

2D weak potential band structure - single square BL

R.L. in square with $\vec{K} = K(n\hat{x} + m\hat{y})$ n, m integers

$$K = 2\pi/a$$

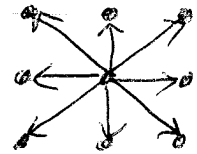
$a =$ lattice constant BL

The smallest R.L. vectors are

$$\vec{K}_0 = 0$$

$$\{\vec{K}_1\} = \{K\hat{x}, -K\hat{x}, K\hat{y}, -K\hat{y}\}$$

$$\{\vec{K}_2\} = \{K(\hat{x}+\hat{y}), K(\hat{x}-\hat{y}), K(-\hat{x}+\hat{y}), K(-\hat{x}-\hat{y})\}$$



For $\vec{g} = g\hat{x}$ in 1st BZ, i.e. $0 \leq g \leq \frac{K}{2}$, we will plot the band structure, in the reduced zone scheme, for all bands corresponding to the above 8 R.L. vectors.

$$E_i(\vec{g}) = \frac{\hbar^2}{2m} (\vec{g} + \vec{K}_i)^2 \quad \text{measure energy in units of} \quad E_x = \frac{\hbar^2}{2m} \left(\frac{K}{2}\right)^2$$

R.L. vector

$$\vec{K}_0 = 0$$

$$E = \frac{\hbar^2 g^2}{2m}$$

energy

$$E/E_x = 4(g/K)^2$$

degeneracy

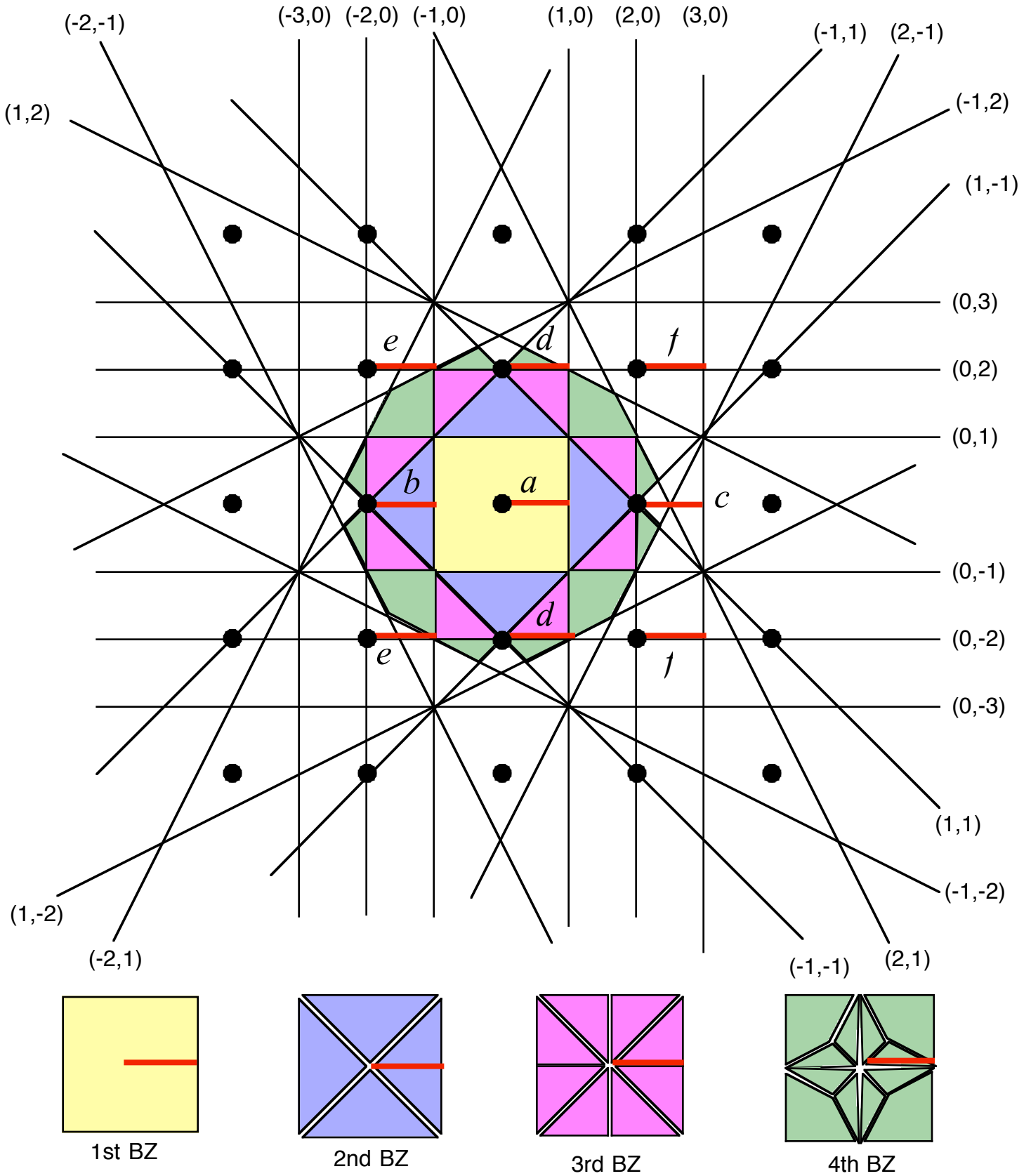
$$1 \quad (a)$$

