Band Theory and Electronic Properties of Solids

Phys 674

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Lecture No. 08

Electrons in a Weak Periodic Potential Part II

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Electrons in a Weak Periodic Potential

Introduction

- *Introduction*
- *SCHRODINGER EQUATION WHEN THE POTENTIAL IS WEAK*
- *Cases of Weak Periodic Potential*
- *ENERGY LEVELS NEAR A SINGLE BRAGG PLANE*
- *ENERGY Bands in One Dimension*
- *THE ENERGY GAP*
- *BRILLOUIN ZONES*

Weak Periodic Potential

- From last lectrure:
- We have arrived into the following equation:

$$\left(\varepsilon - \varepsilon^{0}_{\mathbf{k}-\mathbf{K}_i}\right) c_{\mathbf{k}-\mathbf{K}_i} = \sum_{j=1}^{m} U_{\mathbf{K}_j - \mathbf{K}_i}\, c_{\mathbf{k}-\mathbf{K}_j} \qquad i = 1, \ldots, m \tag{9.19}$$

Electrons in a Weak Periodic Potential

We have the general equation

$$(\epsilon - \epsilon^{0}_{k-\bar{k}_i})\, C_{k-\bar{k}_i} = \sum_{j=1}^{m} U_{\bar{k}_j - \bar{k}_i}\, C_{k-\bar{k}_j} \qquad i = 1, 2 \cdots m \qquad (1)$$

(9.19)

Now: we need to find Energy levels near a single Bragg plane:

What is Bragg plane?

we have $n\lambda = 2d\sin\theta$

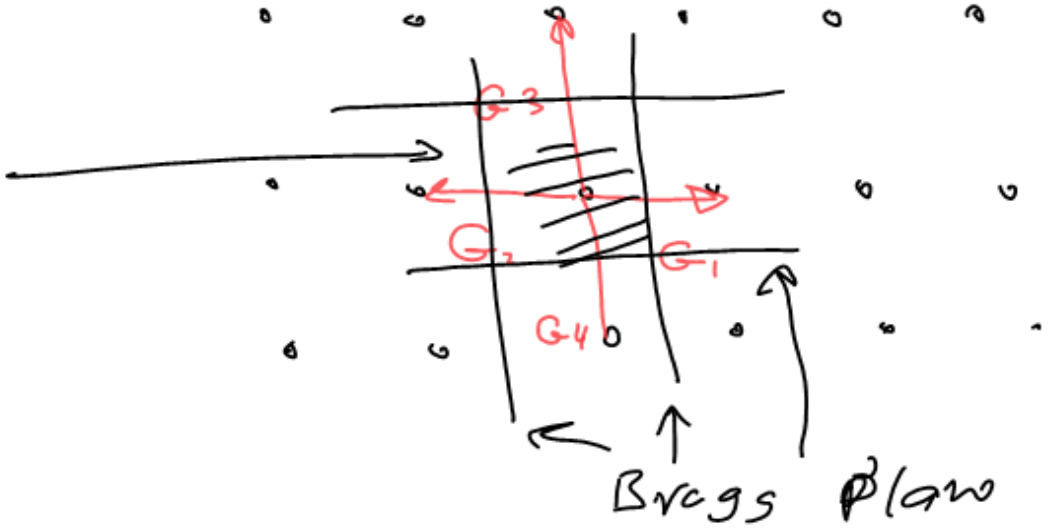
To have Peaks; we must have a Bragg plane

To have a Bragg Plane; we must have a reciprocal vector:

$$\bar{G} = h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$$

(hkl) are the Miller indices

First B.Z.



You can safely use $\bar{k}$ instead of $\bar{G}$

To find Energy Levels Near B.P.

We Consider Two free electrons with two Energy Levels within the order of U of each other.

Electrons in a Weak Periodic Potential

$$\textcircled{1}\quad \left(\epsilon - \epsilon^{\circ}_{k-\bar{k}_1}\right) C_{k-\bar{k}_1} = U_{\bar{k}_2-\bar{k}_1}\, C_{k-\bar{k}_2} \quad \cdots \textcircled{2}$$

$$\textcircled{2}\quad \left(\epsilon - \epsilon^{\circ}_{k-\bar{k}_2}\right) C_{k-\bar{k}_2} = U_{\bar{k}_1-\bar{k}_2}\, C_{k-\bar{k}_1} \quad \cdots \textcircled{3}$$

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let

$$\left.\begin{aligned} q &= \bar{k} - \bar{k}_1 \\ \bar{k} &= \bar{k}_2 - \bar{k}_1 \end{aligned}\right\} \cdots \textcircled{4}$$

$$\textcircled{2} \Rightarrow \left(\epsilon - \epsilon^{\circ}_{q}\right) C_q = U_{\bar{k}}\, C_{q-\bar{k}}$$

$$\left.\textcircled{3} \Rightarrow \left(\epsilon - \epsilon^{\circ}_{q-\bar{k}}\right) C_{q-\bar{k}} = U_{-\bar{k}}\, C_q = U^{*}_{\bar{k}}\, C_q \right\} \cdots \textcircled{5}$$

doing some approximation:

