of an electron. The charge of a proton is equal and opposite to the charge of an electron. The number of protons in a neutral atom must equal the number of electrons in the atom. This number is called the atomic number, while the number of the nucleons (protons and neutrons) in the nucleus is called the mass number.

1.2 Orbits

There was a belief that electrons in an atom follow trajectories or orbits around the nucleus in a way similar to the planetary orbits of planets around the sun. However, this model fell apart on account of Maxwell-Hertz law, which predicts that a charged particle subject to acceleration or deceleration emits electromagnetic radiation. If so, then an electron orbiting around the nucleus in a fixed circle of radius r and with velocity v undergoes acceleration $\frac{v^2}{r}$. Since the electron is charged, it is expected then that such an electron will emit electromagnetic radiation, and hence lose energy, then spiral down and eventually collapse onto the nucleus. Since the universe exists, this model cannot be adopted. So, we cannot say that an electron follows a fixed path around the nucleus. No orbits or known trajectories can be predicted for the motion of an electron inside the atom.

1.3 Confinement

An electron in an atom is confined to the atom. It cannot leave the atom on its own. Since the electron has a negative charge and the nucleus has a positive charge an attractive force sets in and keeps the electron attached to the nucleus within the radius of an atom, estimated to be in the order of $1Å$ ($10^{-10}m$). This attractive force, however will not cause the electron to fall onto the nucleus because the electron does not follow a fixed or known path.

1.4 Binding Energy

One of the mysteries of the atom is: "What keeps it together?". Another more challenging mystery is: "What keeps the nucleus together, despite the immerse repulsive force on account of the similarly charged protons packed together in such a small size?". An answer to both questions is usually found in terms of the binding energy. In other words, the reason why an electron enters into bondage in an atom in the first place is that the energy of the constituents of the atom before the atom is formed is higher than the energy of the atom after it is formed as a whole system. The difference is the binding energy. It is the saving in energy that causes the formation of the atom. Similarly, the binding energy of the nucleus is the driving force which makes a nucleus stable. There are other explanations as far as the nucleus is concerned, namely, the existence of even more fundamental particles within the nucleus that exert an exchange force which overrides the electrostatic repulsive force (Coulomb's force) of the similar charges within the nucleus. But the binding energy model is good enough for our purpose. In fact, to break up an atom, we must supply it with that much energy, called the binding energy of an electron (or ionization energy) to release an electron from the atom, in which case the atom becomes a positive ion and the electron becomes free. Similarly, the binding energy of the nucleus must be supplied to break up a nucleus to its free constituents.

1.5 Free and Bound

We can thus distinguish between two conditions for an electron, a bound (or confined) electron and a free electron. It has been found that the classical laws of physics as we know them-including Newton's second law-applies well to free electrons (and other free particles) but do not apply to an electron confined within an atom.

For an electron in an atom, a new set of laws exist. A body of evidence substantiates this paradigm shift. This has given rise to the quantum theory.

1.6 Quantization

One of the most important tenets of the quantum theory is quantization. This concept is alien to the classical world or the world of classical physics. We are used to continuous physical quantities such as energy, velocity, momentum etc. We can accelerate our cars smoothly and continuously. There is no restriction on the value of any speed we desire to attain. In the case of an electron in an atom it is found that the energy of a confined electron is discrete (quantized or discontinuous). The electron cannot assume any value of energy at will. It assumes only one of a set of allowed values at a time. The lowest level is the ground level (ground state).

It is also found that light energy is quantized. This means that a light beam consists of a stream of individual packets of energy, called photons. Thus, the photons are the units of energy of light as much as an atom is the unit of mass of matter. The energy of a photon E is proportional to υ the frequency of light, the constant of proportionality is *h*, called Planck's constant, $(h = 6.6x10^{-34} Js)$

$$E = h\upsilon \qquad (1\text{-}1)$$

1.7 Bohr's Model

Bohr's model of an atom envisions a set of allowed energy levels in which electrons may exist. These levels are separated by forbidden gaps. An electron can exist only in one of the allowed levels. Given enough energy, the electron may be raised from one level E_1 to another level E_2. But the energy given to the electron must exactly equal the energy difference between the levels $E_2 - E_1$. This energy may be supplied either in the form of thermal energy or radiation energy (i.e. a photon of energy $h\upsilon$ is absorbed to raise an electron from level E_1 to level E_2). But the photon energy must exactly equal the energy difference ΔE.

$$\Delta E = E_2 - E_1 = h\upsilon \qquad (1\text{-}2)$$

If the photon energy is less than or greater than ΔE the electron would not interact. This condition is called atomic resonance.

After a certain time - called lifetime of the excited electron (electron raised to a higher state) - it relaxes back to its original state. In so doing, the electron must give off the energy it originally used up in the excitation process This may appear again in the form of thermal energy or radiation energy.

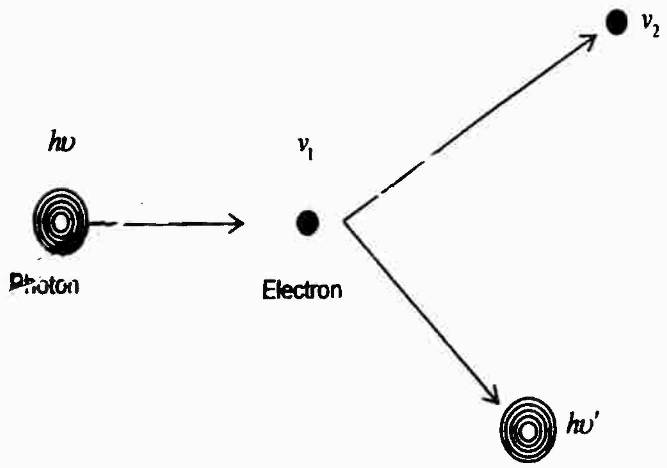

Fig. (1.1) Compton Effect

1.8 Particle Nature of Light

We know that light is a wave. This is manifested in our daily life in so many ways. Light is reflected and refracted. It also undergoes superposition, interference and diffraction. These are all wave properties. But light manifests particle properties a well through being quantized as photons. This is manifested in atomic absorption, in which electrons are excited to higher states. When they relax they emit a line spectrum. This is a conclusive evidence of the quantized nature of light.

Additionally, there have been other experiments giving credence to the particle nature of light. One of these experiments is called the photoelectric effect. It is found that when light falls on a metal, electrons may acquire enough energy to be liberated from the metal provided that the frequency of light υ exceeds a certain threshold υ_0. Einstein postulated an explanation which won him a Nobel Prize. If the energy of the incident photon is $h\upsilon$. Then

$$h\upsilon = E_w + \frac{1}{2}m\upsilon^2 \qquad (1\text{-}3)$$

The energy of the photon is consumed in overriding the binding energy of the electron in the metal - called work function E_w - and the rest is borne by the electron as kinetic energy in which the velocity of the liberated electron is v. If the energy of the photon falls below $h\upsilon_0$

$$h_{\upsilon_0} = E_w \qquad (1\text{-}4)$$

then the electron cannot escape from the metal. This explains why the photoelectric effect depends on the frequency of light.

If the frequency of light is below υ_0, no photoelectric effect occurs regardless of the intensity of light. We must note that the word light is loosely used here for a broad part of the electromagnetic spectrum not just visible light.

The second experiment consolidating the particle nature of light is called Compton effect (Fig. 1.1). It is found that X-rays falling on a beam of free electrons result in a shift in the frequency of X-rays as well as a change in the velocity and direction of the electron beam, in a manner very similar to collisions of billiard balls. Thus the laws of conservation of energy and conservation of momentum apply as in collisions between particles.

