



Phys 570

Lecture #7

Physics & Astronomy Dept.

College of Science

King Saud University

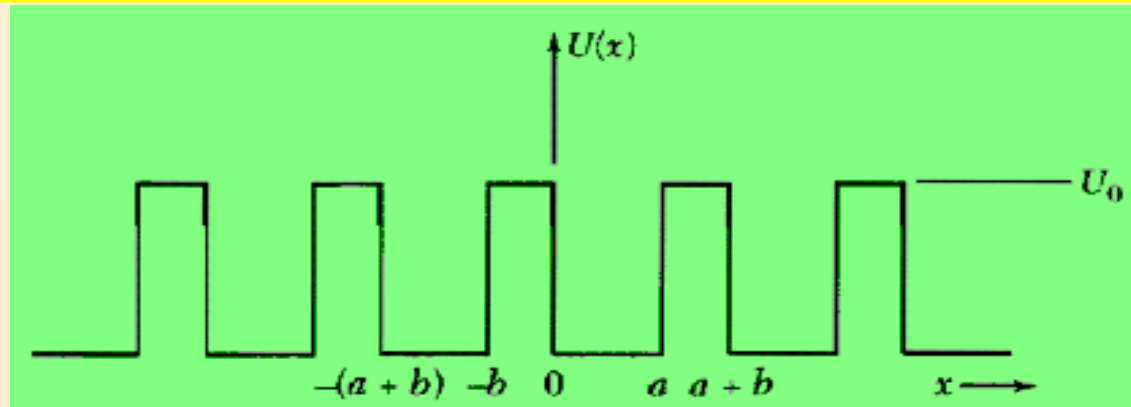
Nasser S. Alzayed

nalzayed@ksu.edu.sa

Chapter 7: Energy Bands

Kronig-Penny Model

- This model solves for periodic potential in a form of a square-well array:



- Schrodinger wave equation for this potential can take the form:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U(x)\psi = \varepsilon\psi \quad (11)$$

where $U(x)$ is the potential energy and ε is the energy eigenvalue.

We have 2 regions: $0 < x < a$ ($U = 0$) and $-b < x < 0$ ($U \neq 0$)

Chapter 7: Energy Bands

Kronig-Penny Model

□ For the first region we have the wave function:

$$\psi = Ae^{iKx} + Be^{-iKx} \quad (12)$$

This is a combination of plane waves traveling to the right and to the left, with energy:

$$\varepsilon = \frac{\hbar^2 K^2}{2m} \quad (13)$$

□ In the 2nd region, wave function takes the form:

$$\psi = Ce^{Qx} + De^{-Qx} \quad (14)$$

with energy:

$$U_o - \varepsilon = \frac{\hbar^2 Q^2}{2m} \quad (15)$$

Chapter 7: Energy Bands

Kronig-Penny Model

- ❑ Solution of this equation shall be on the Bloch form (7) because it is a periodic potential.
- ❑ Thus the solution in the region $a < x < a + b$ must be related to the solution (14) in the region $-b < x < 0$ by the Bloch theorem:

$$\psi_k(r) = u_k(r) e^{ik \cdot r} \quad (7)$$

$$\psi(a < x < a + b) = \psi(-b < x < 0) e^{ik(a+b)} \quad (16)$$

- ❑ The constants A, B, C, D are chosen so that ψ and ψ' are continuous at $x=0$ and $x=a$. same as in square potential wells.
- ❑ At $x = 0$ we have (for both conditions): (12) + (14):

$$A + B = C + D \quad (17)$$

Derivatives of (12) and (14) at $x = 0$ provides:

$$iK(A - B) = Q(C - D) \quad (18)$$

Chapter 7: Energy Bands

Kronig-Penny Model

□ for the case of $x = a$; and applying continuity of ψ and ψ' we will get:

$$Ae^{iKa} + Be^{-iKa} = (Ce^{-Qb} + De^{Qb})e^{ik(a+b)} \quad (19)$$

$$iK(Ae^{iKa} - Be^{-iKa}) = Q(Ce^{-Qb} - De^{Qb})e^{ik(a+b)} \quad (20)$$

□ Solving equations from (17) to (20) can be done by putting all coefficients of A, B, C, D in a determinant. However, such solution is very difficult. We will only write down the final equation:

$$\left[\frac{Q^2 - K^2}{2QK} \right] \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b) \quad (21a)$$