Electrons in a Weak Periodic Potential

let $\quad \varepsilon^{\circ}_{q} \simeq \epsilon^{\circ}_{q-\bar{\kappa}}$

and $\quad |\, \varepsilon^{\circ}_{q} - \varepsilon^{\circ}_{q-\bar{\kappa}'} \,| >> U \qquad \bar{\kappa}' \neq \bar{\kappa}$

Electrons in a Weak Periodic Potential

Weak Periodic Potential

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- The simplest example of the preceding discussion is *when two free electron levels are within order U of each other*, but far compared with *U* from all other levels. For this, (9.19) reduces to the two equations:

$$\because \left(\varepsilon - \varepsilon^0_{\mathbf{k}-\mathbf{K}_i}\right) c_{\mathbf{k}-\mathbf{K}_i} = \sum_{j=1}^{m} U_{\mathbf{K}_j-\mathbf{K}_i}\, c_{\mathbf{k}-\mathbf{K}_j} \qquad i = 1,\ldots,m \qquad (9.19)$$

$$\left.\begin{aligned} \left(\varepsilon - \varepsilon^0_{\mathbf{k}-\mathbf{K}_1}\right) c_{\mathbf{k}-\mathbf{K}_1} &= U_{\mathbf{K}_2-\mathbf{K}_1}\, c_{\mathbf{k}-\mathbf{K}_2} \\ \left(\varepsilon - \varepsilon^0_{\mathbf{k}-\mathbf{K}_2}\right) c_{\mathbf{k}-\mathbf{K}_2} &= U_{\mathbf{K}_1-\mathbf{K}_2}\, c_{\mathbf{k}-\mathbf{K}_1} \end{aligned}\right\} \qquad (9.20)$$

$$\text{let:} \quad \mathbf{q} = \mathbf{K} - \mathbf{K}_1 \quad \& \quad \mathbf{K} = \mathbf{K}_2 - \mathbf{K}_1 \qquad (9.21)$$

$$(9.20) \Rightarrow$$

$$\left.\begin{aligned} \left(\varepsilon - \varepsilon^0_{\mathbf{q}}\right) c_{\mathbf{q}} &= U_{\mathbf{K}}\, c_{\mathbf{q}-\mathbf{K}} \\ \left(\varepsilon - \varepsilon^0_{\mathbf{q}-\mathbf{K}}\right) c_{\mathbf{q}-\mathbf{K}} &= U_{-\mathbf{K}}\, c_{\mathbf{q}} = U^*_{\mathbf{K}}\, c_{\mathbf{q}} \end{aligned}\right\} \qquad (9.22)$$

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- We can do some approximations:

$$\left.\begin{aligned} &\varepsilon_{\mathbf{q}}^{0} \approx \varepsilon_{\mathbf{q}-\mathbf{K}}^{0} \\ &\left|\varepsilon_{\mathbf{q}}^{0} - \varepsilon_{\mathbf{q}-\mathbf{K}'}^{0}\right| >> U \quad \text{for } \mathbf{K}' \neq \mathbf{K}, 0 \end{aligned}\right\} \qquad (9.23)$$

- Now $\varepsilon_{\boldsymbol{q}}^{o}$ is equal to $\varepsilon_{\boldsymbol{q}-\boldsymbol{K}}^{o}$ for some reciprocal lattice vector only when $|\mathbf{q}| = |\mathbf{q} - \mathbf{K}|$. This means that **q** must lie on the Bragg plane bisecting the line joining the origin of **k** space to the reciprocal lattice point **K**. The assertion that $\varepsilon_{\boldsymbol{q}}^{o} - \varepsilon_{\boldsymbol{q}-\boldsymbol{K}'}^{o}$ only for **K'** = **K** requires that **q** lie *only* on this Bragg plane, and on no other.

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

(a) If $|\mathbf{q}| = |\mathbf{q} - \mathbf{K}|$, then the point $\mathbf{q}$ must lie in the Bragg plane determined by $\mathbf{K}$. (b) If the point $\mathbf{q}$ lies in the Bragg plane, then the vector $\mathbf{q} - \frac{1}{2}\mathbf{K}$ is parallel to the plane.