$$\{\vec{K}_1\} \begin{cases} -K\hat{x} & E = \frac{\hbar^2}{2m} (g-K)^2 & E/E_x = 4\left(\frac{g}{K} - 1\right)^2 & 1 & (b) \\ +K\hat{x} & E = \frac{\hbar^2}{2m} (g+K)^2 & E/E_x = 4\left(\frac{g}{K} + 1\right)^2 & 1 & (c) \\ \pm K\hat{y} & E = \frac{\hbar^2}{2m} (g^2 + K^2) & E/E_x = 4\left[\left(\frac{g}{K}\right)^2 + 1\right] & 2 & (d) \end{cases}$$

$$\{\vec{K}_2\} \begin{cases} K(-\hat{x} \pm \hat{y}) & E = \frac{\hbar^2}{2m} [(g-K)^2 + K^2] & E/E_x = 4\left[\left(\frac{g}{K} - 1\right)^2 + 1\right] & 2 & (e) \\ K(+\hat{x} \pm \hat{y}) & E = \frac{\hbar^2}{2m} [(g+K)^2 + K^2] & E/E_x = 4\left[\left(\frac{g}{K} + 1\right)^2 + 1\right] & 2 & (f) \end{cases}$$

we plot the above curves of E/E_x vs g/K in reduced zone scheme

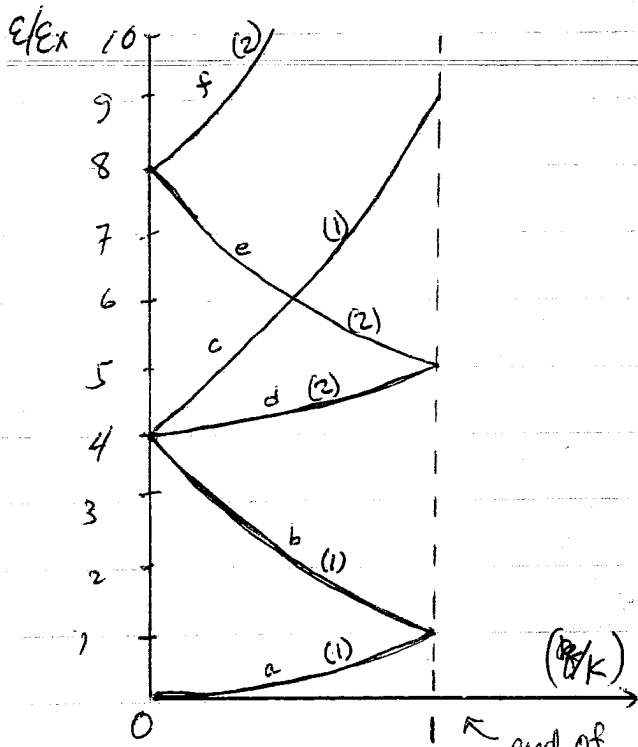
Reciprocal Lattice and k-space for a two-dimensional square Bravais Lattice of lattice constant a . Bragg planes are labeled by the reciprocal lattice vector that they bisect, $\mathbf{K} = (2\pi/a)(n, m)$.



