

Solid State Physics Phys(471) Lecture 16-18









Third band

The *amount of splitting* depends strongly on:
 interatomic distance: the closer the atoms, the greater the splitting.

• **atomic orbital:** the higher the energy, the greater the splitting.

➤ The wave function describing the electronic states in a band, known as the crystal orbital, can extend throughout the solid, unlike the atomic orbital which is localized.

> The wavelike properties of an electron in a crystalline solid can be described using the following form of Schrodinger equation:



Distance of nearest neighbors,  $a_0$ 

$$-\frac{\hbar^2}{2m}\nabla^2 + V(r) \bigg| \psi(r) = E\psi(r)$$
 (1)

Where  $V(\mathbf{r})$  is the *crystal potential* seen by the electron and  $\psi(\mathbf{r}) \& E$  are the *wave function* and *energy* of this electron.



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### **The Bloch Function**

The solution of (1) for *a periodic potential* is given by

$$\psi(r) = f(r)u(r) \tag{2}$$

Where both the function  $\mathbf{u}(\mathbf{r})$  and the *probability density*  $|\psi(\mathbf{r})^2|$  must have the same translational symmetry as the lattice , i.e,

u(r+R) = u(r) $\left|f(r+R)\right|^{2} = \left|f(r)\right|^{2}$ 



The only function that satisfies this is **e**<sup>ikr</sup>, hence **(2)** can be written as

$$\psi_k(r) = e^{ik.r} u_k(r)$$
 (3)

Which known as **Bloch function**.





➤ This state function has the form of a traveling plane wave so it propagates through the crystal like a free particle.

> This function represents the *crystal orbital* of the solid.







Third band Second band First band ➤ The energy spectrum in a solid is composed of a set energy bands. Regions separating these bands are **energy gaps**, i.e. *regions of forbidden energy*.

➤ Each band covers a certain range of energy, extending from the lowest to the highest value it takes when plotted in k-space.

> Within each band the electron states can be classified according to their momentum  $(p=\hbar k)$ .



Second band -

### The crystal potential

V(r) is the crystal potential "seen" by the electron. The most important property of this potential is its *periodicity*.
 This potential is composed of two parts; ionic & electronic:

 $V(r) = V_i(r) + V_e(r)$  (4)

Since electron-electron interaction is very weak and has some difficulties to be calculated, the second term in **(4)** can be dropped out. The major effect of this interaction is to screen the ions from other electrons and hence to **weaken** the electron-ion interaction.

Thus,

$$V(r) = V_i(r) = \sum_j v_s(r - R_j)$$

Where  $v_s(r-R_j)$  is the potential of the screened ion located at  $R_j$ .



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#### Number of States in the Band



Since each Bloch function  $\psi(\mathbf{r})_{n,k}$  defines a specific electron state, let see how many states there are in each band.

**For 1D case:**  $\psi_k(x) = e^{ik \cdot x} u_k(x)$ Applying the periodic boundary condition on this function shows that the allowed number of k is ;  $k = n \frac{2\pi}{L}$ For the first zone, the **number of states** is  $(\frac{2\pi}{a})/(\frac{2\pi}{L}) = \frac{L}{a} = N$ 

Third band

Where **N** is the number of unit cells. Hence, we end with these two important facts:

In each band the number of states (crystal orbital) inside the first zone is equal to the number of unit cells in the crystal N.
 In each band the maximum number of electrons is equal to 2N.



### SOME APPROXIMATE MODELS

To obtain a specific values of *E* and  $\psi$ , one needs to solve Schrodinger equation for the *actual potential V(r)* in the solid of interest. But since this is a very tough task, it is preferable to solve Schrodinger equation using some simplified potentials.

### **Empty-lattice model:**

\* In this simplest case the crystal potential is assumed to be exactly zero ; V(r)=0.

i.e. the electron is completely free.\* For **1D**; the state functions and energies are:

Third band —

 $\psi_k^0 = \frac{1}{L^{1/2}} e^{ik.x}$  (5)

 $=\frac{\hbar^2 k^2}{k^2}$ 

and



where L = Na is the length a long x axis and the superscript 0 indicates that these solutions obtained at V(x)=0.

(6)







### Nearly-free-electron model (NFE):

•In this model the crystal potential is assumed to be so weak ; i.e. the electron is nearly free.