□ to simplify the solution; we represent the potential by a Delta Function. Let: $b \rightarrow 0$ and $U_0 \rightarrow \infty$

Chapter 7: Energy Bands

Kronig-Penny Model

□ We do some approximation:

$$Q \gg K \quad Qb \ll 1$$

$$\sinh Qb \rightarrow Qb$$

$$\cosh Qb \rightarrow 1$$

$$\cos k(a+b) \rightarrow \cos ka$$

notice that: $Q^2 \gg K^2$, hence: (21a) \Rightarrow

$$\frac{Q^2}{2QK} Qb \sin Ka + \cos Ka = \cos ka$$

$$\left[\frac{P}{Ka} \right] \sin Ka + \cos Ka = \cos ka \quad (21b)$$

$$\text{with } P = \frac{Q^2 ba}{2}$$

Chapter 7: Energy Bands

Kronig-Penny Model

- The ranges of K for which this equation has solutions are plotted in Fig. 5, for the case $P = 3\pi/2$. The corresponding values of the energy are plotted in Fig. 6. Note the energy gaps at the zone boundaries.

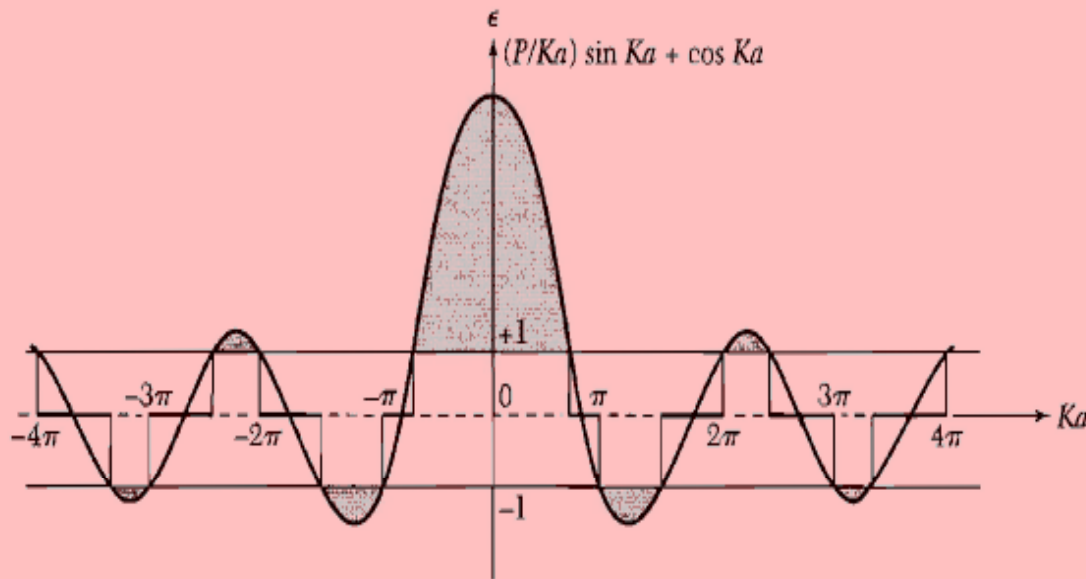
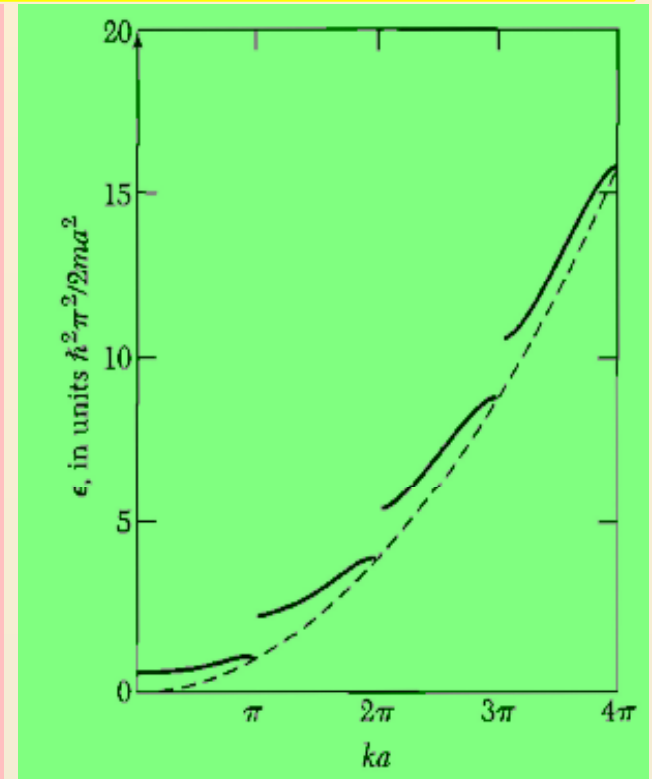