Pieces of the n th Brillouin Zone translated back into the 1st BZ

red lines indicate the values of k for the free electron states giving rise to the band structure plotted in the reduced scheme on the next page

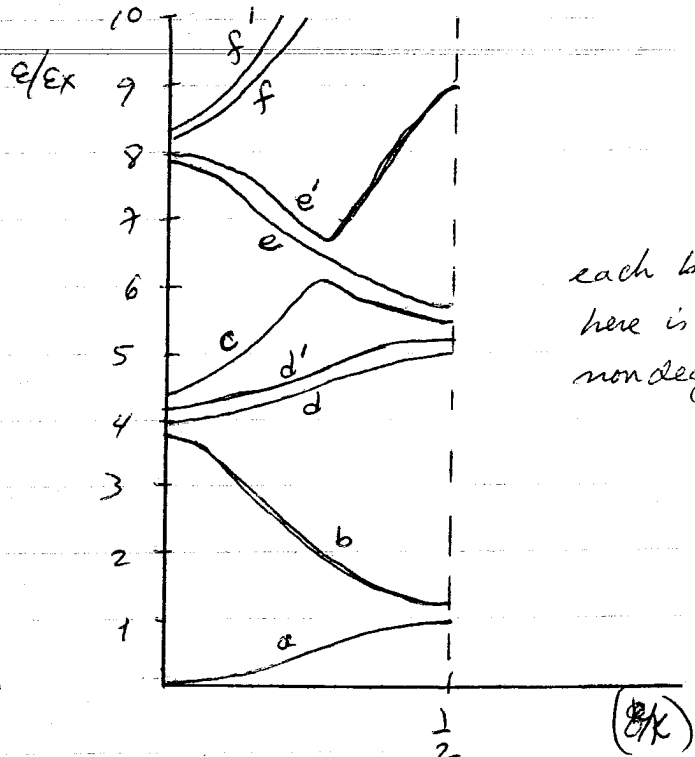
free electrons



reduced zone scheme

$\frac{1}{2}$ ← end of 1st BZ in \hat{x} direction

weak potential



each band here is non degenerate

- a) 1st BZ
- b) 2nd BZ
- d) 3rd + 4th BZs
- c) 5th + 7th BZs
- e) 5th, 6th + 7th BZs
- f) 8th + 9th BZ + higher

- a) 1st BZ
- b) 2nd BZ
- d) 3rd BZ
- d') 4th BZ
- c) 5th BZ
- e) 6th BZ
- e') 7th BZ
- f) 8th BZ
- f') 9th BZ

