



Part I Fundamentals

Electron Theory : Matter Waves

Chap. 1 Introduction

Chap. 2 The Wave-Particle Duality

Chap. 3 The Schödinger Equation

Chap. 4 Solution of the Schödinger Equation for
Four Specific Problems

Chap. 5 Energy Bands in Crystals

Chap. 6 Electrons in a Crystal

Electromagnetic Theory : Maxwell Equations

Chap. 4 Light Waves

(Electrons in Solids, 3rd Ed., R. H. Bube)





6. Electrons in a Crystal



6.1 Fermi Energy and Fermi Surface

The Fermi energy, E_F :

- An important part of an electron band diagram
- Defined as “**the highest energy that the electrons assume at $T = 0 \text{ K}$** ”
- Fermi energy for Al and Cu : see Fig 5.21, 5.22

Fermi energy for semiconductor:

- The above definition can occasionally be misleading, particularly when dealing with semiconductors
- Fermi function at E_F , $F(E_F) = \frac{1}{2}$: see Section 6.2 for more accurate definition

Fermi surface (in 3-d k -space) for Cu : see Fig 5.27



6. Electrons in a Crystal

6.2 Fermi Distribution Function

Fermi function, $F(E)$: The probability that a certain energy level is occupied by electrons

$$F(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$

Fermi distribution for $T = 0$ K (Fig 6.1)

and for higher T ($T \neq 0$ K) (Fig 6.2)

At high energy ($E \gg E_F$), $F(E)$ is approximated by classical Boltzmann distribution

$$F(E) \approx \exp\left[-\left(\frac{E - E_F}{k_B T}\right)\right]$$

“Boltzmann tail”

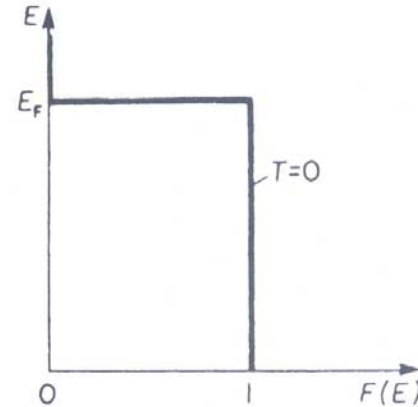


Figure 6.1. Fermi distribution function, $F(E)$, versus energy, E , for $T = 0$.

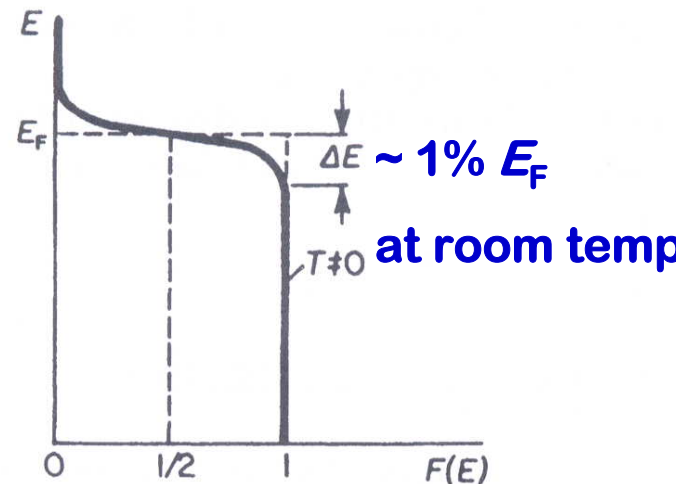


Figure 6.2. Fermi distribution function for $T \neq 0$.

6. Electrons in a Crystal



6.3 Density of States

“How energy levels are distributed over a band?”