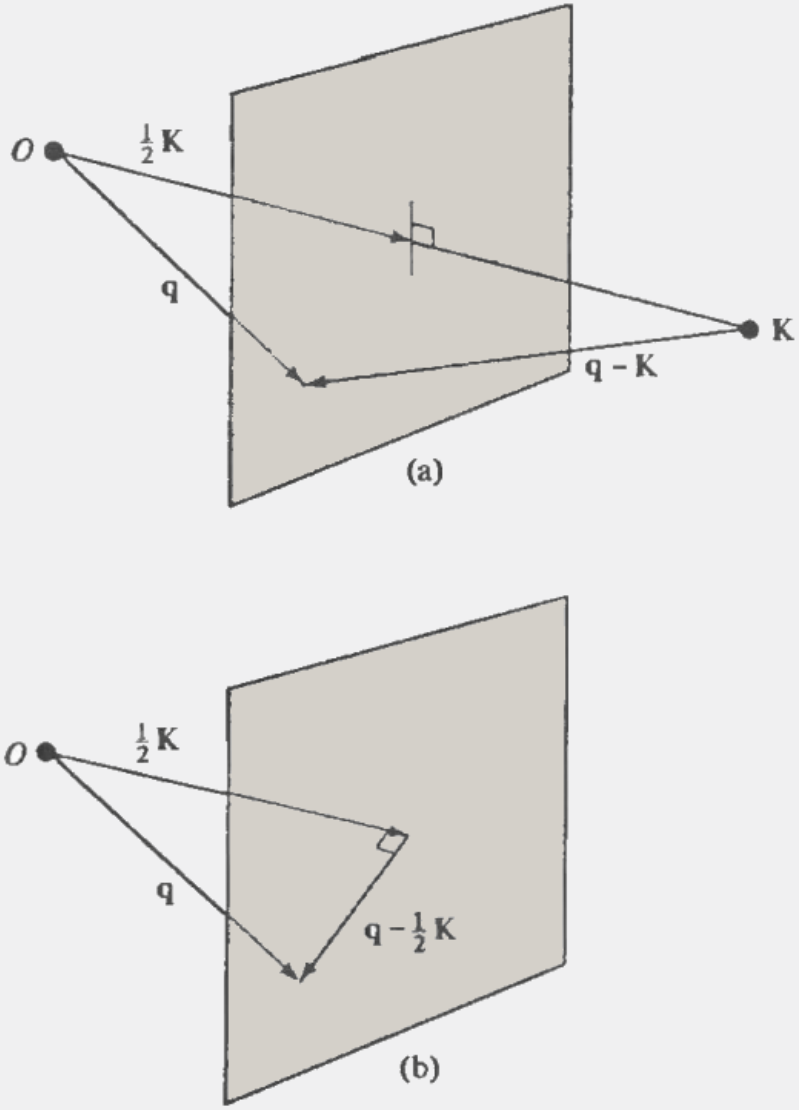


Fig. 5.1

Brag Plane Fig 5.1 :

$\Rightarrow$ if $\bar{K}$ is a reciprocal vector that connects O to point $\bar{K}$:

Then There is a plane that bisects it any wavevector $\bar{q}$ that satisfies the condition $|\bar{q}| = |\bar{q} - \bar{K}|$ $\Rightarrow$ point $\bar{q}$ must be on that plane.

$\Rightarrow$ # Energy degeneracy : ##

$$\epsilon_q \hat{\approx} \epsilon_{q-K}$$

∴ if electron wavevector q is close to but not exactly on Bragg plane $\Rightarrow$ nearly degenerate Energy

* When electron wavevector is near multiple B. Plane

⇒ Leads degenerate of many Energy Levels.

⇒ "Complex Band structures"

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- Thus conditions (9.23) have the geometric significance of requiring **q** to be close to a Bragg plane (but not close to a place where *two* or more Bragg planes intersect).
- Therefore the case of two nearly degenerate levels applies to an electron whose wave vector very nearly satisfies the condition for a single Bragg scattering
- Hence, *a weak periodic potential has its major effects on only those free electron levels whose wave vectors are close to ones at which Bragg reflections can occur.*
- Next; we examine the level structure when only a single Bragg plane is nearby, as determined by (9.22)

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- We solve eq. (9.22) using determinants:

$$\begin{vmatrix} \varepsilon - \varepsilon_{\mathbf{q}}^{0} & -U_{\mathbf{K}} \\ -U_{\mathbf{K}}^{*} & \varepsilon - \varepsilon_{\mathbf{q}-\mathbf{K}}^{0} \end{vmatrix} = 0 \qquad (9.24)$$

$$\Rightarrow$$

$$\left(\varepsilon - \varepsilon_{\mathbf{q}}^{0}\right)\left(\varepsilon - \varepsilon_{\mathbf{q}-\mathbf{K}}^{0}\right) = \left|U_{\mathbf{K}}\right|^{2} \qquad (9.25)$$

Solution is:

$$\varepsilon = \frac{1}{2}\left(\varepsilon_{\mathbf{q}}^{0} + \varepsilon_{\mathbf{q}-\mathbf{K}}^{0}\right) \pm \left[\left(\frac{\varepsilon_{\mathbf{q}}^{0} - \varepsilon_{\mathbf{q}-\mathbf{K}}^{0}}{2}\right)^{2} + \left|U_{\mathbf{K}}\right|^{2}\right]^{1/2} \qquad (9.26)$$

- Eq. (9.26) gives the dominant effect of the periodic potential on the energies of the two free electron levels $\varepsilon_{\boldsymbol{q}}^{o}$ and $\varepsilon_{\boldsymbol{q}-\boldsymbol{K}}^{o}$ when **q** is close to the Bragg plane determined by **K.**

Electrons in a Weak Periodic Potential

To get eq. (9.26):

$$\therefore (\epsilon - \epsilon^0_q)(\epsilon - \epsilon^0_{q-k}) - U_k^2 = 0$$

$$\Rightarrow \epsilon^2 - \epsilon\epsilon^0_{q-k} - \epsilon\epsilon^0_q + \epsilon^0_q \epsilon^0_{q-k} = U_k^2$$

$$\Rightarrow \epsilon^2 - \epsilon\underbrace{(\epsilon^0_q + \epsilon^0_{q-k})}_{b} + \underbrace{\epsilon^0_q \epsilon^0_{q-k} - U_k^2}_{c} = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\therefore \epsilon = \frac{1}{2}(\epsilon^0_q + \epsilon^0_{q-k}) \pm \left[\left(\frac{\epsilon^0_q - \epsilon^0_{q-k}}{2}\right)^2 + U_k^2\right]^{1/2} \quad \# \quad (9.26)$$

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

E in (9.26) represents the modified Energy Levels of the electron wavefunctions due to periodic pot.