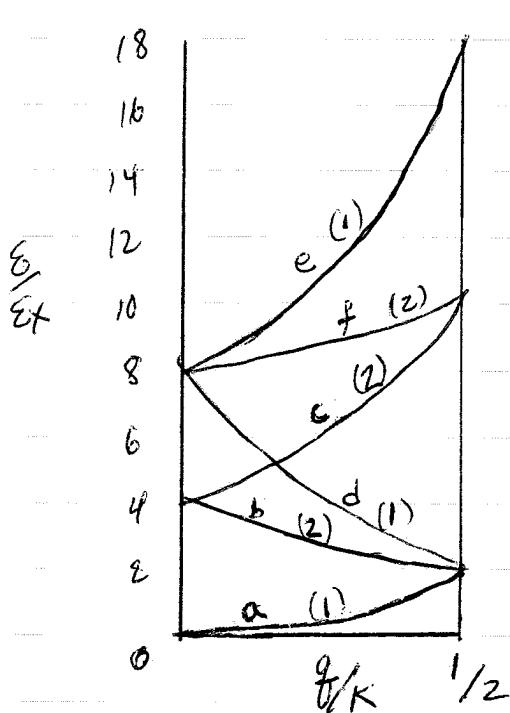
Weak potential splits degeneracies

More complicated band structure than in 1 dimension

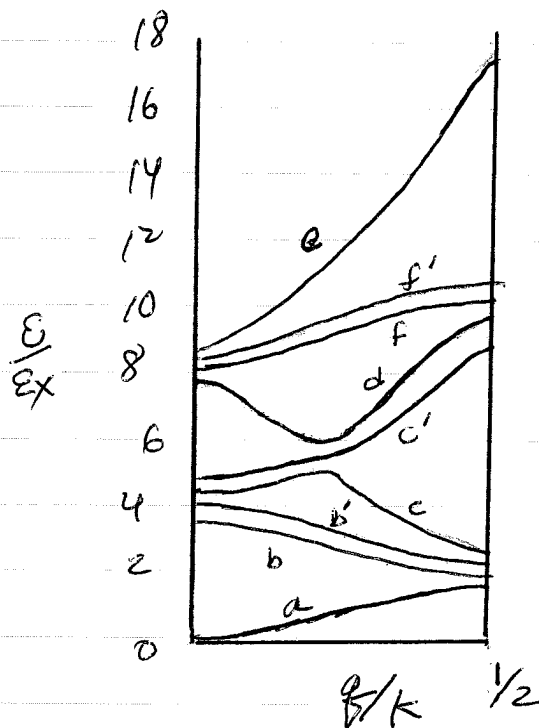
Not necessarily true that $\max[E_n(\vec{k})] \leq \min[E_{n+1}(\vec{k})]$

We can do the same thing for wave vectors along the diagonal of the 1st BZ, i.e. $\vec{q} = q(\hat{x} + \hat{y})$, $0 \leq q \leq k/2$

	R.L.	energy	degeneracy
	$\vec{k}_0 = 0$	$E = \frac{\hbar^2 q^2}{2m} (2)$	$E/E_x = 8(P/K)^2$ 1 (a)
$\{\vec{k}_1\}$	$-K\hat{x}, -K\hat{y}$	$E = \frac{\hbar^2}{2m} [(q-K)^2 + q^2]$	$E/E_x = 4[(\frac{q}{K}-1)^2 + (\frac{q}{K})^2]$ 2 (b)
	$+K\hat{x}, +K\hat{y}$	$E = \frac{\hbar^2}{2m} [(q+K)^2 + q^2]$	$E/E_x = 4[(\frac{q}{K}+1)^2 + (\frac{q}{K})^2]$ 2 (c)
$\{\vec{k}_2\}$	$-K\hat{x} - K\hat{y}$	$E = \frac{\hbar^2}{2m} [2(q-K)^2]$	$E/E_x = 8[\frac{q}{K}-1]^2$ 1 (d)
	$+K\hat{x} + K\hat{y}$	$E = \frac{\hbar^2}{2m} [2(q+K)^2]$	$E/E_x = 8[\frac{q}{K}+1]^2$ 1 (e)
	$-K\hat{x} + K\hat{y}$ $K\hat{x} - K\hat{y}$	$E = \frac{\hbar^2}{2m} [(q+K)^2 + (q-K)^2]$	$E/E_x = 4[(\frac{q}{K}+1)^2 + (\frac{q}{K}-1)^2]$ 2 (f)