•This model can serve as a rough approximation to the valence bands in the simple metals such as: Na, K, Al, etc.

• On the basis of *perturbation method* one finds that the crystal potential will only affect the regions near the zone boundaries. This effect is to smooth over the sharp corners, and hence, to create energy gaps at these regions with values of,











- \* Physically, *energy gaps* can be explained according to *Bragg reflection* of electron waves in crystal:
- 1. When Bragg condition  $k = \pm n\pi/a$  is satisfied at the zone boundaries, a wave traveling to the right is Bragg reflected to the left forming a *standing wave*.
- 2. Two different standing waves  $\psi(+) \& \psi(-)$  will be formed from the two traveling waves  $e^{ikr} \& e^{-ikr}$ .
- **3**. Each of these standing wave will pile up electrons at two different directions for the same *k*, and this the origin of the energy gap.



### tight-binding model (TB):

• In this model the crystal potential is assumed to be strong so that the electron is captured by ions for some intervals. During each interval the electron orbits around a single ion, i.e. its state function is that of an atomic orbital.

• This model can serve as a rough approximation to the narrow, inner bands in solids.







### Metals, Insulators & Semiconductors

• The fact that used to distinguish between these types of solids is:

A band which is completely full carries no electric current, even in the presence of an electric field.

• If the gap between the valance band and the band immediately above it is small, electrons may be thermally excited across the gap and the solid is called a *semiconductor*.

• At room temperature a substance behaves as a semiconductor if  $E_g$  is less than 2eV. In insulators  $E_g \sim 7eV$ .









Dispersion relation is given by;

$$E_k = \frac{\hbar^2 k^2}{2m^*} \qquad (7)$$

Second band

The corresponding energy contours in k-space are spheres surrounding the origin.

Volume of shell confined between *E* & *E*+*dE* is:  $4\pi k^2 dk$ 



First band

Hence:

 $g(E)dE = \frac{V}{\left(2\pi\right)^3}$  $= \frac{1}{(2\pi)^3} 4\pi k^2 dk$  $= \frac{1}{4\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2} dE$ 

Taking into account the spin degeneracy leads to

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

Second band

➤ The larger the energy the greater the radius, and hence the larger the number of states.

> The greater the mass the larger the number of states.



### For regions near the zone boundaries: > Dispersion relation given by (7) is not valid. > As a result the density of states will has a more complicated formula. The following Fig. shows how g(E) will vary with E near the zone boundaries. g(E) $E^{1/2}$ Higher band Gap kr **Insulator or Semiconductor** g(E)g(E) $E_{\rm F}$ $E_{\rm F}$ **Monovalent** metal **Divalent metal**



Second band

#### THE FERMI SURFACE



► **Recall:** *FS* is the surface in k-space inside which all states are occupied by valence electrons.

≻The significance of this surface derives from the fact that only those electrons lying near it contribute to thermal and electrical processes.

We will determine the Fermi energy  $E_F$  in the regions where the relation (7) is applicable.

From definition;

Or

Third band Second band First band

$$\int_{0}^{1} g(E)dE = n$$
(9) we get;  $E_{F} = \frac{\hbar^{2}}{2m^{*}} (3\pi^{2}n)^{2/3}$ 

 $E_F$ 

$$E_F = \frac{\hbar^2 k_F^2}{2m^*}$$

where





Second hand \_\_\_\_\_





### Velocity of The Bloch Electron

➢ for a free electron the velocity is given by

$$v = \frac{p}{m_0} = \frac{\hbar k}{m_0}$$

### **Constant velocity**

> Consider an electron in a state  $\psi_k$ , the velocity by which it moves through the crystal should be related to the energy of the state according to;









Near the center of the zone , where (7) is valid, the relation (10) lead to;

$$v = \frac{1}{\hbar} \frac{\partial}{\partial k} E(k) = \frac{1}{\hbar} \frac{\partial}{\partial k} \left( \frac{\hbar^2 k^2}{2m^*} \right) = \frac{\hbar k}{m^*}$$

Which is of the same form as the relation for a free particle, except that  $m_0$  has been replaced by  $m^*$ .

The velocity is proportional to the slope of the energy curve

### Constant velocity



zero velocity (standing waves)