(9.26) has 2 solutions $\pm$ corresponding to the split energy levels due to interaction with Periodic Potential. (Compare to 9.13)

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- The result (9.26) is particularly simple for points lying *on* the Bragg plane since, when **q** is on the Bragg plane, $\varepsilon_{\mathbf{q}}^{o} = \varepsilon_{\mathbf{q}-\mathbf{K}}^{o}$ Hence,

$$\varepsilon = \varepsilon_{\mathbf{q}}^{0} \pm \left|U_{\mathbf{K}}\right| \qquad (9.27)$$

- *Thus, at all points on the Bragg plane, one level is uniformly raised by $|U_K|$ and the other is uniformly lowered by the same amount.*

$$\because \frac{\hbar^2}{2m}(\mathbf{q}-\mathbf{K})^2 = \varepsilon_{\mathbf{q}-\mathbf{K}}^{0} \qquad (9.4)$$

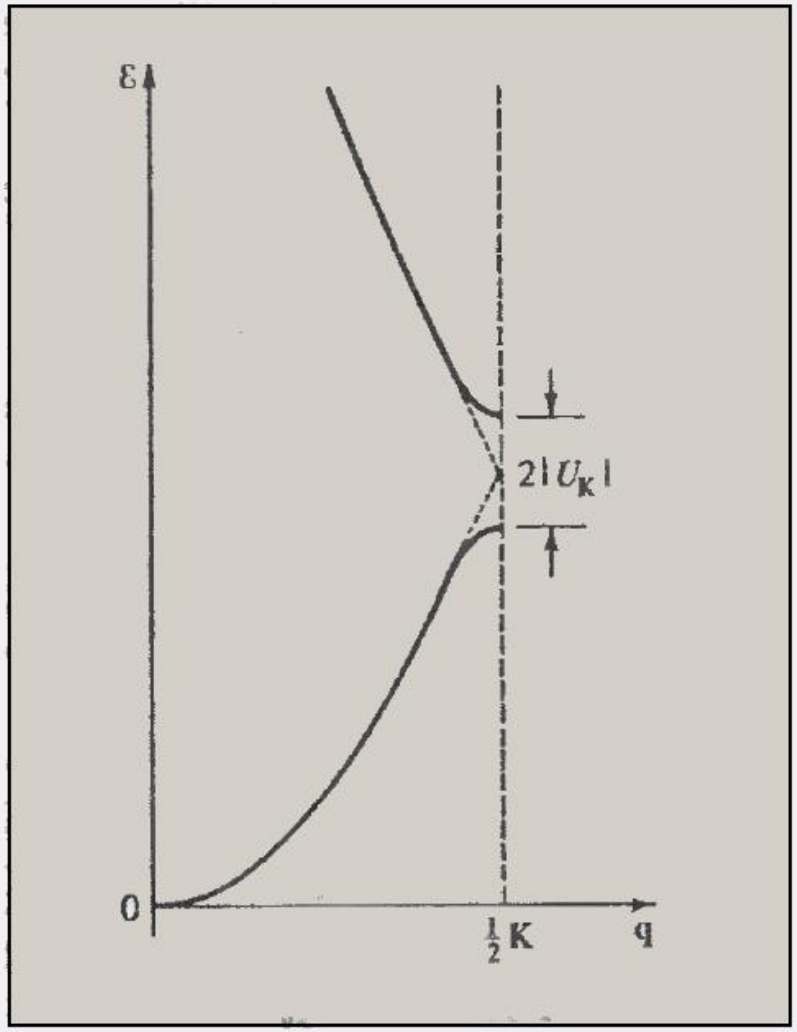
$$\text{if : } \varepsilon_{\mathbf{q}}^{0} = \varepsilon_{\mathbf{q}-\mathbf{K}}^{0},\ (9.26) \Rightarrow$$

$$\varepsilon = \frac{1}{2}\left(\frac{\hbar^2}{2m}\mathbf{q}^2 + \frac{\hbar^2}{2m}(\mathbf{q}-\mathbf{K})^2\right) \pm U_{\mathbf{K}} = \frac{1}{2}\left(\frac{\hbar^2}{2m}\mathbf{q}^2 + \frac{\hbar^2}{2m}(\mathbf{q}^2+\mathbf{K}^2-2\mathbf{q}\mathbf{K})\right) \pm U_{\mathbf{K}}$$

$$\therefore \frac{\partial \varepsilon}{\partial \mathbf{q}} = \frac{\hbar^2}{m}\left(\mathbf{q} - \frac{1}{2}\mathbf{K}\right) \qquad (9.28)$$

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE



Plot of the energy bands given by Eq. (9.26) for **q** parallel to **K**. The lower band corresponds to the choice of a minus sign in (9.26) and the upper band to a plus sign. When $\mathbf{q} = \frac{1}{2}\mathbf{K}$, the two bands are separated by a band gap of magnitude $2|U_K|$. When **q** is far removed from the Bragg plane, the levels (to leading order) are indistinguishable from their free electron values (denoted by dotted lines).