free electrons

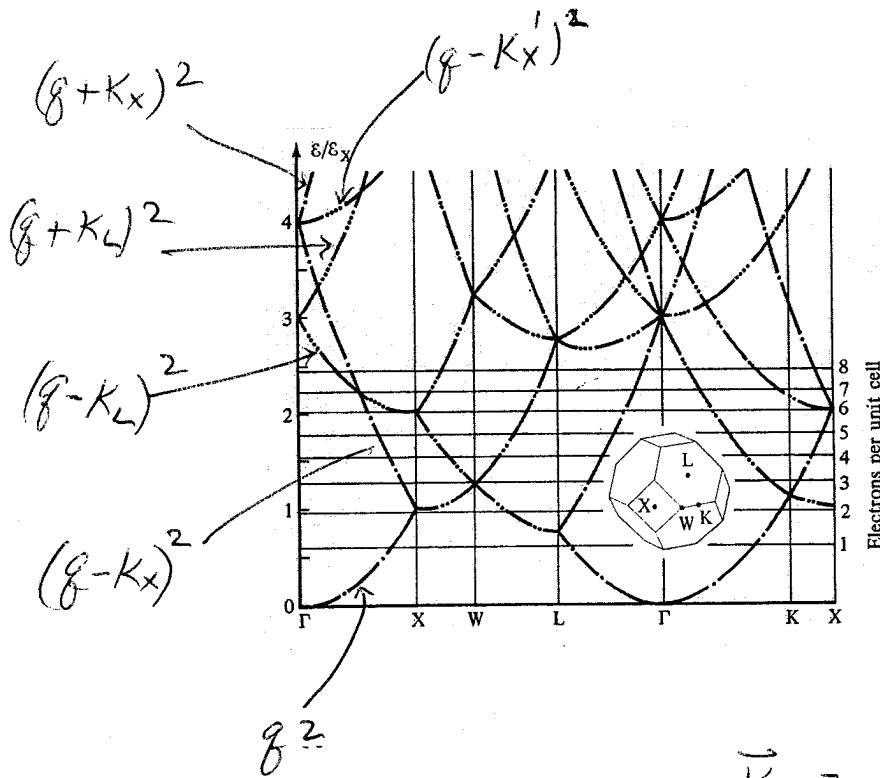


weak potential

gaps open up where free electron states are degenerate
weak potential "lifts" degeneracies

To represent band structure in 2D or 3D one picks \vec{q} in certain symmetry directions, and plots $E_n(\vec{q})$ vs $|\vec{q}|$ along these directions, as done above.

3 Dimensional free electron band structure



A+M

Figure 9.5

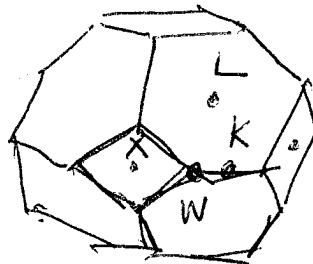
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points Γ ($k = 0$), K, L, W, and X. ϵ_x is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

plot E_{q-k}^0 for \vec{q} in special directions for all \vec{k} in R-L.

$$\vec{k}_x = (1, 0, 0)$$

$$\vec{k}_L = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

$$\vec{q}_x = (\frac{1}{2}, 0, 0)$$

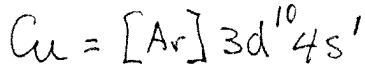
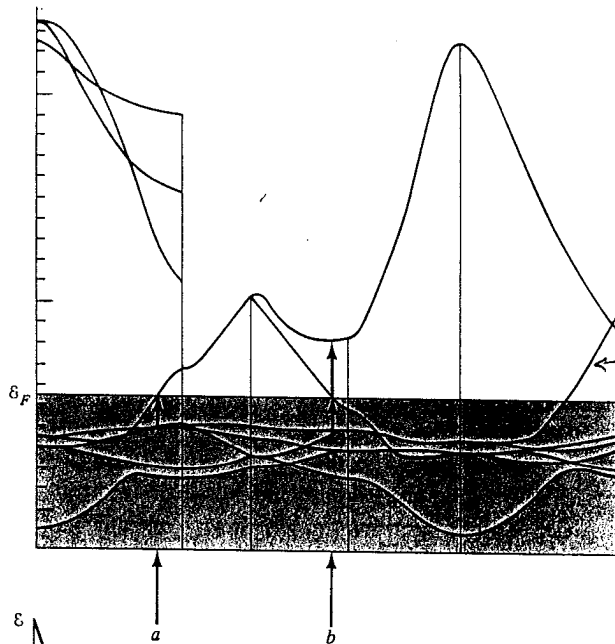