1.9 Wavelength

Light waves may be characterized by frequency υ and wavelength λ, where

$$\lambda = \frac{c}{\upsilon} \qquad (1\text{-}5)$$

where c is the electromagnetic wave velocity (velocity of light). We may envision the relation between light waves and photons as follows. A light beam consists of a stream of tiny photons propagating together in a certain direction. Collectively, they demonstrate wave properties. They have an electric field and a magnetic field perpendicular to each other and to the direction of propagation. Each field oscillates at the light frequency. This is the wave concept. Alternatively we may think of a photon as being the germ of light. It has the genetic properties of light, namely, the oscillating nature and the wavelength. It has energy $E = h\upsilon$. According to the special theory of light the photon must have mass.

$$E = h\upsilon = mc^2 \qquad (1\text{-}6)$$

$$m = \frac{h\upsilon}{c^2} \qquad (1\text{-}7)$$

A photon moving always at a constant speed $c = 3\text{x}10^8 m/s$ must then have linear momentum p

$$p = mc = \frac{h\upsilon}{c^2} \times c = \frac{h\upsilon}{c} = \frac{E}{c} \qquad (1\text{-}8)$$

This means that when light falls on a surface it exerts a force on that surface equal to the rate of change of momentum. The change of momentum per collision in case of reflected light is Δp normal to the surface.

$$\Delta p = 2mc = \frac{2E}{c} \qquad (1\text{-}9)$$

If we have $I\ watts/m^2$ as intensity of light, the photon flux (photons per unit area) is $I/h\upsilon$ and the pressure P exerted by photons falling on - and reflected off - a surface (called radiation pressure) which is force per unit area is given by

$$P = \frac{I}{h\upsilon} \times \frac{2E}{c}$$

$$= \frac{I}{h\upsilon} \times \frac{2h\upsilon}{c}$$

$$= \frac{2I}{c} \qquad (1\text{-}10)$$

Applying this result to Compton's experiment shows that when a photon collides with an electron it exerts such a large force on the electron that deflects it away, whereas if light falls on a wall it is hardly felt by the wall. This is because the mass of the photon is so small, i.e., the mass of the wall is so great that it hardly moves at all.

The concept of the wavelength for a photon can be visualized as a representation of the spatial extent of the photon. So we may visualize photons as small oscillating spheres of radius equal to the wavelength. An X-ray photon is extremely small $(0.5A)$, whereas a photon of visible light may be $0.5\mu m$ or $5000A$ $(1\mu m = 10^{-6}, m = 10^4 A,$ and $1A = 10^{-10} m)$

1.10 Wave Particle Duality

De Broglie extended the concept of the dual nature of light - being a photon on the atomic or subatomic scale and a wave on the collective (macroscopic scale) - to particles as well. He postulated that a particle may also demonstrate wave properties.

As much as a photon has a wavelength given using eqn. (1-8) by

$$\lambda = \frac{c}{\upsilon} = \frac{ch}{h\upsilon} = \frac{h}{p} \qquad (1\text{-}10)$$

So he postulated that particles moving with linear momentum p have a wavelength

$$\lambda_{particle} = \frac{h}{p} \qquad (1\text{-}11)$$

This proved true through the invention of the electron microscope.

1.11 The Dividing Line

The wave particle duality leads to understanding the limitations due to localization, namely quantization. It looks as if a particle has feelers in the sense of the wavelength. If the wavelength is in the order of magnitude of the physical size in which the particle is confined (i.e., the particle feels the bounds in which it is placed) it behaves as a wave, and thus obeys the laws of quantum theory rather than classical physics. If however, the wavelength of the particle is so small compared to the physical dimensions then the particle does not feel that it is confined at all, and thus behaves as a free particle. In such case, the quantization restriction is removed and all levels of energy are allowed.

Since there is no absolute freedom, we can say that if the physical dimension is much bigger than the particle wavelength (10 times bigger or as big as the whole universe the result being nearly the same) the particle is considered free.

Thus, the dividing line between quantum and classical realms is the ratio of the particle wavelength to the physical dimension of its confining space. In an atom, this physical dimension is in the same order of magnitude as the wavelength of the electron, and hence, the electron can be described in terms of quantum theory. Thus, quantization results in this case. Whereas if the particle is given enough energy E_{bond} (binding or ionization energy) to leave the atom altogether (Fig. 1.2) then it is confined in a space as big as the universe. The quantization effect ceases to take hold, and the particle behaves classically. If the given energy is in excess of E_{bond} it moves with kinetic energy given by

$$h\upsilon = E_{bond} + \frac{1}{2}mv^2 \qquad (1\text{-}12)$$

As a result to the dual nature of particles, when an electron and a photon collide the collision does not have to be in a classical way. Wavelengths play a role for particles and photons feeling each other out before any physical contact actually takes place.

1.12 Localization

From Compton effect, it is clear that it is impossible to localize an electron. Since to localize an electron, we need to shine light on it to locate it. The reflected light should give information about its whereabouts. However, the very fact of using light to locate the electron will cause the electron to be deflected away, so that the information gathered from the reflected light is already obsolete. This has led Heisenberg to formulate his uncertainly principle, namely that it is impossible to precisely locate an electron of known energy or velocity, i.e. it is impossible to determine both momentum and position with accuracy at the same time.

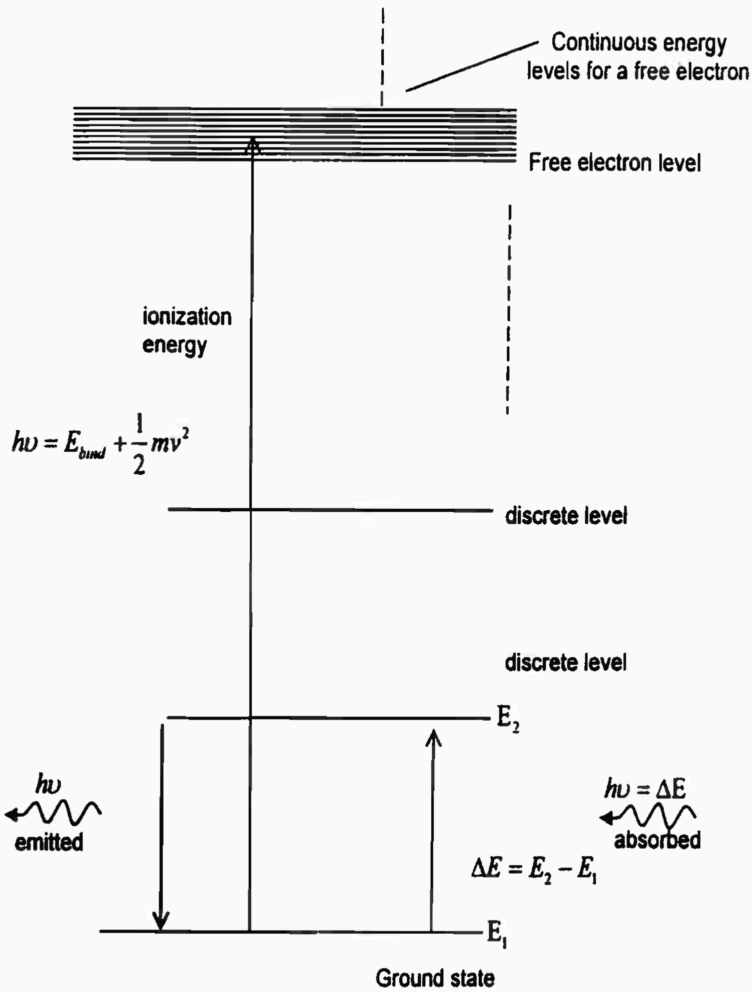

Fig. (1.2) Energy diagram for an electron in an atom

1.13 Ensemble

When we consider a large number of atoms (say hydrogen atoms) the electron in each atom need not be in the ground state. Granted most of these atoms will be in the ground state. However, some will have their electrons in the first excited state (level). Less number of atoms will have their electron in the second excited state and so on. As the energy level becomes higher and higher less and less atoms will be excited into that level. The excited electrons will not remain in their excited state forever but will soon relax into the ground state and other atoms will be excited and so on.