Fig. 5.2

Eq. (9.27) :

When $\bar{q}$ is on Brags plane

(9.26) simplifies to: $\varepsilon_q^\circ = \varepsilon_{q-\bar{h}}^\circ$

$$\varepsilon = \varepsilon_q^\circ \pm |U_k| \quad ---(9.27)$$

It means: all points on the Brags plane have two levels of Energy:

① one is raised by $|U_k|$

② " " lowered " $|U_k|$

at perpendicular bisector

Q. derive the Energy Levels near Bragg plane (9.26) and simplify it in case of $\varepsilon_q^\circ \approx \varepsilon_{q-\bar{h}}^\circ$ (9.27)

Explain the meaning. Also show that in this case (9.28) the gradient of ϵ is // to the plane

Electrons in a Weak Periodic Potential

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

ENERGY LEVELS NEAR A SINGLE BRAGG PLANE

- The result (9.28) means that when the point **q** is on the Bragg plane the gradient of ε is parallel to the plane.
- Since the gradient is perpendicular to the surfaces on which a function is constant, the constant-energy surfaces at the Bragg plane are perpendicular to the plane

Electrons in a Weak Periodic Potential

ENERGY Bands in One Dimension

- In the absence of any interaction the electronic energy levels are just a parabola (figure 9.4 a)
- To leading order in the weak one-dimensional periodic potential this curve remains correct except near Bragg "planes"
- When *q* is near a Bragg "plane" corresponding to the reciprocal lattice vector *K* (i.e., the point ½K) the corrected energy levels are determined by drawing another free electron parabola centered around *K* (figure 9.4 b)

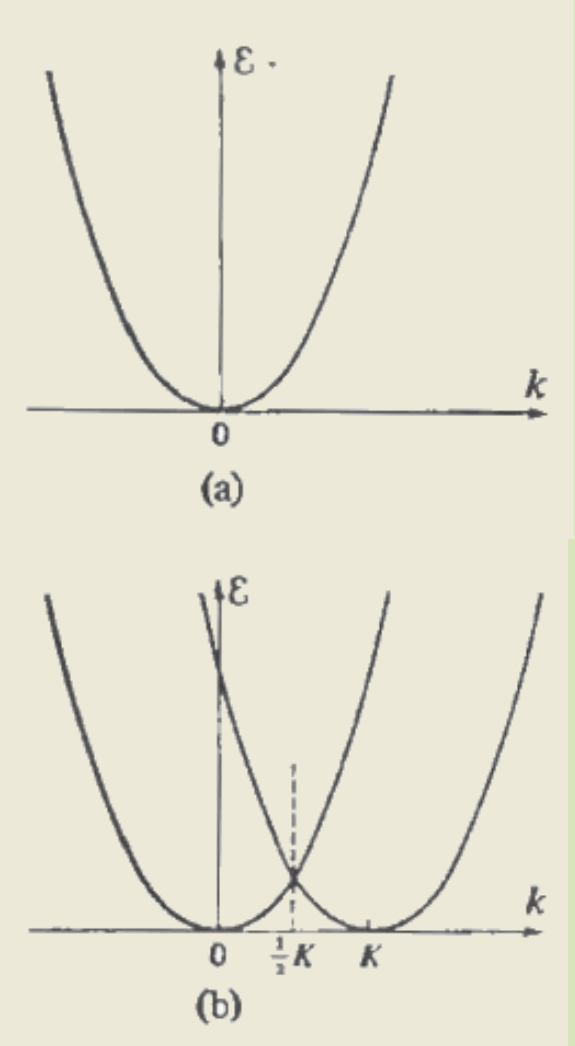


Fig. 9.4

ENERGY Bands in One Dimension

- noting that the degeneracy at the point of intersection is split by $2|U_K|$ in such a way that both curves have zero slope at that point, and redrawing Figure 9.4 b to get 9.4 c
- The original free electron curve is therefore modified as in Fig 9.4 d. When all Bragg planes and their associated Fourier components are included, we end up with a set of curves such as those shown in Figure 9.4 e