X' ← 1st BZ of fcc

A+M

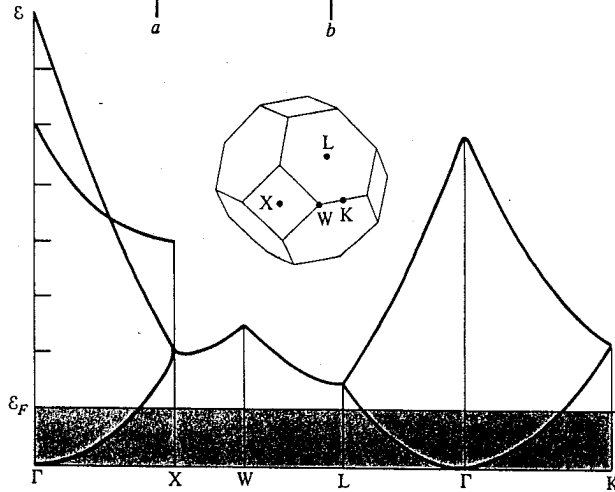
Figure 15.11

Burdick's calculated bands for copper, illustrating that the absorption threshold for transitions up from the conduction band is about 4 eV, while the threshold for transitions from the *d*-band to the conduction band is only about 2 eV. (The energy scale is in tenths of a rydberg (0.1 Ry = 1.36 eV).) Note the resemblance of the bands other than the *d*-bands to the free electron bands plotted below.



~~Free electron bands~~

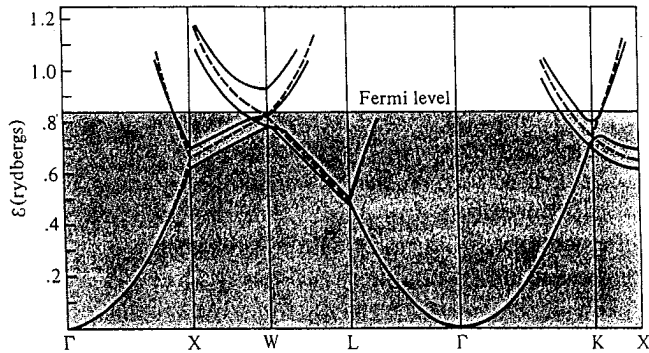
Free electron bands →



A+M

Figure 11.9

Calculated valence bands for aluminum (three electrons outside of a closed-shell neon configuration) compared with free electron bands (dashed lines). The bands are computed by the KKR method. (B. Segall, *Phys. Rev.* 124, 1797 (1961).)



$Z = 3$

Bravais Lattice with a basis

Suppose we have a monatomic BL with a basis (all atoms identical). If $\phi(\vec{r}-\vec{r}_0)$ is the potential from the ion centered at \vec{r}_0 , then the periodic ion potential is

$$U(\vec{r}) = \sum_i \sum_j \phi(\vec{r}-\vec{R}_i-\vec{d}_j)$$

since ions are located at positions $\vec{R}_i+\vec{d}_j$
Fourier transform is:

$$U_{\vec{k}} = \frac{1}{V} \int_{\text{primitive cell}} d^3r e^{-i\vec{k}\cdot\vec{r}} \sum_{ij} \phi(\vec{r}-\vec{R}_i-\vec{d}_j)$$

$$= \frac{1}{V} \int_{\text{all space}} d^3r e^{-i\vec{k}\cdot\vec{r}} \sum_{ij} \phi(\vec{r}-\vec{R}_i-\vec{d}_j)$$

$$= \sum_i \frac{1}{V} \int_{\text{all space}} d^3r e^{-i\vec{k}\cdot\vec{r}} \sum_j \phi(\vec{r}-\vec{R}_i-\vec{d}_j)$$