We can safely say that at a given temperature the number of atoms in a certain excited state E_n is constant, but the electron per se in that excited state will not be the same all the time. Continuous shuffling of electrons takes place.

We call a group of atoms an ensemble, and we may express the probability of finding an electron in a given excited state E_n as the number of atoms in state E_n divided by the total number of atoms. This ratio can also represent the likelihood of a certain atom to have its electron in state E_n. Of course, we cannot label a particular electron in a given state. But we are content to gain that much information about the electron in an atom or about the atoms in the ensemble. This statistical (probabilistic) approach is usually the best we could do, given the limitations of Heisenberg's uncertainty principle. Thus, we express the probability of an electron having energy E_n as $f(E_n)$

$$\frac{n(E_n)}{n_o} = f(E_n) = Ae^{-E_n/kT} \qquad (1\text{-}13)$$

where A is a constant, k is Boltzmann constant ($k = 1.38\text{x}10^{-23} J/\overset{o}{K}$), T is absolute temperature, $n(E_n)$ is the number of atoms in state E_n and n_0 is the total number of atoms in the ensemble. This formula is known as Maxwell-Boltzmann probability function.

1.14 Forms of Matter

It is known that matter may exist in one of 4 forms, gas, liquid, solid and plasma. In a gas, the atoms are far apart and a weak force of interaction exists among different atoms or molecules. In a liquid, the distance is smaller and the interactive force is bigger. In a solid, atoms are closer and the interactive forces are the greatest. In plasma, different ions and free particles coexist as in gas discharge. It is possible for matter to transform from one form to another. For example, increasing temperature causes a solid to melt and thus convert to liquid. Upon increasing temperature even further, the liquid may transform to vapor or gas. In case of electrical discharge, the gas may convert into plasma.

1.15 The Crystal

The atoms of a liquid may fall into a certain arrangement upon cooling, forming what is called crystal. Thus, a crystal is an orderly arrangement of atoms. There are other ways of solidification in which such an orderly arrangement does not take place, such as amorphous and polycrystalline structures. But let us concentrate on the crystalline structure. The key parameters in the crystal include the interatomic distance and the shape or structure of the crystal. If we imagine a row of atoms and we try to bring them closer, we note that as they get near each other the attractive forces of one nucleus of one atom on the electron cloud of the second atom draws the two atoms closer. If these atoms get too close, however, the repulsive force of the electron clouds pushes the atoms apart.

Thus, there must be an equilibrium position where the two Coulomb (electrostatic) forces cancel out. This atomic separation under equilibrium is called interatomic distance at which the net force is zero. In this case, the energy of the solid is minimum. In fact, energy is given off in the process, so that the solid remains together. This is the binding energy of the crystal.

1.16 Hanging in Space

It must be clear that in equilibrium the atoms of a crystal are held in space by the balanced interactive (attractive and repulsive) forces which hold these atoms together, hanging in space by what may resemble virtual springs connecting each pair of atoms. Actually, these atoms may exercise local vibrations around their equilibrium positions due to thermal energy. In fact, these vibrations give a measure of temperature or internal energy. As the solid is heated, the vibrations get more intense. Ultimately, the solid may melt and the crystal structure collapses.

What is also interesting is to note that the interatomic distance is in the order of $1\text{A} = 10^{-10}\text{m}$, while the size of the nucleus is in the order of $10^{-15}m$. If somehow Coulomb forces were to vanish altogether and we manage to pack up all nuclei and electrons together we will reduce the size of an object by roughly 10^{15} times (in 3D). This will make giant objects virtually invisible, assuming the mass to be conserved. Thus, the wholistic figures we see around owe their extended shape to Coulomb's law; but they virtually consist of empty space.

So far we have considered a metal crystal. Another related type of crystal is ionic crystals such as $NaCl$. In this case the sodium atom is ionized to Na^+ ion and the chlorine atom to $C\ell^-$ ion. Again, electrostatic forces set in, and equilibrium determines the interatomic distance.

1.17 The Surface

Consider a metal crystal. The atoms usually become ionized even at room temperature, giving off one or more electrons. These electrons become free within the metal. They can wander around throughout the crystal. An overall force exists between the electron cloud and the conglomerate of ions. It is called ionic bond. If we consider a single electron, however, we find that all ions in the neighborhood exert attractive forces on it, the net of which is zero. Thus, such electrons move freely. If one of these electrons tries to penetrate through the outermost layer of atoms (which we call surface) it will experience a net force inwardly, since there is no additional layer of atoms to balance out this inward attraction, as is the case of an electron in the bulk. Thus, such an escaping electron will be pulled back inwardly. This keeps the electron cloud within the crystal. We call this effect surface potential, meaning that for an electron to overcome the forces of attraction at the surface, it needs an external stimulus, which could be in the form of heat, electric field or a photon. The surface potential or barrier represents the binding energy of the free electron in the solid, which we called before work function E_w.

The question that arises now is this: "Since there is no really a continuous surface but only an outermost layer of atoms, why do we see a continuous surface for practically all solids?". Again, to see an object we must use a light beam which when reflected to our eyes we see the object. Now, if we use visible light, the wavelength is in the order of $0.5\mu m\,(5000A)$, which is roughly 5000 times the interatomic distance. Thus, the distance between the atoms are not visible to the naked eye. However, if we use X-rays - whose wavelength is in the order of $1A$ or less - then we may recognize the existence of the atoms through what is called X-rays diffraction. This is similar to batting a tennis ball with a tennis racket versus batting a handful of sand with the same racket (Fig. 1.3).

1.18 Band Theory

We may classify solids from the point of view of electrical conductivity to conductors, insulators and semiconductors. Conductors (such as metals) conduct easily electrical current and heat. Insulators are bad conductors. Semiconductors are somewhere in between. One way to understand the reason is what is called band theory. To comprehend the band theory, consider a row of atoms. For each separate atom the potential barrier is a function of $1/r$ where r is the distance from the nucleus. The total energy of an electron is negative, meaning that the electron needs an external energy to surmount the barrier and escape from the atom. So the electron remains confined to what looks like a potential well within its parent atom. In one dimensional model, the potential barrier varies as $1/x$ and an electron in energy level E_n can move between two limiting points $x_{0n}, -x_{0n}$ beyond which the kinetic energy becomes negative, meaning that the velocity becomes imaginary, i.e., not allowed. To illustrate this point (Fig. 1.4) let us assume the energy E_n to be $-3eV$. The potential energy at point x_1 is $-4eV$. Then

$$E_n = PE + KE \qquad (1\text{-}14)$$

$$-3 = -4 + \frac{1}{2}mv^2$$

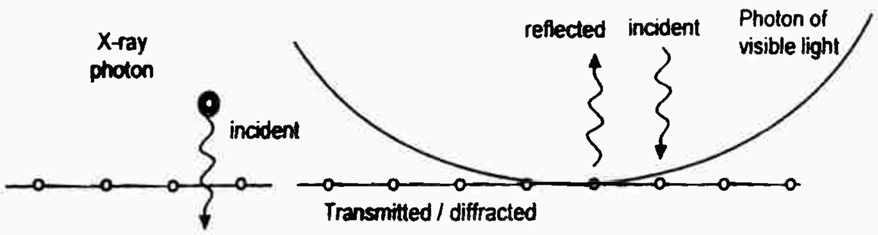

Fig. (1.3) Relation between interatomic distance and wavelength

Thus, $KE = leV$, which is as expected to be always positive.
If the electron reaches point x_{0n} it has $PE = -3eV_1$ then $KE = 0$. At x_2 PE is $-2eV$, then KE is negative. Thus the electron is confined between x_{0n} and $-x_{0n}$. We note that as n is closer to the ground state the margin through which the electron moves, i.e., $2x_{0n}$ is quite limited, and as n increases the margin increases. When we bring closer the second atom we superimpose the PE due to the two atoms. We note that a hump exists in between the two atoms, while the potential barriers remain intact at the free ends. This effect is repeated when we bring in a whole row of atoms (Fig. 1.5).

