### **University of Anbar**



## **College of Science – Dept. of Physics**

## **Lectures of Semiconductors #1**

# for 3th level of physics students Lecture 5 : Introduction to the Quantum Theory of Solids/1 by Assist. Prof. Dr. Mazin A. Al-Alousi 2021-2022

#### **3.1 : ALLOWED AND FORBIDDEN ENERGY BANDS.**

### **3.1.1** : Formation of Energy Bands.

• The radial probability density function for the lowest electron energy state of the single, noninteracting hydrogen atom

- The same probability curves for two atoms that are in close proximity to each other.
- The wave functions of the two atoms' electrons overlap, which means that the two electrons will interact. This interaction or perturbation results in indiscretion in the quantum energy level splitting into two discrete energy levels

The splitting of the discrete state into two states is consistent with the Pauli exclusion principle.



If the hydrogen atoms start with a regular periodic arrangement that is initially very far apart and begins pushing the atoms together, the initial quantum energy level will split into a band of discrete energy levels.



### • As an example,

suppose that we have a system with  $10^{19}$  one-electron atoms and also suppose that, at the equilibrium interatomic distance, the width of the allowed energy band is 1 **eV**. For simplicity, we assume that each electron in the system occupies a different energy level and, if the discrete energy states are equidistant, then the energy levels are separated by  $10^{-19}$  eV. This energy difference is extremely small, so that fur all practical purposes, we have a quasi-continuous energy distribution through the allowed energy band. The fact that  $10^{-19}$  eV very small difference between two energy state can be seen from the following example.

#### Example :

Calculate the change in kinetic energy of an electron when the velocity changes by a small value. Consider an electron traveling at a velocity of  $10^7$  cm/s Assume the velocity increases by a value of 1 cm/s.

#### Solution

The increase in kinetic energy is given by:

$$\begin{split} \Delta E &= \frac{1}{2} m \left( v_2^2 - v_1^2 \right) \\ let \quad v_2 &= v_1 + \Delta v \\ \Delta E &= \frac{1}{2} m \left[ (v_1 + \Delta v)^2 - v_1^2 \right] = \frac{1}{2} m \left[ v_1^2 + 2 v_2 \Delta v + \Delta v^2 - v_1^2 \right] \\ But \quad \Delta v \ll v_1 \text{ , So we have that :} \\ \Delta E &= \frac{1}{2} m \left( 2 v_2 \Delta v \right) = m v_2 \Delta v \\ \Delta E &= (9.11 \times 10^{-31})(10^5)(0.01) = 9.11 \times 10^{-28} J \\ \Delta E &= \frac{9.11 \times 10^{-28}}{1.6 \times 10^{-19}} = 5.7 \times 10^{-9} eV \end{split}$$

A change in velocity of 1 cm/s compared with  $10^7$  cm/s results in a change in energy of  $5.7 \times 10^{-19}$  eV, which is orders of magnitude larger than the change in energy of  $10^{-19}$  eV between energy states in the allowed energy band. This example serves to demonstrate that a difference in adjacent energy states of  $10^{-19}$  eV is indeed very small, so that the discrete energies within an allowed band may be treated as a quasi-continuous distribution.

- Consider a regular periodic arrangement of atoms. Suppose the atom in this imaginary crystal contains electrons up through the n = 3 energy level. If the atoms are initially very far apart, the electrons in adjacent atoms will not interact and will occupy the discrete energy levels.
- If these atoms are brought closer together, the outermost electrons in the n = 3 energy shell will begin to interact initially, so that this discrete energy level will split into a band of allowed energies.
- If the atoms continue to move closer together, the electrons in the n = 2 shell may begin to interact and will also split into a band of allowed energies.



 Finally, if the atoms become sufficiently close together, the innermost electrons in the n = 1 level may interact. so that this energy level may also split into a band of allowed energies



There are now N electrons occupying this 3s band. They go into the lowest energy levels they can find.

The shaded area represents available states, not filled states. At the selected separation, these are the available states.

#### **3.2 : ELECTRICAL CONDUCTION IN SOLIDS**

**3.2.1** The Energy Band and the Bond Model

To the silicon atom be stabile the atoms combine So as to have eight electrons in the valence orbit .For this each atom arranges itself with four other atoms so that each neighbor shares an electron with the central atom .



The semiconductor is neutrally charged. This means that as the negatively charged electron breaks away from its covalent bonding position, a positively charged "empty state" is created in the original covalent bonding position in the valence band. As the temperature further increases, more covalent bonds are broken, more electrons jump to the conduction band, and more positive "empty states" are created in the valence band.





The *E* versus, *k* diagram at the conduction and valence bands of a semiconductor



#### Current is due to the net flow of charge

If we had a collection of positively charged ions with a volume density N (cm<sup>-3</sup>) and an average drift velocity  $V_d$  (cm/s), then the drift current density would be :

$$J = qNv_d \qquad (\frac{A}{cm^2}) \qquad \dots \dots \dots \dots \dots (1)$$

the drift current density

q~ is the charge of ion ,  $v_d~$  is drift velocity of ion

If instead of considering the average drift velocity, we considered the individual ion velocities, then we could write the drift current density as :

net drift of electrons in the conduction band will give rise to a current. The electron distribution in the conduction band, as in the beside figure. is an even function of k when no external force is applied.

Mazin A. Alalousi.....Ch.3



Recall that k for a free electron is related to momentum so that, since there are as many electrons with a (+k) value as there are with a (-k) value, the net drift current density due to these electrons is zero. This result is certainly expected since there is no externally applied force. 9 If a force is applied to a particle and the particle moves, it must gain energy. this effect is expressed as:

where F is the applied force, dx is the differential distance the particle moves, v is the velocity, and dE is the increase in energy

If an external force is applied to the electrons in the conduction band, there are empty energy states into which the electrons can move: therefore, because of the external force, electrons can gain energy and a net momentum. The electron distribution in the conduction band may look like that shown in beside Figure, which implies that the electrons have gained a net momentum.



We may write the drift current density due to the motion of electrons as:

n

$$J = -e \sum_{i=1}^{n} v_i \qquad : q = -e \ (electron \ charge) \qquad \dots \dots \qquad (4)$$

where *e* is the magnitude of the electronic charge and *n* is the number of electrons per unit volume in the conduction hand. Again, the summation is taken over a unit volume so the current density is  $A/cm^2$ 

We may note from eq.(4) that the current is directly related to the electron velocity; that is, the current is related to how well the electron can move in the crystal.

Mazin A. Alalousi.....Ch.3