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**Unit III: Application of Quantum Mechanics to Electrical transport in Solids** 



- >Suggested Reading
  - 1. Fundamentals of Physics, Resnik and Halliday, Chapter 41
  - 2. Solid state Physics, S.O Pillai, Chapter 6
  - 3. Concepts of Modern Physics, Arthur Beiser, Chapter 9
  - 4. Learning materials prepared by the department-unit III
- > Reference Videos
  - 1. Physics Of Materials-IIT-Madras/lecture-24.html

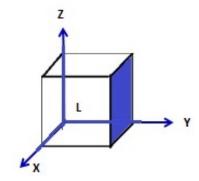
**Unit III: Application of Quantum Mechanics to Electrical transport in Solids** 



**Class# 25** 

Density of states derivation

## **Density of states derivation**



The x component of the particle motion described by

the SWE 
$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+E\psi(x)=0$$

the SWE  $\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + E\psi(x) = 0$ Eigen energy value for the x component  $E_{n_x} = \frac{h^2 n_x^2}{8mL^2}$ 

Similarly other two dimensions can be evaluated as

$$E_{n_y} = \frac{h^2 n_y^2}{8mL^2}$$
 and  $E_{n_z} = \frac{h^2 n_z^2}{8mL^2}$ 



## **Density of states derivation**



The total energy of the electron is given by

$$E_n = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2) = E_o R^2$$

Where 
$$R^2 = n_x^2 + n_y^2 + n_z^2$$
 and  $E_o = \frac{h^2}{8mL^2}$ 

The number of states with energy E can be evaluated by varying the combinations of  $n_x$ ,  $n_y$  and  $n_z$ 

### Example:

If 
$$n_x$$
,  $n_y$  and  $n_z$  is (111), then  $E_{111} = 3E_o$ , similarly

If  $n_x$ ,  $n_y$  and  $n_z$  is (121), (112), (211) all these states have energy equal to  $6E_o$ 

## **Density of states derivation**

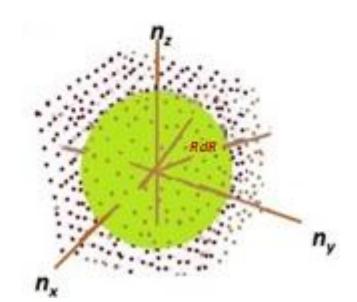
- The distribution of energy states depend on the combinations of  $n_{x'}$ ,  $n_{v}$  and  $n_{z}$  and can be evaluated by analyzing the n space formed by  $n_x$ ,  $n_v$  and  $n_z$  all positive.
- Every point in n-space given by the co-ordinates  $(n_x, n_y)$ n,) and the points are at a distance R from the origin.
- Every combination of  $n_x$ ,  $n_v$  and  $n_z$  result in an additional unit volume in n space.
- Hence evaluating the number of states is equivalent to evaluating the volume of the n space.





 $\uparrow$   $n_z$ 

## **Density of states derivation**





■Hence it is sufficient to find the volume of sphere of radius Rto evaluate the number of energy states up to R



## **Density of states derivation**



The sensitivity of increase in the states with increasing  $n_x$ ,  $n_y$  and  $n_z$  can be found from the change in the volume of the octant if the radius changes from R to R+dR

$$V = \frac{1}{8} \left( \frac{4}{3} \pi (R + dR)^3 - \frac{4}{3} \pi R^3 \right)$$
 Where  $R >> dR$ 

$$dV = \frac{\pi R^2 dR}{2}$$

This gives the number of energy states available between R and R+dR

## **Density of states derivation**



The energy expression is given by 
$$E_n = E_o R^2$$
 where  $E_o = \frac{h^2}{8mL^2}$ 

We can write 
$$R^2=rac{E_n}{E_o}$$
 and  $dR=rac{dE}{2\{E_nE_o\}}$ 

Therefore the number of energy states between E and E+dE is given

$$\frac{by}{2} = \frac{\pi R^2 dR}{4} = \frac{\pi}{4} \frac{E_n}{E_o} \frac{dE}{\{E_n E_o\}}^{1/2}$$

$$= \frac{\pi}{4} \cdot \frac{E_n^{1/2}}{E_o^{3/2}} dE$$

## **Density of states derivation**

Substituting for 
$$E_o = \frac{h^2}{8mL^2}$$



$$= \frac{\pi}{4} \cdot \left(\frac{8mL^2}{h^2}\right)^{3/2} E^{1/2} \cdot dE$$

Now we have to apply a factor of 2 for the spin factor

$$= 2.\frac{\pi}{4} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

Therefore density of states per unit volume is given by

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

This shows that the distribution of electrons in energy states vary non-linearly with increasing energy E.



### Class 25. Quiz ...

#### The concepts which are correct are....

- 1. When  $n_x$ ,  $n_y$  and  $n_z$  have values 1,2,3, the degree of degeneracy of this level is 3.
- 2. If the Eigen value of energy of the particle in a cubical box is  $11h^2/8mL^2$ , then the quantum numbers of the states are (3 1 1).
- 3. The degenerate states with the same energy values lie on the surface of a sphere.
- 4. The density of states for electrons in a metal gives the number of electron states per unit volume with energy E.





## **THANK YOU**

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