Assume free electrons are confined in a square potential well of crystal. Similar to the case in Sec. 4.2, by using B.C., the solution of the Schrödinger equation

$$E_n = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)$$

$$n^2 = n_x^2 + n_y^2 + n_z^2$$

where n_x, n_y, n_z are principal quantum numbers,
 a is the length of the crystal

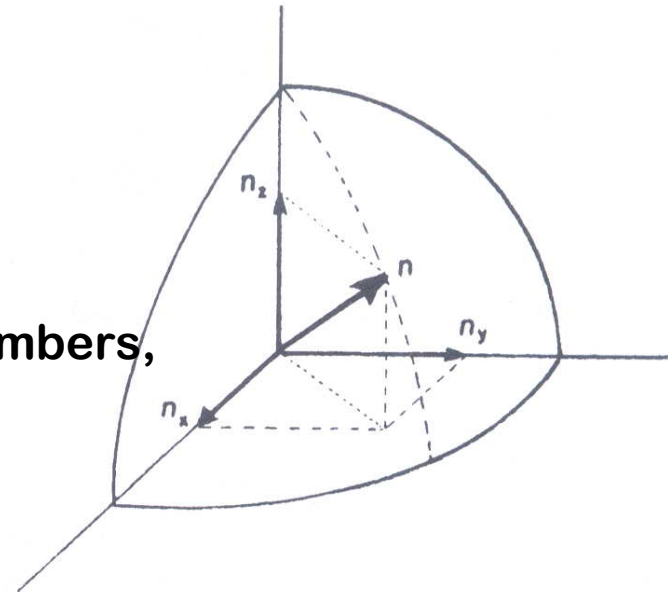


Figure 6.3. Representation of an energy state in quantum number space.





6. Electron in a Crystal



6.3 Density of States

A specific energy level, E_n for each set of n_x, n_y, n_z , called “**energy state**”

- Equal values of the energy, E_n lie on the surface of sphere with radius n

- All points within the sphere represent quantum states with energy smaller

than E_n

- **The # of quantum state, η** , with an energy equal to or smaller than E_n , is proportional to the volume of the sphere

(n values can be defined in positive octant of the n -space)

In a one-eighth of the volume of the sphere with radius n

(# of energy state η),

$$\eta = \frac{1}{8} \cdot \frac{4}{3} \pi n^3 = \frac{\pi}{6} \left(\frac{2\pi a^2}{\pi^2 \hbar^2} \right)^{3/2} E^{3/2}$$





6. Electrons in a Crystal



6.3 Density of States

Density of state, $Z(E)$: # of energy states per unit energy in the energy interval dE

($a^3 =$ volume that the electrons can occupy)

$Z(E)$: differentiation of η with respect to the energy, E

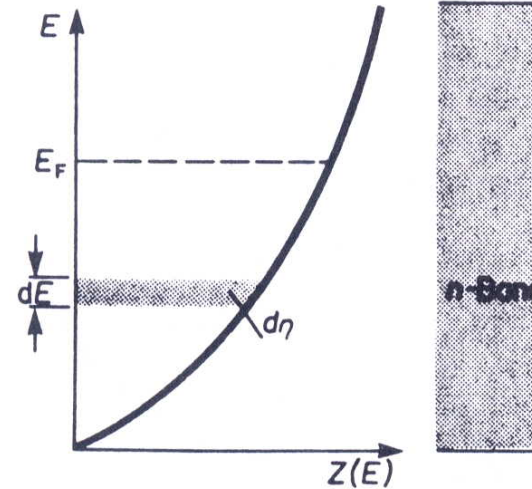


Figure 6.4. Density of states $Z(E)$ within a band. The electrons in this band are considered to be free.

$$\frac{d\eta}{dE} = Z(E) = \frac{\pi}{4} \left(\frac{2ma^2}{\pi^2 \hbar^2} \right)^{3/2} E^{1/2} = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2}$$

$$d\eta = Z(E) \cdot dE$$



6. Electrons in a Crystal

6.4 Population Density

Pauli principle : each energy state can be occupied by one electron of positive spin and one of negative spin

Population density $N(E) = 2 \cdot Z(E) \cdot F(E)$

$$N(E) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$

For $T \rightarrow 0$ and $E < E_F \rightarrow N(E) = 2 \cdot Z(E)$, $F(E) = 1$

For $T \neq 0$, $E \approx E_F$, \rightarrow the Fermi distribution function causes a smearing out of $N(E)$

(Fig 6.5)

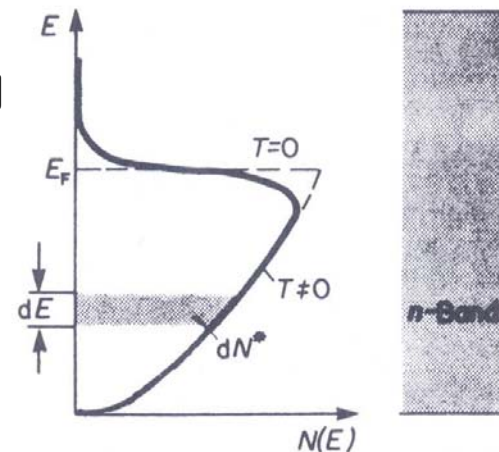


Figure 6.5. Population density $N(E)$ within a band for free electrons. dN^* is the number of electrons in the energy interval dE .

