Band Theory

The free electron theory of Summerfield was successful in explaining the various electronic and thermal properties of metals such as specific heat, Para magnetism, electrical conductivity, electron emission, etc. However, there are various other properties which could not be explained by this theory. For example, the theory could not explain why certain solids have a large number of free electrons and thus behave as good conductors while certain others have hardly any electrons and are, therefore, insulators. It also could not account for the variation of resistivity with temperature for the latter type of materials. Moreover, the properties of semiconductors also could not be explained on the basis of this theory. The failure of the free electron theory is due to the oversimplified assumption that a conduction electron in a metal experiences a constant or zero potential due to the ion cores and hence is free to move about in a crystal; the motion being restrained only by the surface of the crystal. In fact, the potential due to ion cores is not constant and may change with position of the electron in the crystal. Some contribution to potential may also arise because of the other electrons present in the crystal. Obviously, the actual nature of potential under which an electron moves in a crystal is very complicated. The band or zone theory of solids explains this with the concept of periodic potential field by assuming that the electrons move in a region of constant potential. The electrons move in a periodic potential field provided by crystal lattice. We have already mentioned in the discussion on periodic table of elements that the atomic arrangement is periodic in all solids, i.e., within any real metal there is a periodic arrangement of positively charged ions through which the electrons move. To a reasonable approximation, the ion cores may be considered at rest and the potential experienced by an electron in a crystal is assumed to be periodic with period equal to the lattice constant *a* as shown in Fig. 5.9. The deep attractive wells mark the positions of the positive ions. We note that a deep potential well is located at each ion due to the Coulomb forces when the potential *V* varies periodically with distance *x*. The motion of an electron in a periodic potential yields the following conclusions:

(i) There exist allowed energy bands separated by forbidden regions or energy gaps.

(ii) The electronic energy functions *E*(*k*) are periodic in wave vector *k*

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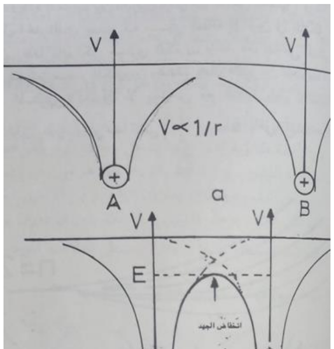
Energy Levels and Energy Band

Now the question what is happen of these levels when collective many atoms together ? supose we take one atom so the electron move arround nuclious under nuclious attractive and can be free if we have potential gerter than potential well and this potential depends on (r) as $V \propto \frac{1}{r}$ see Fig (2)

Fig (2) : (a) –Energy level for singl atom (b)- Energy level when two atom be compound



Now if we take two atoms A, B we see whenever icreases the convergens between two atoms the force betwwen the single nuclious and other electrons becomes very strong and resultant potential barrier be lowers see Fig (3).

Increases in convergens between two atoms leads interpenetration of leveles so potential barrier be lower fig (2) . So if we have N atoms in material the singl levele disintegrate to N levels and each level can occupied two electrons so singl level transform to level band have energy band . The quantum of saparation for each energy level (uniform shell) depends on destance between two nuclei of atoms and atomic shell.

Periodic Potential and Bloch Theory

The positive ions in perfect crystal arrengs in uniform periodic raws in unstable state and vibated arround eqilibrium position. Free electrons move in periodic potential because the arrengment of positve ions core as we see in Fig (3).

Since the function lW(x. t)12 represents the probability density function, then for a single particle. we must have that

$$\left| \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \right|$$

The probability of finding the particle somewhere is certain. Equation (2.18) allows us to normalize the wave function and is one boundary condition that is used to determine some wave function coefficients. The remaining boundary conditions imposed on the wave function and its derivative are postulates. However. we may state the bounda~y conditions and present arguments that justify why they must be imposed. The wave function and its first derivative must have the following properties if the total energy Eand the potential V(x) are finite everywhere.

Condition 1. Ψ(x) must be finite, single-valued and continuous.

Condition 2. $\frac{d\psi(x)}{dx}$ must be finite, single-valued, and continuous

Bloch study periodic potential for lattice (crystal potential) and concludes that the potential consists two part :

1-Statics potential V_i(r) form from interaction between conduction electron with all positive ion cores which form crystal lattice .This part $V_{(r)}$ have the same periodic transformatiom of perfect crystal (R) .

2-potential V_e(r) form from interaction of conduction electron (Bloch electron) with other conduction electrons moves through crystal lattice .