Figure 5 Plot of the function $(P/Ka) \sin Ka + \cos Ka$, for $P = 3\pi/2$. The allowed values of the energy e are given by those ranges of $Ka = (2m\epsilon/\hbar^2)^{1/2}a$ for which the function lies between ± 1 . For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.



Chapter 7: Energy Bands

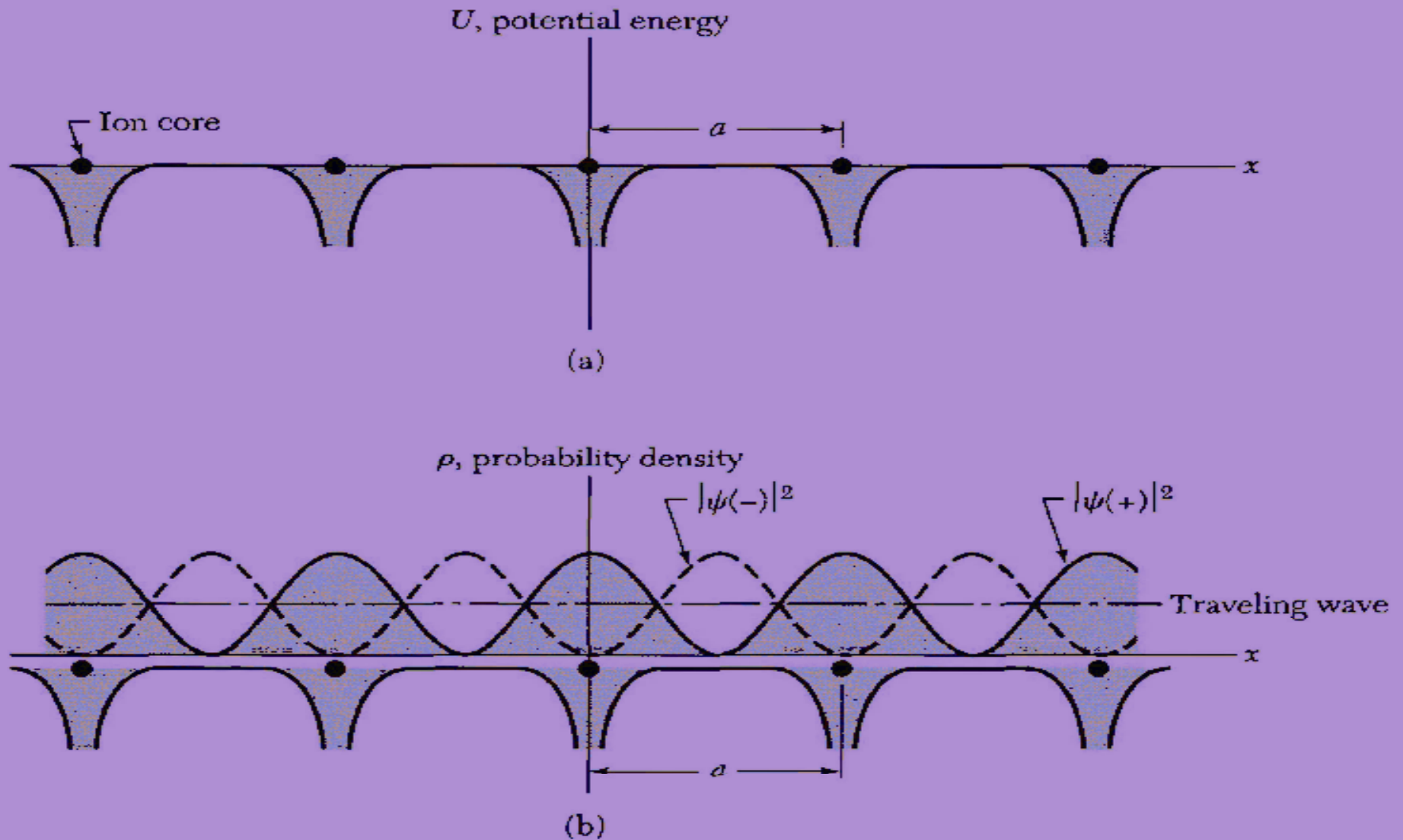
WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- We considered in Fig. 3 the approximate form we expect for the solution of the Schrödinger equation if the wave vector is at a zone boundary, as at $k = \pm\pi/a$.
- Here, we treat in detail the wave equation for a general potential, at general values of k .
- Let $U(x)$ denote the potential energy of an electron in a linear lattice of lattice constant a . Potential energy is invariant under the lattice translation. Hence: $U(x) = U(x + a)$.
- A function invariant under a crystal lattice translation may be expanded as a Fourier series in the reciprocal lattice vectors G .
- As a rule: **There is periodicity : There is Fourier Transform**
- We write the Fourier series for the potential energy as:

$$U(x) = \sum_G U_G e^{iGx} \quad (22)$$

Chapter 7: Energy Bands

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL



Chapter 7: Energy Bands

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- ❑ Please review Fourier Analysis.