6. Electrons in a Crystal

6.4 Population Density

of electrons N^* , that have an energy equal to or smaller than the energy E_n (The area within the curve in Fig 6.5) For an energy interval between E and $E + dE$

$$dN^* = N(E)dE$$

From (6.8) and (6.9) and consider simple case $T \rightarrow 0$ and $E < E_F$, $F(E) = 1$

$$N^* = \int_0^{E_F} N(E)dE = \int_0^{E_F} \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} dE = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E_F^{3/2}$$

$$E_F = \left(3\pi^2 \frac{N^*}{V} \right)^{2/3} \frac{\hbar^2}{2m}$$

If we define #of electrons per unit volume as $N' = N^*/V$,

$$E_F = (3\pi^2 N')^{2/3} \frac{\hbar^2}{2m}$$

6. Electrons in a Crystal

6.5 Complete Density of States Function Within a Band

Evs. $Z(E)$ in actual crystals

- Low energy : free-electronlike

- Higher energy : fewer energy state available (Fig 5.26)

→ $Z(E)$ decrease with increasing E

- The corners of the BZ : $Z(E)$ dropped to zero

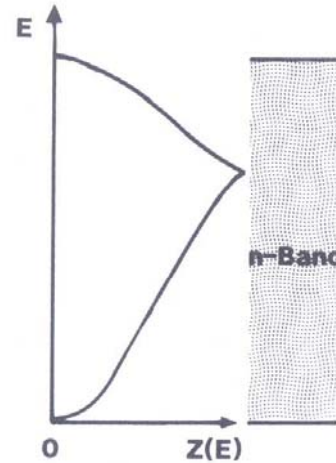


Figure 6.6. Schematic representation of the complete density of states function within a band.

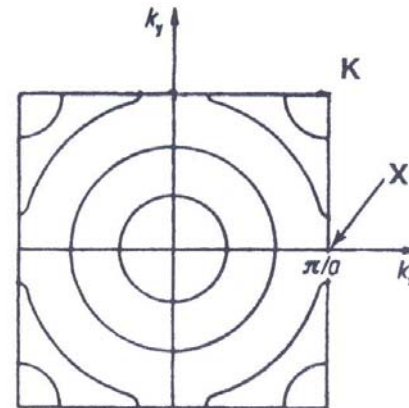


Figure 5.26. Curves of equal energy inserted into the first Brillouin zone for a two-dimensional square lattice.

6. Electrons in a Crystal



6.6 Consequences of the Band Model

Insulators : solids in which the highest filled band is completely occupied by electron

Alkali metal: the valence band is essentially half-filled, electrons can drift under external field