It looks now like we must distinguish between two sets of electrons. Electrons deep within the potential well (representing the parent atom) are called tightly bound electrons, which hardly interact with neighboring atoms. The second class of electrons are those which have large n and their energy level exceeds the hump. Such electrons will have freedom to move around from one atom to its neighbors, and eventually throughout the whole crystal, and hence are called free electrons (actually nearly free since they cannot leave the crystal). These electrons are restricted by the surface potential barrier and are contained in a bigger well or box of the dimensions of the crystal rather than the box of the atom. When the electron is localized within the atom, the energy is quantized and the energy levels are clearly separated. For free electrons, the box is much bigger and localization effect is much weaker and the energy levels are very close to one another. A group of very closely spaced energy levels is called energy band.

This concept is in harmony with Pauli's exclusion principle, namely that there is restriction on the number of electrons sharing the same energy level. Therefore, as electrons from different atoms transfer back and forth between neighboring atoms they cannot share the same energy values. Therefore, due to interaction or coupling between neighboring atoms, the energy levels contributed by each atom slightly differ from those contributed by neighboring atoms, leading to fine splitting of energy levels, which is the origin of the energy band. In any case, we conclude that for tightly bound electrons, atoms are noninteracting and isolated from one another, and they occupy energy levels pertaining to their individual parent atoms. Whereas for loosely bound (valence) electrons, the energy levels due to neighboring atoms nearly merge forming a band. We can safely say that each level for such electrons in one atom fans out into a band of levels in the crystal. In the metal, all bands for the valence electrons merge into one continuous (almost continuous) band called conduction band. It contains all free electrons liberated from their parent atoms. This ionization does not need much energy and it is safe to assume that metal crystals contain free (or conduction) electrons even at absolute zero. These electrons are on the move.

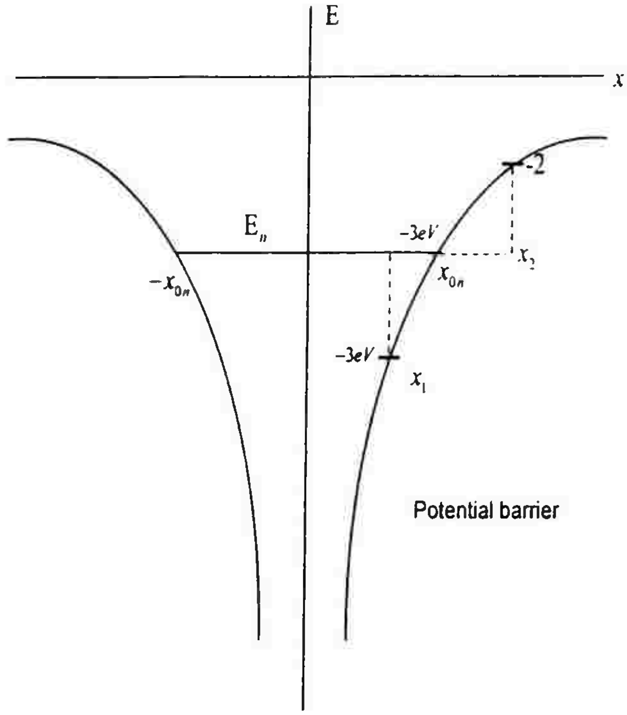

Fig. (1.4) Potential well of a single atom

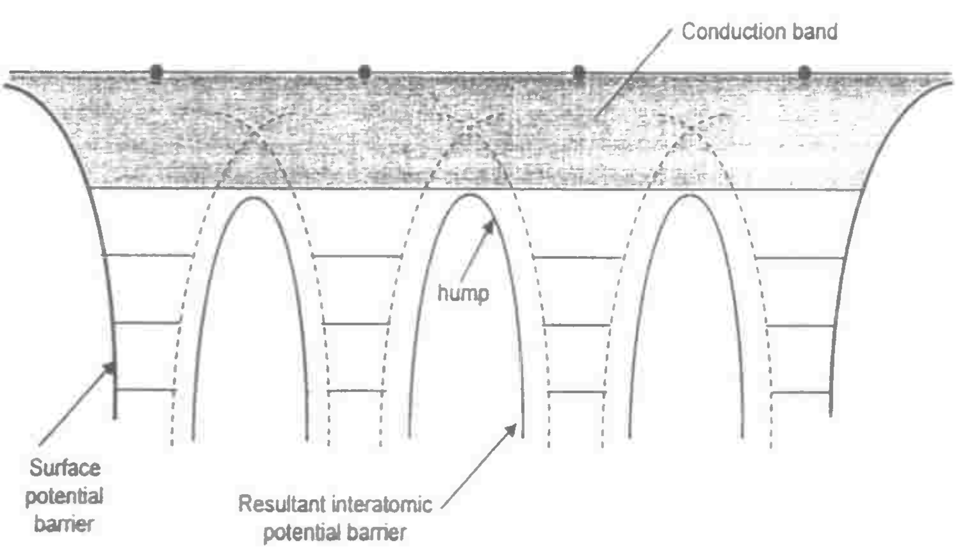

Fig. (1.5) Row of atoms in a metal crystal

It might appear awkward that electrons at absolute zero have kinetic energy, since we expect that absolute zero means everything is at rest or on freeze. If that were true it would bring contradiction to Heisenberg's principle, since we could then locate and point at an electron which would be at rest. Since this is impossible, it means that even at absolute zero there is still energy in the electrons. This energy is what Einstein called rest energy and he used it to correct formulas for specific heat in metals.

We should also note that when the electron is confined within its parent atom the quantization effect is quite obvious. When the electron becomes free to move through the crystal – a much wider box – the quantization effect becomes less conspicuous. If the electron is liberated from the crystal it becomes completely free and the confining box is the whole wide universe. In this case, the spacings between its energy levels are extremely small, and we can safely say that its energy is seamlessly continuous band, and classical physics then applies.

1.19 Fermi Level

We have seen that free electrons exist in a metal even at absolute zero. These free electrons do not fill out all energy levels of the conduction band, but they may fill up to a maximum level above which energy levels are empty. This energy level is called Fermi level E_F. It can thus be defined as the maximum energy an electron can have at absolute zero. If we think of the conduction band as a vessel partly filled by a liquid, the Fermi level is the surface of that liquid. We will see that Fermi level plays a central role in understanding the operation of electron devices.