- ❑ For actual crystal potentials; the values of the coefficients U_G tend to decrease rapidly with increasing magnitude of G . For a coulomb potential: U_G decreases as $1/G^2$
- ❑ In equation (22), we did not specify the x -values. We want to use only **real** values. Accordingly: (22) can be rewritten as:

$$U(x) = \sum_{G>0} U_G (e^{iGx} + e^{-iGx}) = 2 \sum_{G>0} U_G \cos Gx \quad (23)$$

- ❑ The wave equation of an electron in the crystal is $H\psi = \epsilon\psi$ where H is the Hamiltonian and ϵ is the energy eigenvalue.
- ❑ The full equation is then:

$$\left[\frac{p^2}{2m} + U(x) \right] \psi(x) = \left[\frac{p^2}{2m} + \sum_G U(x) e^{iGx} \right] \psi(x) = \epsilon \psi(x) \quad (24)$$

Chapter 7: Energy Bands

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- Equation (24) is written in the one-electron approximation in which the orbital $\psi(x)$ describes the motion of one electron in the potential of the ion cores and in the average potential of the other conduction electrons.
- The wavefunction $\psi(x)$ may be expressed as a Fourier series summed over all values of the wavevector permitted by the boundary conditions, so that:

$$\psi = \sum_k C(k) e^{ikx} \quad (25)$$

- The set of values of k has the form $2\pi n/L$.
- To solve the wave equation, substitute (25) in (24) to obtain a set of linear algebraic equations for the Fourier coefficients.
- We will take the solution as term by term:

Chapter 7: Energy Bands

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

□ The kinetic energy term is:

$$\frac{p^2}{2m} \psi(x) = \frac{1}{2m} \left(-i\hbar \frac{d}{dx} \right)^2 \psi(x) = \frac{-\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = \frac{\hbar^2}{2m} \sum_k k^2 C(k) e^{ikx} \quad (i)$$

and the potential energy term is :

$$U(x) \psi(x) = \left(\sum_G U_G e^{iGx} \right) \psi(x) = \sum_G \sum_k U_G e^{iGx} C(k) e^{ikx} \quad (ii)$$

The full Schrodinger Eq. becomes:

$$\frac{\hbar^2}{2m} \sum_k k^2 C(k) e^{ikx} + \sum_G \sum_k U_G C(k) e^{i(k+G)x} = \varepsilon \sum_k C(k) e^{ikx} \quad (26)$$

For 1 K value, this equation becomes:

$$\frac{\hbar^2 k^2}{2m} C(k) + \sum_G U_G C(k-G) = \varepsilon \sum_k C(k) e^{ikx} \quad (26)$$

Chapter 7: Energy Bands

Solution of the Central Equation

- Each Fourier component must have the same coefficient on both sides of the equation. Thus we have the **central equation**:

$$(\lambda_k - \varepsilon)C(k) + \sum_G U_G C(k - G) = 0 \quad (27)$$

with :

$$\lambda_k = \hbar^2 k^2 / 2m \quad (28)$$

- Eq. (27) is the Algebraic form of the well know Schrodinger equation in a periodic potential (24).
- It is not easy to solve it, but usually one can use only few terms.
- No. of solutions of this equation = no. of equations it has = No. of Fourier coefficients $C(K - G)$.

Chapter 7: Energy Bands

Solution of the Central Equation

- Eq. (27) represents a set of simultaneous linear equations that connect the coefficients $C(k - G)$ for all reciprocal lattice vectors G . It is a set because there are as many equations as there are coefficients C .
- To solve it, the determinant of the coefficients must vanish.
- As an application: for the case when $G = g$ (Shortest values of G):

$$\begin{bmatrix} \varepsilon_{k-2g} - \varepsilon & U_g & 0 & 0 & 0 \\ U_g & \varepsilon_{k-g} - \varepsilon & U_g & 0 & 0 \\ 0 & U_g & \varepsilon_k - \varepsilon & U_g & 0 \\ 0 & 0 & U_g & \varepsilon_{k+g} - \varepsilon & U_g \\ 0 & 0 & 0 & U_g & \varepsilon_{k+2g} - \varepsilon \end{bmatrix} \begin{bmatrix} C(k-2g) \\ C(k-g) \\ C(k) \\ C(k+g) \\ C(k+2g) \end{bmatrix} = 0 \quad (32)$$

- The solution of the determinant (32) gives a set of energy eigenvalues ε_{nk} .

Chapter 7: Energy Bands

Empty Lattice Approximation

- ❑ Band structures are usually plotted as energy versus wavevector in the first Brillouin zone. When wavevectors are outside this zone, they are carried back into the first zone by translation.
- ❑ We look for a G such that a k' in the first zone satisfies: $k' + G = k$
- ❑ where k is the free electron wavevector in the empty lattice.
- ❑ We can drop the ' from k since G can be - or + :

$$\varepsilon(k_x, k_y, k_z) = \frac{\hbar^2}{2m} (k + G)^2 = \frac{\hbar^2}{2m} \left[(k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2 \right]$$

- ❑ We consider as an example free electron bands of a simple cubic lattice. Suppose we want to exhibit the energy as a function of k in the [100] direction. Let $\hbar^2 / 2m = 1$. We show several bands in this empty lattice approximation with their energies $\varepsilon(000)$ at $k = 0$ and $\varepsilon(k_x 00)$ along the k_x axis in the first zone:

Chapter 7: Energy Bands

Empty Lattice Approximation

Band	$Ga/2\pi$	$\epsilon(000)$	$\epsilon(k_x, 00)$
1	000	0	k_x^2
2,3	100,100	$(2\pi/a)^2$	$(k_x \pm 2\pi/a)^2$
4,5,6,7	010,0 $\bar{1}$ 0,001,00 $\bar{1}$	$(2\pi/a)^2$	$k_x^2 + (2\pi/a)^2$
8,9,10,11	110,101,1 $\bar{1}$ 0,10 $\bar{1}$	$2(2\pi/a)^2$	$(k_x + 2\pi/a)^2 + (2\pi/a)^2$
12,13,14,15	$\bar{1}$ 10, $\bar{1}$ 01, $\bar{1}\bar{1}$ 0, $\bar{1}$ 0 $\bar{1}$	$2(2\pi/a)^2$	$(k_x - 2\pi/a)^2 + (2\pi/a)^2$
16,17,18,19	011,0 $\bar{1}$ 1,01 $\bar{1}$,0 $\bar{1}\bar{1}$	$2(2\pi/a)^2$	$k_x^2 + 2(2\pi/a)^2$

Chapter 7: Energy Bands

Empty Lattice Approximation

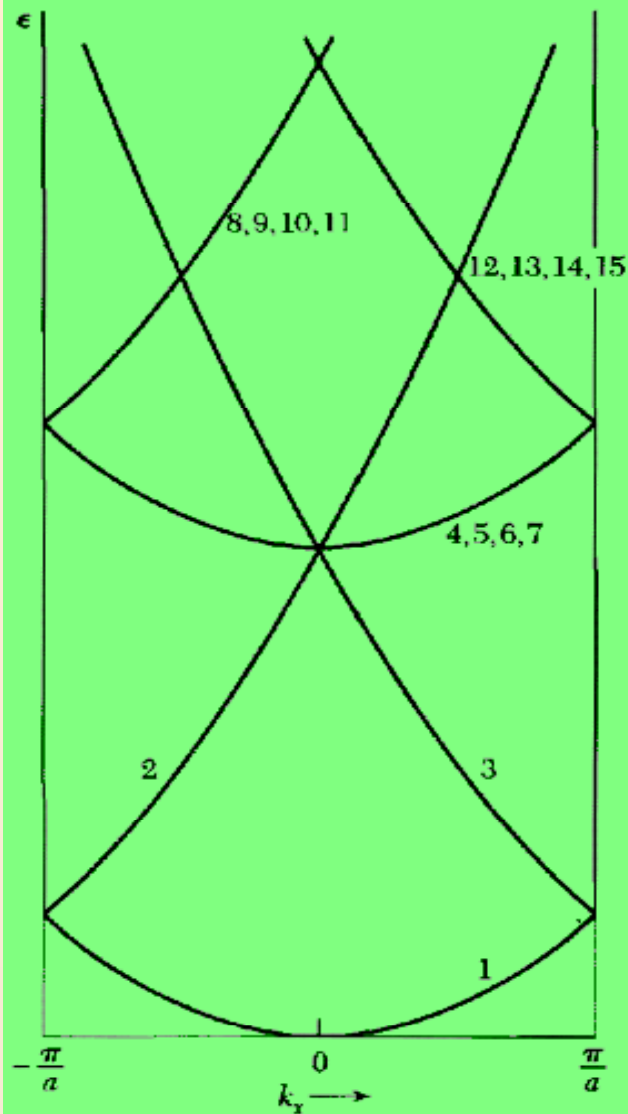


Figure 8 Low-lying free electron energy bands of the empty *sc* lattice, as transformed to the first Brillouin zone and plotted vs. $(k_x, 0, 0)$. The free electron energy is $\hbar^2(\mathbf{k} + \mathbf{G})^2/2m$, where the \mathbf{G} 's are given in the second column of the table. The bold curves are in the first Brillouin zone, with $-\pi/a \leq k_x \leq \pi/a$. Energy bands drawn in this way are said to be in the reduced zone scheme.