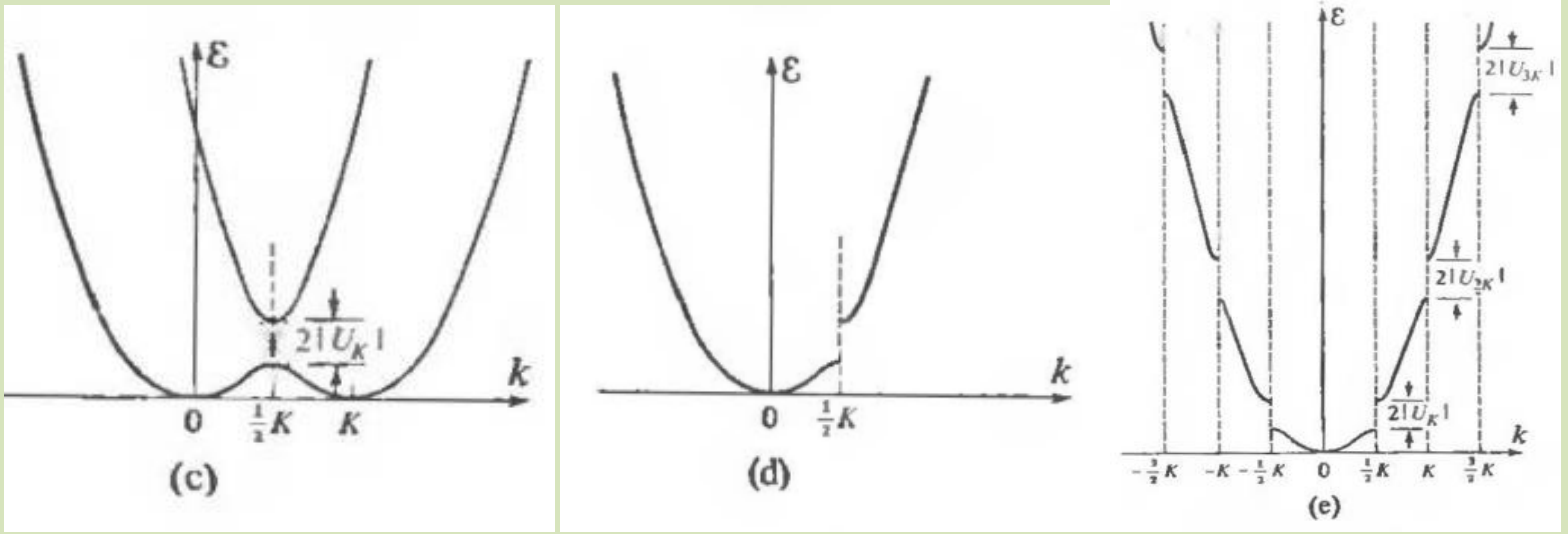


Fig. 9.4

Electrons in a Weak Periodic Potential

ENERGY Bands in One Dimension

- This particular way of depicting the energy levels is known as the *extended-zone scheme.* If we insist on specifying all the levels by a wave vector *k* in the first Brillouin zone, then we must translate the pieces of Figure 9.4 e, through reciprocal lattice vectors. into the first Brillouin zone. The result is shown in Figure 9.4 f. The representation is that of the *reduced-zone scheme*

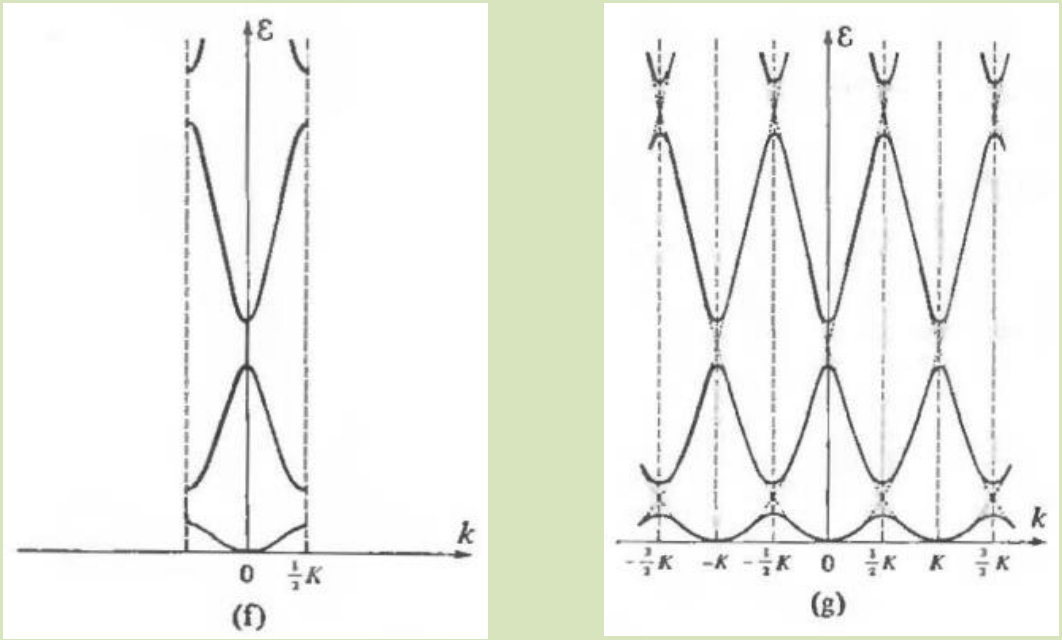


Fig. 9.4

Electrons in a Weak Periodic Potential

THE ENERGY GAP

- *Quite generally, a weak periodic potential introduces an "energy gap" at Bragg planes. By this we mean the following:*
- When $U_K = 0$, as **k** crosses a Bragg plane the energy changes continuously from the lower root of (9.26) to the upper, as illustrated in Figure 9.4b.
- When $U_K \neq 0$; this is no longer so. The energy only changes continuously with **k,** as the Bragg plane is crossed, if one stays with the lower (or upper) root, as illustrated in Figure 9.4 c.
- To change branches as **k** varies continuously it is now necessary for the energy to change *discontinuously* by at least $2|U_K|$