1.20 Fermi Dirac Statistics

We have seen from eqn. (1-13) that Maxwell-Boltzmann statistics describes the population (numbers) of gas atoms as the probability of an electron residing in an excited state of a single atom. For electrons in a metal, a different form of statistics exists, namely, Fermi – Dirac statistics. Thus, the probability of finding an electron at energy E in the conduction band is given by:

$$f(E) = \frac{1}{1+e^{(E-E_F)/kT}} \qquad (1\text{-}15)$$

At $T = 0°K$, and $E < E_F$, $f(E) = 1$, *i.e.*, 100% while for $E > E_F$, $f(E) = 0$

where E_F is Fermi level and k is Boltzmann constant. This confirms the definition of Fermi level as the highest level that can be occupied by an electron in a metal at absolute zero.

As temperature increases, at $E = E_F$ we find that $f(E_F) = \frac{1}{2}$. Thus, we may alternatively, define Fermi level as the level at which the probability of finding an electron is half (50%) for any temperature above $T = 0°K$.

As temperature increases, we find that the sharp edge of $f(E)$ slackens into a curve (Fig. 1.6). For $\frac{(E-E_F)}{kT} \gg 1$, we find that eqn. (1-15) reduces to

$$f(E) = \frac{1}{1+e^{(E-E_F)/kT}} \qquad (1\text{-}16)$$

$$= e^{E_F/kT} e^{-E/kT}$$

$$= A\, e^{-E/kT} \qquad (1\text{-}17)$$

which is similar to eqn. (1-13), noting that A is constant but temperature-dependent.

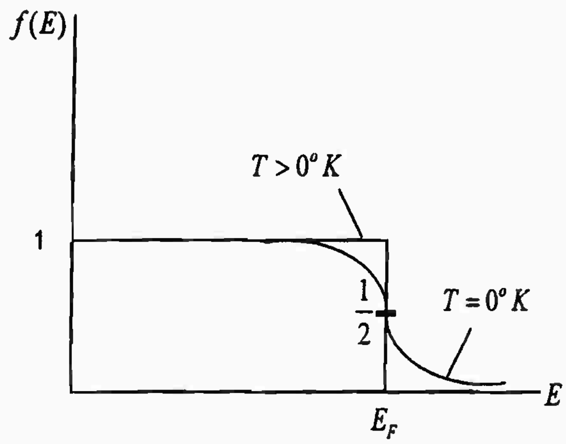

Fig. (1.6) Fermi Dirac probability function

This means that Fermi-Dirac probability function reduces to Maxwell-Boltzmann probability function for sparce population of energy levels, i.e., $\frac{(E-E_F)}{kT} \gg 1$.

In fact we may visualize electrons in the metal as a liquid filling a vessel. When we heat the liquid to boiling point, it splashes above the surface.

1.21 Density of States

We must introduce here the concept of density of states. To find an electron at level E we must have first an available (allowed) energy level E. Since the energy levels in the conduction band are packed up so closely, we may consider the band as a continuum of levels, it is not appropriate to count energy levels one by one. Instead we may define the number of levels (states) in the continuum that are contained within a sub band defined by the interval E to $E+dE$ per unit volume of the crystal as $S(E)dE$. The function $S(E)$ is called density of states function (DOS). It is the number of states between E and $E+dE$ per unit energy dE per unit volume (Fig. 1.7).

1.22 Density of Electrons

To count the number of electrons in the conduction band, again we define the interval E to $E+dE$. The number of electrons in this interval per unit volume $N(E)dE$ is given by the product of the number of allowed states in that interval times the probability of filling a representative state within this interval.

$$N(E)dE = f(E)S(E)dE \qquad (1\text{-}18)$$

Thus, $N(E)$, is called the electron distribution function, i.e., the number of electrons within the interval E to $E+dE$ per unit dE per unit volume.

The total number of electrons in the conduction band per unit volume is called density of conduction (free) electrons n_0 and is given by (Fig. 1.8).

$$n_o = \int_0^{\infty} f(E)S(E)dE \qquad (1\text{-}19)$$

It is found that $S(E)$ is given by

$$S(E) = C\sqrt{E} \qquad (1\text{-}20)$$

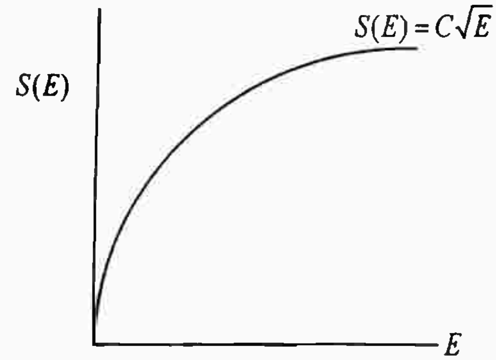

Fig. (1.7) Density of states function

where C is a constant.
Thus, eqn. (1-19) reduces - using eqn. (1-15) - to

$$n_o = \int_0^\infty N(E)dE = \int_0^\infty \frac{C\sqrt{E}}{1+e^{(E-E_F)/kT}}dE \qquad (1\text{-}21)$$

We should note here that the limits of the integral are taken from the edge (start) of the conduction band to the end of the band (free electron level or space level). Actually, infinity here is relative. For an exponential function (as that which appears in the integral), for $\frac{E-E_F}{kT} > 10$, we will have well reached infinity (very large number). Noting that $kT = 0.025eV$ at room temperature, we note therefore that the exponential tail tapers off quickly even at room temperature to zero (Fig. 1.9). We note that the total number of electrons per unit volume (density of electrons) n_0 as given by eqn. (1-21) is the area under the $N(E)$ curve.

We see that the total area under $N(E)$ curve at $T > 0^o K$ is equal to the area of the curve at $T > 0^o K$, i.e. the density of free electrons in a metal does not change with temperature, a characteristic property of conductors (metals). It is easier to perform the integration at $T = 0^o K$.

Thus,
$$n_o = \int_0^{E_f} C\sqrt{E}dE = \frac{2}{3}CE_F^{3/2} \qquad (1\text{-}22)$$

$$E_F = (\frac{3n_o}{2C})^{2/3} \qquad (1\text{-}23)$$

Inserting the numerical value (6.82 x 10^{27}) for the constant C, we have for E_F expressed in eV, and $n_o\,(m^{-3})$,