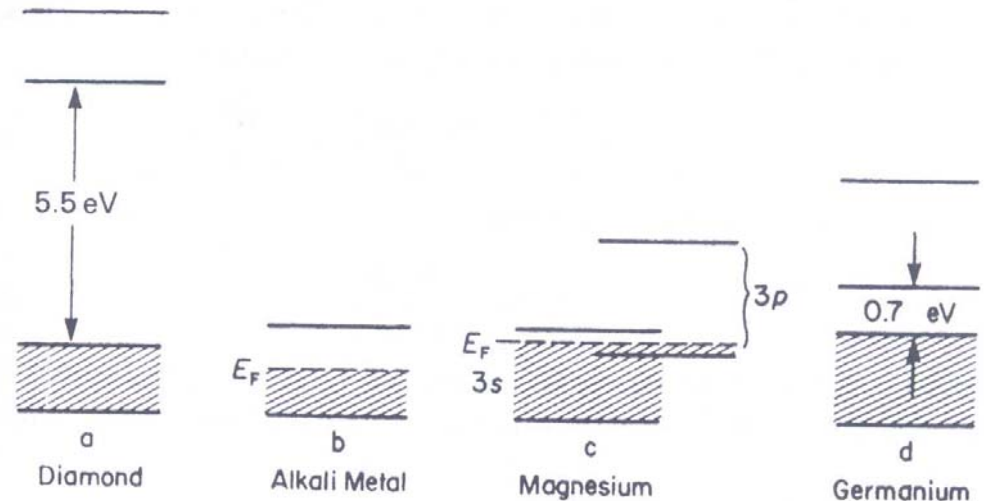


Figure 6.7. Simplified representation for energy bands for (a) insulators, (b) alkali metals, (c) bivalent metals, and (d) intrinsic semiconductors.

Bivalent metals: upper band partially overlapped ; weak binding forces of the valence electrons on atom

Semiconductors: valence band is completely filled with electron; relatively narrow band gap (intrinsic semiconductors); a sufficiently large energy can excite electron from valence band to conduction band → some electron conduction





6. Electrons in a Crystal



6.7 Effective Mass

Effective mass (of electron), m^*

experimentally determined electron mass


- Deviation of m^* from free electron mass m_0 : usually attributed to interaction between drifting electrons and atoms in a crystal

- For example,

Electron accelerated in an electric field might be slowed down slightly due to “collisions” with some atom \rightarrow ratio $m^*/m_0 > 1$

The electron wave in another crystal might have just the right phase in order that the response to an external electric field is enhanced \rightarrow $m^*/m_0 < 1$

- Derivation of effective mass
group velocity (2.10)
$$v_g = \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{dk} = \frac{d(2\pi E / h)}{dk} = \frac{1}{\hbar} \frac{dE}{dk}$$



6. Electron in a Crystal



6.7 Effective Mass

(continued)
$$a = \frac{dv_g}{dt} = \frac{1}{\hbar} \frac{d^2 E}{dk^2} \frac{dk}{dt}$$

(4.7)
$$p = \hbar k \quad \rightarrow \quad \frac{dp}{dt} = \hbar \frac{dk}{dt}$$

$$a = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \frac{dp}{dt} = \frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} \cdot \frac{d(mv)}{dt} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} F$$

$$a = \frac{F}{m} \quad m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1}$$



6. Electron in a Crystal

6.7 Effective Mass

$$m^* = \hbar^2 \left(\frac{d^2 E}{dk^2} \right)^{-1}$$

Effective mass is inversely proportional to the curvature of an electron band.

In Fig 6.8, m^* is small and positive near the center of BZ

Negative m^* (upper part of the band in Fig 6.8) : “particle travels in the opposite direction to an applied electric force (and opposite to an electron” ; called “electron hole”

cf) exciton : an electron/hole pair

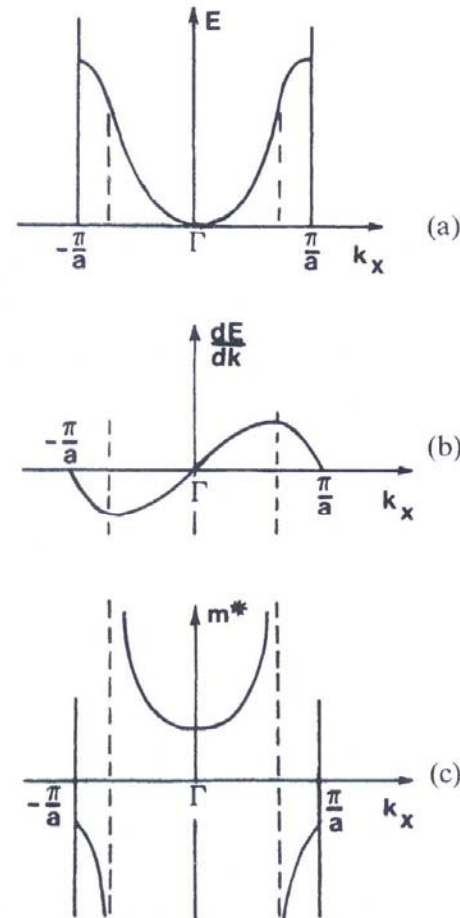


Figure 6.8. (a) Simple band structure, as shown in Fig. 5.4. (b) First derivative and (c) inverse function of the second derivative of the curve shown in (a).