let $\vec{r}' = \vec{r} - \vec{R}_i$ and do change of integration variable

$$U_{\vec{k}} = \sum_i \frac{1}{V} \int_{\text{all space}} d^3r' e^{-i\vec{k}\cdot(\vec{r}'+\vec{R}_i)} \sum_j \phi(\vec{r}'-\vec{d}_j)$$

$$= \sum_i \frac{1}{V} \int_{\text{all space}} d^3r' e^{-i\vec{k}\cdot\vec{r}'} \sum_j \phi(\vec{r}'-\vec{d}_j)$$

since $\vec{k}\cdot\vec{R}_i = 2\pi$

$$= \frac{N}{V} \int_{\text{all space}} d^3r' e^{-i\vec{k}\cdot\vec{r}'} \sum_j \phi(\vec{r}'-\vec{d}_j)$$

Since all the terms in the Σ_i are now identical

$$U_{\vec{k}} = \frac{1}{v} \int_{\text{all space}} d^3r e^{-i\vec{k}\cdot\vec{r}} \sum_j \phi(\vec{r}-\vec{d}_j) \quad \text{as } v \equiv \frac{V}{N}$$

substitute in F.T. of $\phi(\vec{r})$

$$\phi(\vec{r}-\vec{d}_j) = \int \frac{d^3k'}{(2\pi)^3} e^{i\vec{k}'\cdot(\vec{r}-\vec{d}_j)} \phi_{k'}$$

So

$$U_{\vec{k}} = \frac{1}{v} \int d^3k' \phi_{k'} \underbrace{\int_{\text{all space}} \frac{d^3r}{(2\pi)^3} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}}_{\delta(\vec{k}'-\vec{k})} \sum_j e^{-i\vec{k}'\cdot\vec{d}_j}$$

$$= \frac{1}{v} \phi_{\vec{k}} \sum_j e^{-i\vec{k}\cdot\vec{d}_j}$$

$$U_{\vec{k}} = \frac{1}{v} \phi_{\vec{k}} S_{\vec{k}} \quad \text{proportional to geometric structure factor } S_{\vec{k}}$$

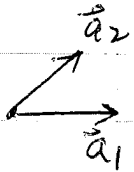
If $S_{\vec{k}}$ vanishes - we saw that there will be no diffraction peak in X-ray scattering at \vec{k} .

Now we see the analogous result, when $S_{\vec{k}} = 0$ then $U_{\vec{k}} = 0$, and there will be no energy gap opening up for electron states with \vec{k} that lie on the Bragg plane bisecting \vec{k} .

An important case where this happens is for hcp crystals

For hcp $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$, $\vec{a}_3 = c\hat{z}$

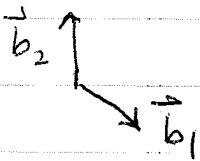
two point basis $\vec{d}_1 = 0$, $\vec{d}_2 = \frac{1}{3}(\vec{a}_1 + \vec{a}_2) + \frac{1}{2}\vec{a}_3$



lies in center of cells of triangular lattice in xy plane, and halfway between the two triangular layers

R.L.

$$\vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3 \quad \left\{ \begin{array}{l} \vec{b}_1 = \frac{4\pi}{\sqrt{3}a} \left(\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y} \right) \\ \vec{b}_2 = \frac{4\pi}{\sqrt{3}a} \hat{y} \\ \vec{b}_3 = \frac{2\pi}{c} \hat{z} \end{array} \right.$$

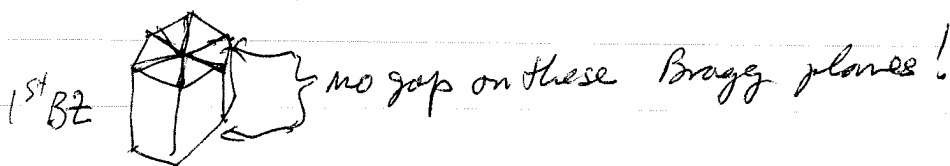


Then $S_{\vec{K}} = e^{-i\vec{K}\cdot\vec{d}_1} + e^{-i\vec{K}\cdot\vec{d}_2}$

$$= 1 + e^{-i(n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3) \cdot \left(\frac{\vec{a}_1}{3} + \frac{\vec{a}_2}{3} + \frac{\vec{a}_3}{2} \right)}$$

$$S_{\vec{K}} = 1 + e^{-2\pi i \left(\frac{n_1}{3} + \frac{n_2}{3} + \frac{n_3}{2} \right)}$$