$$E_F = 3.64\times10^{-19} n_o^{2/3} \qquad (1\text{-}24)$$

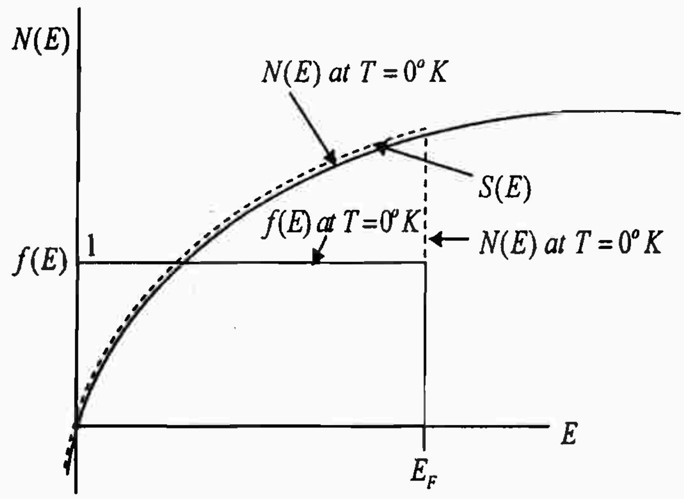

Fig. (1.8) Electron distribution function at $T = 0^{\circ} K$

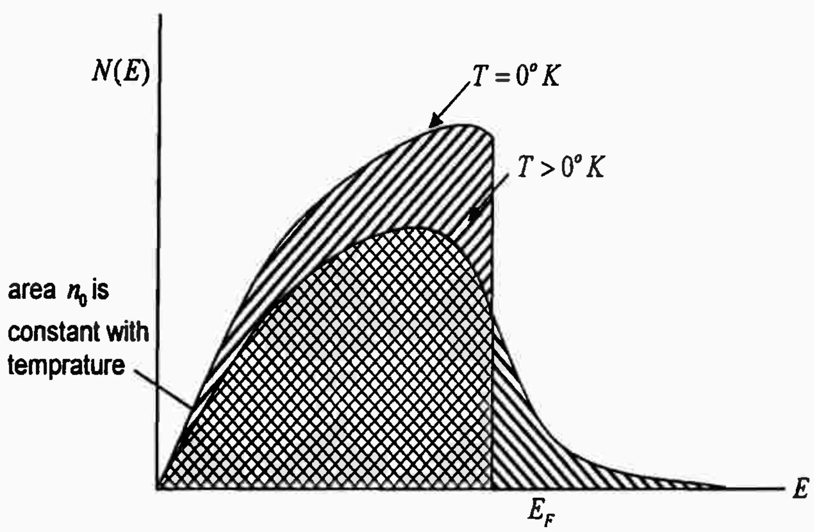

Fig. (1.9) Electron density n_0 **is the integral of electron distribution function** $N(E)$

Ex. 1.1

The specific gravity of tungsten is 18.8, and its atomic weight is 184. Assume two free electrons per atom, calculate n_0 and E_F.

Solution

A quantity of any substance equal to its molecular weight in grams is a mole of that substance. One mole of any substance contains the same number of molecules as one mole of any other substance.
This number is Avogadro's number, $N_{av} = 6.02\text{x}10^{23}\ molecules/mole$. Noting that 1molecule contains 1 atom

$$n_o = 6.02\times10^{23}\frac{molecules}{mole}\times\frac{1mole}{184gram}\times\frac{18.8\ gram}{cm^3}\times2\frac{electrons}{atom}\times\frac{1atom}{molecule}$$

$$=12.3\times10^{22}\frac{electrons}{cm^3}=1.23\times10^{29}\frac{electrons}{m^3}$$

From eqn. (1-24),

$$E_F = 3.64\times10^{-18}(123\times10^{27})^{2/3} = 8.95eV$$

1.23 Drift Velocity

Free electrons in the conduction band at thermal equilibrium exercise a random motion due to their kinetic energy, which is related to temperature. At room temperature the thermal random velocity is around 10^5 m/s. But this velocity keeps changing direction and its average is zero. When a dc external electric field ε is applied (when an external battery is connected), a component of velocity (called drift velocity) is developed, which is quite small (in the order of a few meters/s). But it is characterized by the fact that it is pointed in the same direction, so the motion of the electrons in this case is directed - not randomly oriented - i.e., it adds up giving rise to current. As the electrons are accelerated due to the external field, their velocity increases with time. Ultimately, collisions take place either among the electrons themselves or between the electrons and imperfections in the crystal. Upon collision, the electron loses its kinetic energy and starts drifting anew with zero initial drift velocity, and gains kinetic energy again due to the existence of the electric field. Since we deal with nearly free electrons, we may use Newton's second law of motion, recalling that Coulomb force is the field intensity ε times the electronic charge (numeric value) $|q|$

$$F = mx'' \qquad (1\text{-}22)$$

$$|q|\varepsilon = mx''$$

$$x'' = \frac{|q|\varepsilon}{m}$$

$$x' = |q|\frac{\varepsilon}{m}t \qquad (1\text{-}23)$$

The velocity acquired by the electric field increases linearly, until collision takes place (Fig. 1.10). Calling the average time after which collision takes place collision time or scattering time τ_s, the maximum drift velocity $\hat{\upsilon}_d$ becomes

$$\hat{v}_d = \frac{|q|\varepsilon}{m}\tau_s \qquad (1\text{-}24)$$

Defining the mobility μ as the ratio of the average drift velocity $\bar{v}_d$ to the electric field intensity ε and $\hat{v}_d$ as the maximum drift velocity just before collision, we have

$$\bar{v}_d = \frac{1}{2}\hat{v}_d = \frac{|q|\varepsilon}{2m}\tau_s \qquad (1\text{-}25)$$

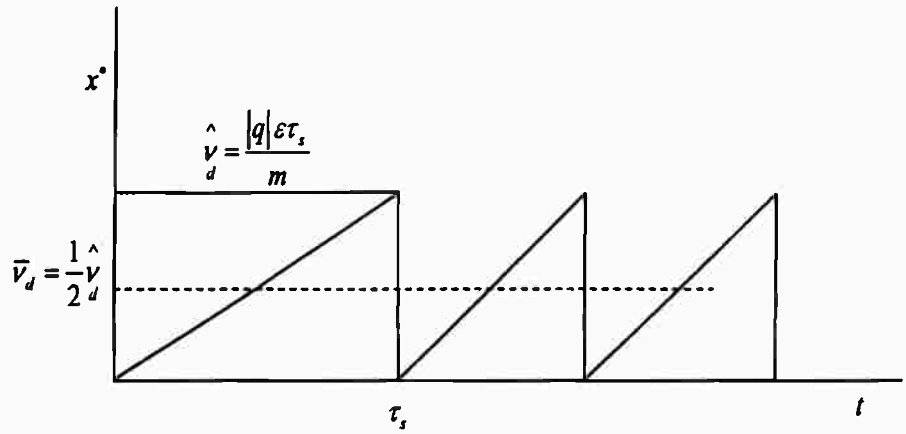

Fig. (1.10) Drift velocity

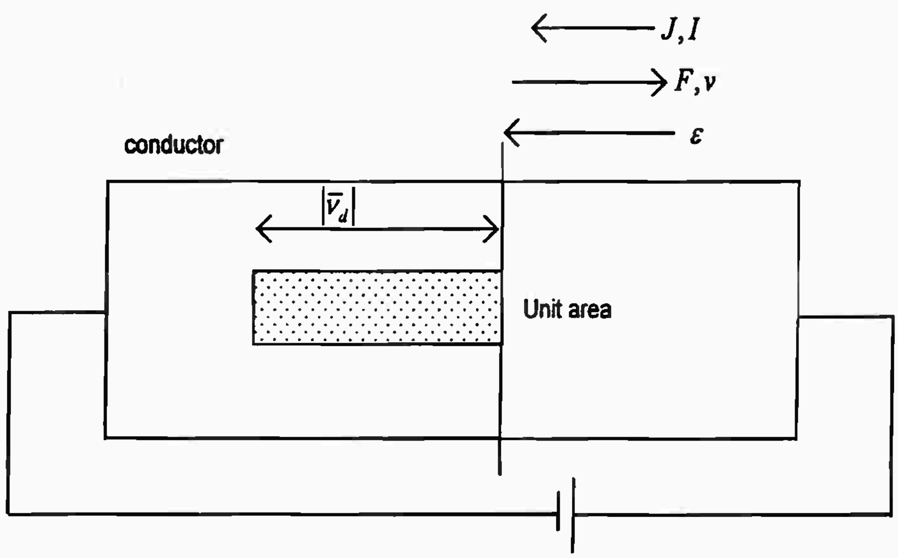

Fig. (1.11) Model for the calculation of conductivity

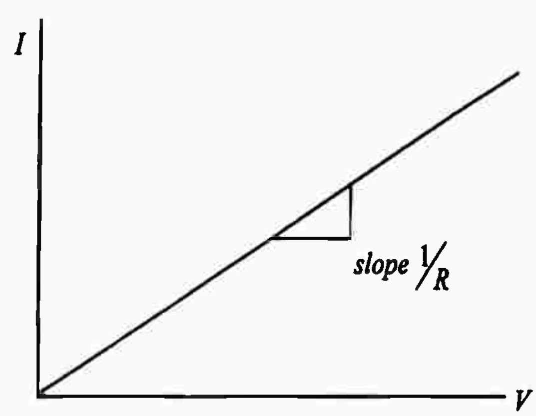

Fig. (1.12) IV characteristic of a linear resistor

Thus, $$\bar{v}_d = \mu\varepsilon \qquad (1\text{-}26)$$

$$\mu = \frac{1}{2}\frac{|q|\tau_s}{m} \qquad (1\text{-}27)$$

The direct proportionality between the average drift velocity and the electric field intensity is in harmony with cause-effect paradigm, meaning that $\bar{v}_d$ is caused by ε therefore, as a first approximation they are linearly related.