Chapter 7: Energy Bands

Empty Lattice Approximation

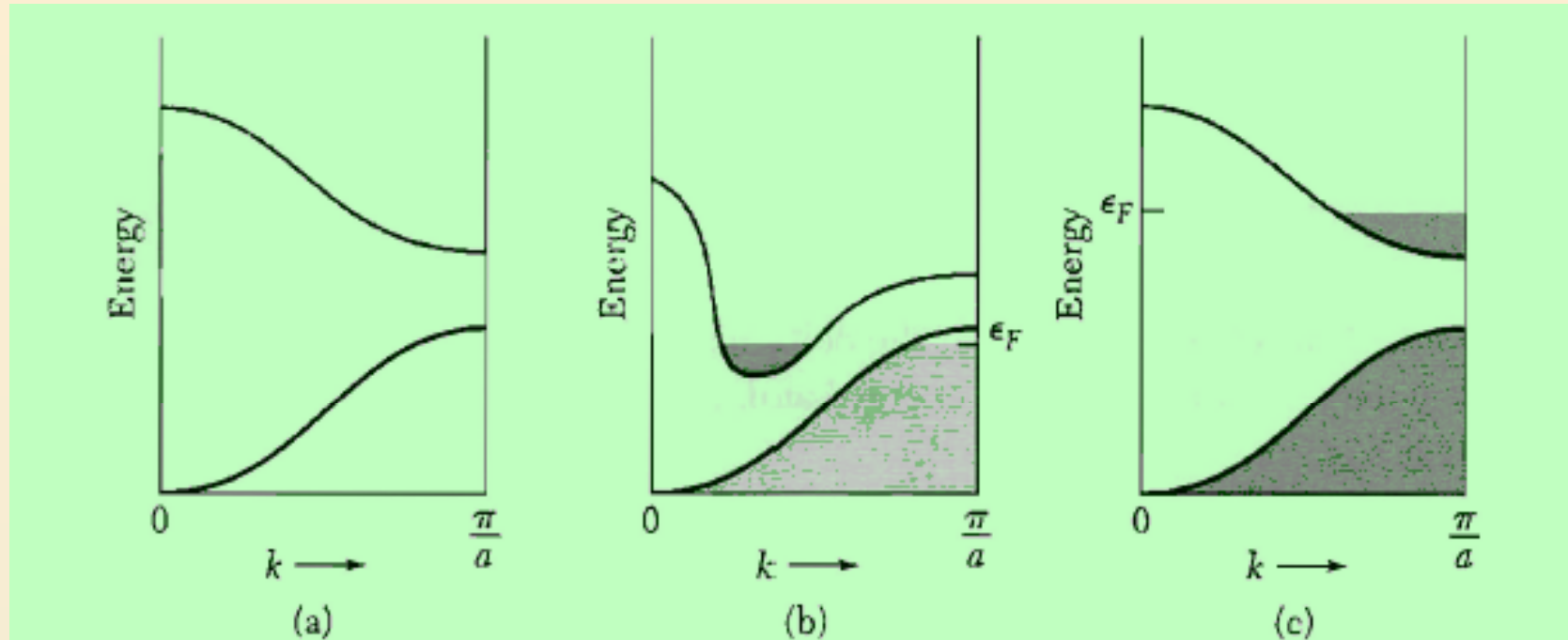


Figure 11 Occupied states and band structures giving (a) an insulator, (b) a metal or a semimetal because of band overlap, and (c) a metal because of electron concentration. In (b) the overlap need not occur along the same directions in the Brillouin zone. If the overlap is small, with relatively few states involved, we speak of a semimetal.