Electrons in a Weak Periodic Potential

BRILLOUIN ZONES

- Using the theory of electrons in a weak periodic potential to determine the complete band structure of a three-dimensional crystal leads to geometrical constructions of great complexity. It is often most important to determine the Fermi surface and the behavior of the $\varepsilon(\mathbf{k})$ in its immediate vicinity. In doing this for weak potentials, the procedure is ***first*** to draw the free electron Fermi sphere centered at $\mathbf{k} = 0$.
- Next, one notes that the sphere will be deformed in a manner of which Figure 9.6 is characteristic when it crosses a Bragg plane and in a correspondingly more complex way when it passes near several Bragg planes.
- When the effects of all Bragg planes are inserted, this leads to a representation of the Fermi surface as a fractured sphere in the extended-zone scheme

Electrons in a Weak Periodic Potential

BRILLOUIN ZONES

- To construct the Fermi surface in the reduced-zone scheme, one can translate all the pieces of the single fractured sphere back into the first zone through reciprocal lattice vectors.
- This procedure is made systematic through the geometrical notion of the higher Brillouin zones.

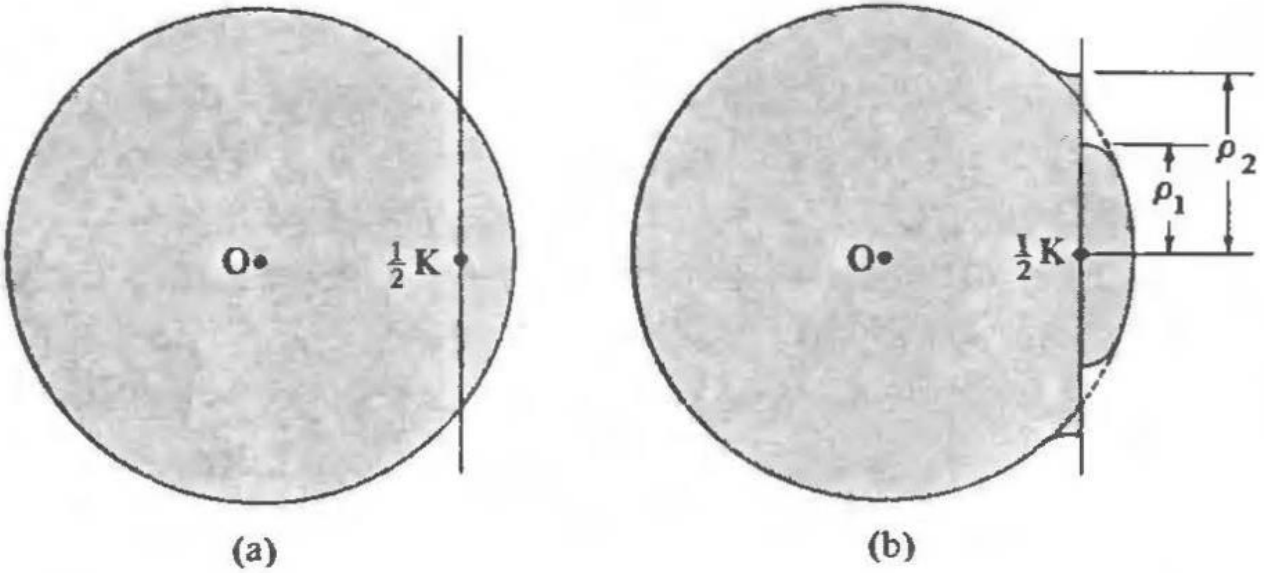


Figure 9.6
(a) Free electron sphere cutting Bragg plane located at $\frac{1}{2}\mathbf{K}$ from the origin ($U_{\mathbf{K}} = 0$). (b) Deformation of the free electron sphere near the Bragg plane when $U_{\mathbf{K}} \neq 0$. The constant-energy surface intersects the plane in two circles, whose radii are calculated in Problem 1.

Electrons in a Weak Periodic Potential

BRILLOUIN ZONES

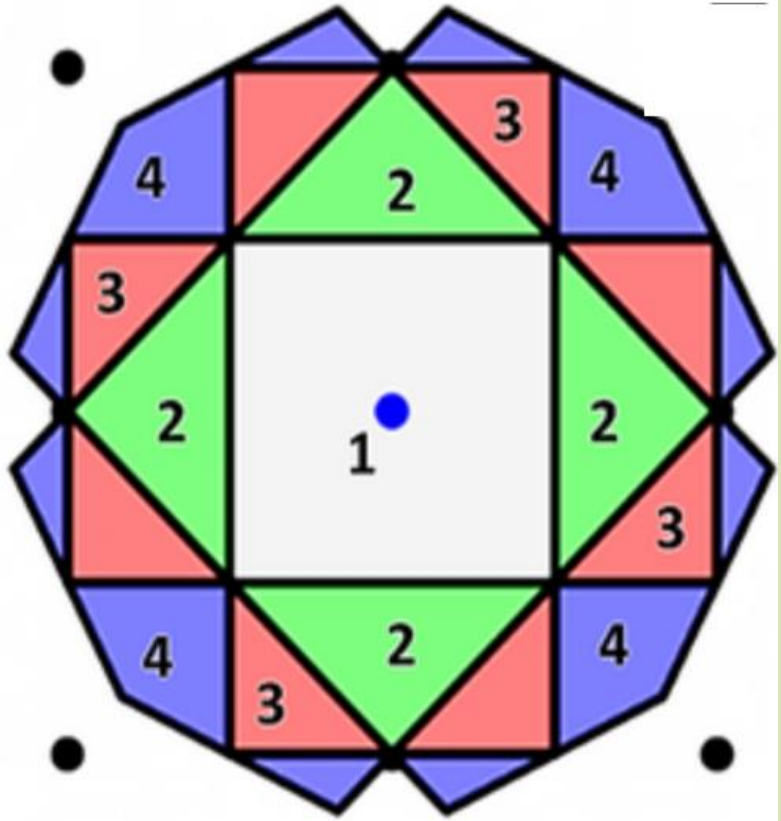
- Recall that the first Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice (pages 73 and 89), i.e. the set of points lying closer to **K** = 0
- Since Bragg planes bisect the lines joining the origin to points of the reciprocal lattice, one can equally well define the first zone as the set of points that can be reached from the origin without crossing any Bragg planes
- Higher Brillouin zones are simply other regions bounded by the Bragg planes defined as follows:
- The *first Brillouin zone* is the set of points in k-space that can be reached from the origin without crossing *any* Bragg plane. The *second Brillouin zone* is the set of points that can be reached from the first zone by crossing only one Bragg plane