1.24 Conductivity of Metals

To calculate the current in a conductor, we note that the current is the charge moving in one second. Construct a cylinder whose base in unit area and whose height is numerically equal to the average drift velocity. We count electrons crossing the cross section of the conductor through the base of the cylinder in one second. We note that the farthest electron to cross the base of the cylinder is the one at the top of the cylinder, since it has to travel a distance numerically equal to $|\bar{v}_d|$ at speed $\bar{v}_d$, i.e., it takes one second to reach the base. Any electron at larger distances in the cylinder will take more than one second to reach the base. Thus, the number of electrons crossing the base per second n_t is equal to the number of electrons contained within the cylinder, which is the electron density n_0 times the volume of the cylinder, which is the area of the base (unit area) times the height of the cylinder (Fig.1.11).

$$n_t = 1 \times \bar{v}_d \times n_o \qquad (1\text{-}28)$$

The current density J is the charge crossing per unit time per unit cross sectional area and n_t is the number of electrons crossing per unit time per unit cross sectional area.

$$J = |q|n_t = |q|\bar{v}_d n_0 \qquad (1\text{-}29)$$

Using eqn. (1-26)

$$J = |q|\mu n_o\varepsilon \qquad (1\text{-}30)$$

Defining conductivity σ as the current density per unit electric field intensity, again assuming a linear relation, which is called Ohmic approximation,:

$$J = \sigma\varepsilon \qquad (1\text{-}31)$$

$$\sigma = |q|\mu n_o \qquad (1\text{-}32)$$

To calculate the current in a conductor of cross sectional area A and length ℓ -noting that the electric field is the voltage per unit length - so for an applied voltage V

$$I = JA = \sigma A\,\varepsilon \qquad (1\text{-}33)$$

$$= \frac{\sigma A}{\ell}V \qquad (1\text{-}34)$$

Defining the resistance R

$$R = \frac{\ell}{\sigma A} \qquad (1\text{-}35)$$

$$I = \frac{V}{R} \qquad (1\text{-}36)$$

$$V = IR \qquad (1\text{-}37)$$

This is the celebrated Ohm's law which states that the current flowing in a conductor (or resistor) is the voltage divided by the resistance. We note here that the voltage source establishes an electric field directed in the semiconductor from the positive terminal to the negative terminal. This electric field acts on the negative charge of the electron causing it to move toward the positive terminal.

It is customary to consider that current due to the electrons is in the direction opposite to the direction of motion of the electrons. This is so to make the current in the circuit look as emanating from the positive terminal of the battery into the resistor back to the battery. The relation between voltage and current is called $I-V$ characteristic. For an ohmic approximation, this relation is linear and the slope is $1/R$ (Fig. 1.12).

The unit of resistance is called Ohm (Ω) which is Volt/Ampere. From eqn. (1-35), the unit of σ is $\Omega^{-1}m^{-1}$. For connecting wires (leads) we usually assume σ to be infinity. This makes wire resistance zero. Thus, the voltage drop on the wire $(V = IR)$ is zero. This is to distinguish a resistor from metallic wires.

1.25 Temperature Effect on the Conductivity of a Metal

We should note that upon the application of an external electric field all the electrons in the conduction band are shifted by the electric force. The electrons keep circulating, which constitutes current, but the electron density at any given time remains constant at n_o.

This is a characteristic feature of metals, since there is no additional source to increase the number of electrons in the conduction band (n_0 is constant). It is found that with increasing temperature the scattering becomes more probable, i.e., τ_s decreases, leading to a decrease in mobility, i.e., electrons have more difficulty getting through with increased temperature.

It is found that

$$\mu = \mu_0 \left(\frac{T}{T_0}\right)^{-3/2} \quad (1\text{-}38)$$

where μ_0 is mobility at T_0

From eqn. (1-32)

$$\sigma = \sigma_0 \left(\frac{T}{T_0}\right)^{-3/2} \quad (1\text{-}39)$$

1.26 Band Tilt in a Metal

Consider a resistor whose terminals are a,b. A voltage source is applied such that $V_a > V_b$. Because of the negative charge of the electron, the potential energy at point a, $PE_a = -|q|V_a$ and at point b, $PE_b = -|q|V_b$. Thus $PE_b > PE_a$ and $E_{c_b} > E_{c_a}$ where E_c is the conduction band edge. Also Fermi level $E_{F_b} > E_{F_a}$. This is called band tilt, which applies to every level in the conduction band. The electric field is given by

$$\varepsilon = -\frac{dV}{dx} \quad (1\text{-}40)$$

$$= \frac{1}{|q|}\frac{dE_c}{dx} = \frac{1}{|q|}\frac{dE_F}{dx} \quad (1\text{-}41)$$

$$E_c = |q|\varepsilon x + E_{c_a} \quad (1\text{-}42)$$

$$E_F = |q|\varepsilon x + E_{F_a} \quad (1\text{-}43)$$

$$E_{c_b} = |q|\varepsilon \ell + E_{c_a} \quad (1\text{-}44)$$

$$E_{F_b} = |q|\varepsilon\ell + E_{F_a} \quad (1\text{-}45)$$

We should note that

$$\Delta E_F = |q|V_{BB} = |q|\varepsilon\ell \quad (1\text{-}46)$$

where $V_{BB} = V_a - V_b$ is the voltage of the battery. The Fermi level measures the external voltage. The Fermi level in the wire at point b is aligned with Fermi level in the resistor at point b, while the Fermi level at point a in the wire is aligned with Fermi level at point in the resistor. We consider the wire to have zero resistance, and hence, has no voltage drop and no band tilt in it

1.27 Energy Exchange

We note from Fig. (1.13) that $PE_b > PE_a$. Consider an electron at Fermi level at point b, which has total energy $E_b = E_{F_b}$. The effect of the electric field is moving the electron from point b toward point a reducing PE, but the total energy should be constant. As a result of the decreasing PE, the saving in PE is converted into kinetic energy.

When collision takes place, the KE gained before collision is totally lost in the collision, and the energy falls to the point on Fermi level locus, which is a tilted straight line. The process is repeated and the energy is dissipated in a cascading process (Fig. 1.14) until the electron reaches point a. The total energy lost can be calculated as total loss in PE which is $|q|V_{BB}$. The total energy lost per second is power P, which is the proauct of $|q|V_{BB}$ times the rate of flow of electrons which is $I/|q|$

$$P = |q|V_{BB} \times \frac{I}{|q|} = IV_{BB} \quad (1\text{-}47)$$

This is the power dissipated in the resistor. Actually, this energy is imparted to the crystal as heat. Using eqn. (1-37)

$$P = I^2R = \frac{V_{BB}^2}{R} \quad (1\text{-}48)$$

The electron is given a potential energy difference, which is converted to heat through collisions, then the electron is pumped up by the battery and so on. The electron transfers the electrical energy from the battery to heat without deducting any energy for itself.

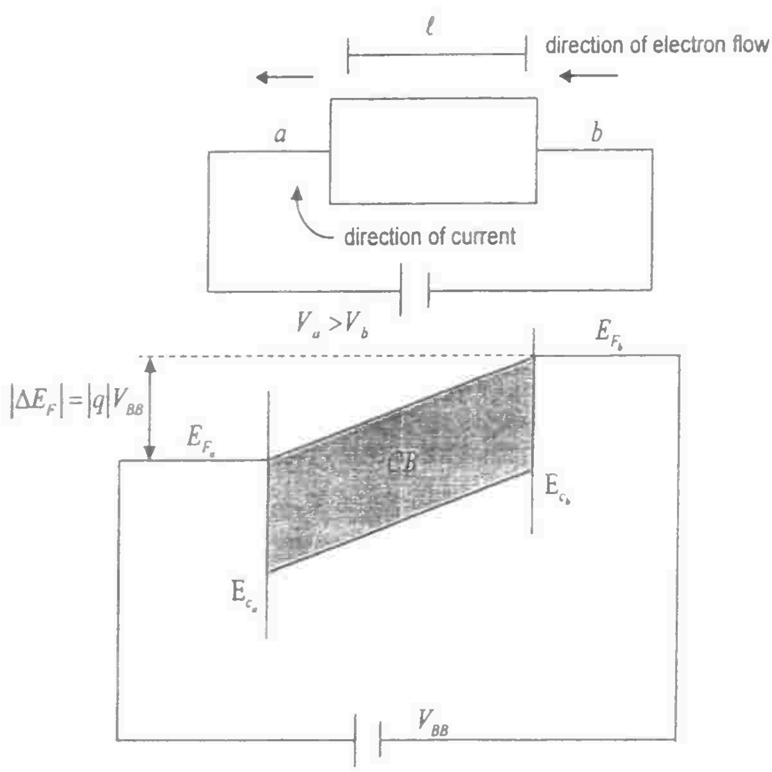

Fig. (1.13) Band tilt in a metallic resistor

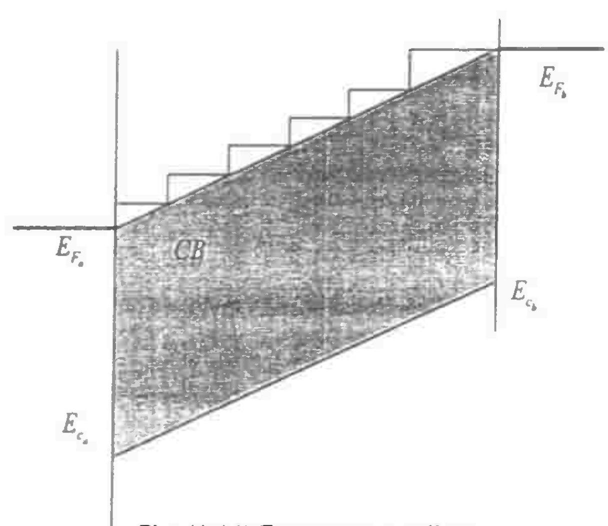

Fig. (1.14) Energy cascading

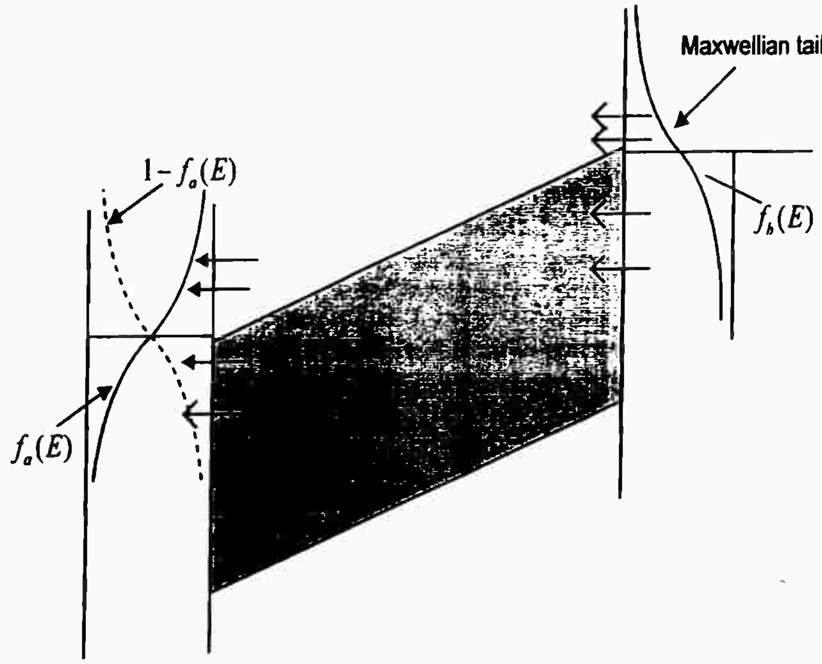

Fig. (1.15) Continuity of current in an Ohmic contact

1.28 Ohmic Contact

Electrons flowing from the metal wire at point b are actually supplied by the Maxwellian tail of the metallic wire, as well as the bulk of the metallic wire, and exit at the other end into the empty levels in the conduction band in the metallic wire at point a. For the continuity of current, the Maxwellian tail at point a must swash in the electron supply uninterruptedly at all working temperatures (Fig. 1.15). Also if the polarity of the battery is reversed the same magnitude of current flows in the opposite direction. Such a contact is called Ohmic contact.

The electron stream flows at a rate of $I/|q|$ electrons per second, while the number of electrons in the resistor remains constant. Since the entire electron population is available for conduction, an Ohmic contact supports current even at $T = 0^o K$ (Prob. 1.10).

Problems

1- A resistor which has $n_0 = 10^{30} electrons/m^3$, $\mu = 2000cm^2/Vs$, $|q| = 1.6\times10^{-19}$ Coulomb and is of length $10cm$ and area $0.01cm^2$. A voltage of $3V$ is applied. Find

a- the drift velocity, J and power loss

b- If the thermal velocity can be obtained from $mv^2 = 3kT$, $m = 9.1\times10^{-31}kg$, $kT = 0.025eV$ at room temperature. Compare the drift velocity with the thermal velocity. What do you conclude?

c- Calculate the electron flow per second?

d- Compare with n_0. What do you conclude?

2- In the above problem calculate E_F and show how it varies with distance under the external voltage.

3- In the above problem, calculate the percentage of electrons which have energy kT above E_F using reasonable approximations.

4- Derive the number of collisions and the average distance an electron may travel before collision (mean free path)

5- In the above problem derive the energy lost per collision, hence show how electrical energy is converted to heat.

6- Two resistors one of 5Ω and the second is 10Ω are connected in series. A total voltage of 1.5 V is applied. Sketch the band diagram.

7- Repeat the above problem if they are connected in parallel.

8- Estimate the percentage of resistance change with 1% change in temperature using data in problem 1. What is the polarity of the change? What do you conclude?

9- In Ohmic contacts at $T = 0^oK$ is there current?
Show why electrons in the bulk of the metal contribute to current at any temperature not only electrons at or the near E_F.

10-Show how the temperature dependence of the resistance of a metal can be used as a thermostat in many electric appliances (Do some research).

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