Electrons in a Weak Periodic Potential

BRILLOUIN ZONES

- The (n + 1)th *Brillouin zone* is the set of points not in the *(n* - 1)th zone that can be reached from the nth zone by crossing only one Bragg plane.

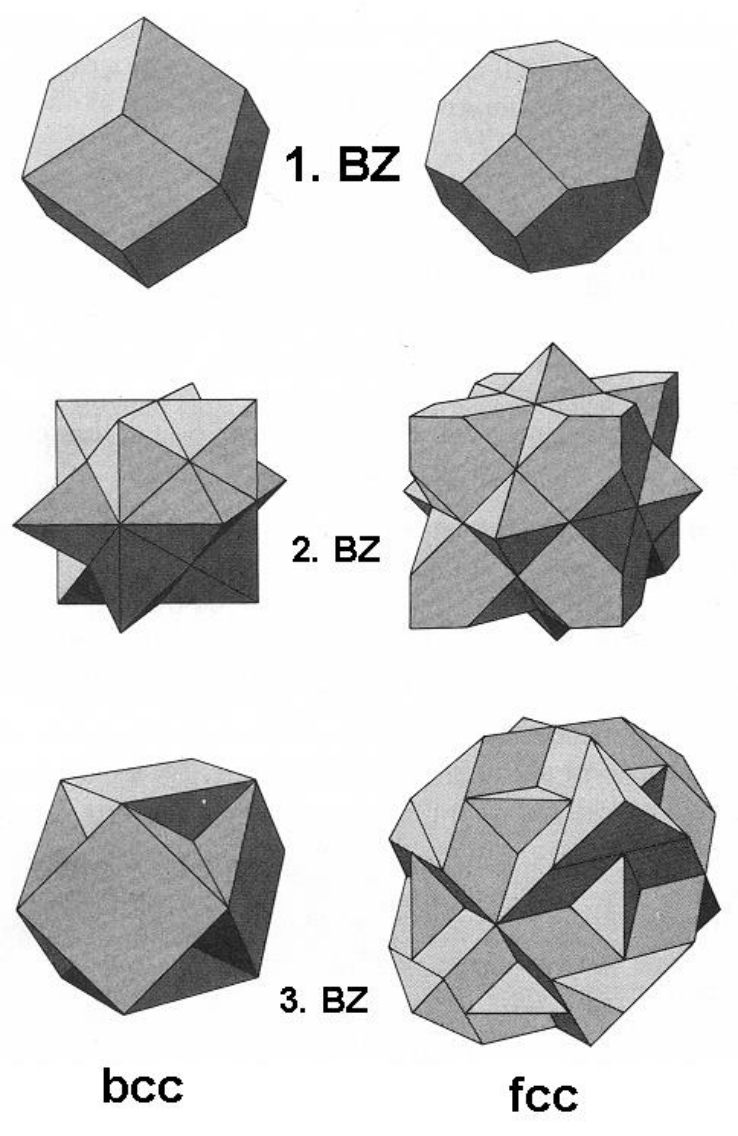
Figure 5.5
Illustration of the definition of the Brillouin zones for a two-dimensional square Bravais lattice. The reciprocal lattice is also a square lattice of side *b*. The figure shows all Bragg planes (lines, in two dimensions) that lie within the square of side 2*b* centered on the origin. These Bragg planes divide that square into regions belonging to zones 1 to 6. (Only zones 1, 2, and 3 are entirely contained within the square, however.)



Electrons in a Weak Periodic Potential

BRILLOUIN ZONES

Surfaces of the first, second and third Brillouin zones for (a) body-centered cubic and (b) face-centered cubic crystals. (Only the *exterior* surfaces are shown. It follows from the definition that the *interior* surface of the nth zone is identical to the exterior surface of the *(n* - 1)th zone. Evidently the surfaces bounding the zones become increasingly complex as the zone number increases. In practice it is often simplest to construct free electron Fermi surfaces by procedures that avoid making use of the explicit form of the Brillouin zones.



Thanks