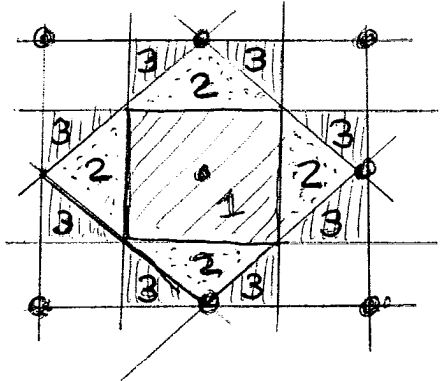
If, for example, $n_1 = n_2 = 0$, $n_3 = \pm 1$, then $S_{\vec{K}} = 0$. So no gap opens on the Bragg plane that bisects $\vec{K} = \pm \frac{2\pi}{c} \hat{z}$ - i.e. the top and bottom surfaces of the 1st BZ.



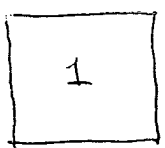
and Fermi Surface

Zones in Two dimensions - single square BL

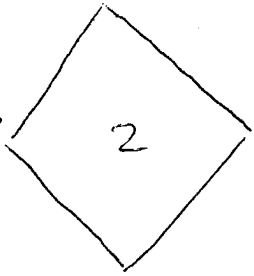
Draw in Bragg p planes



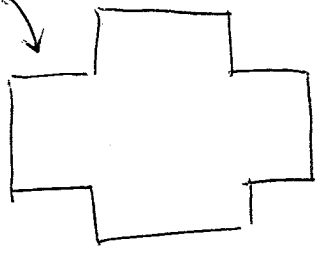
so ^{outer} surface 1st zone looks like



outer surface 2nd zone is →



outer surface 3rd zone is →

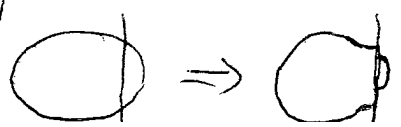


Surface of n th zone gets more complicated as n increases

To find shape of constant energy surface (fermi surface) in weak potential approx:

- 1) Draw free fermi sphere corresponding to desired energy
- 2) See ~~which~~ which zones surface of sphere intersects
There will be branches of surface in each ~~zone~~ ^{band, corresponding to ~~one~~ the} zones
- 3) deform free energy sphere where it intersects zone boundary so that it is \perp to Bragg plane (HW probl

#2)

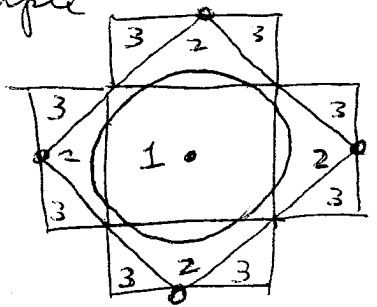


(often ignore this step as 1st approx)

4) This gives constant energy surface in extended zone scheme.
 Translate branches of surface in n th zone back to 1st zone (by adding appropriate recip lattice vector) to get branches of surface in reduced zone scheme.
Or translate through all recip lattice vectors to get repeated zone scheme.

example

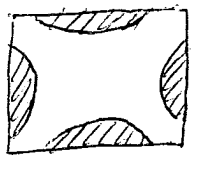
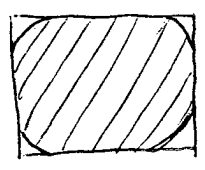
extended zone scheme



This free electron surface ^(of energy E_0) intersects 1st & 2nd zones only

Translate pieces of curves back to 1st BZ

branches of surface in 1st ~~zone~~ band.



branches of surface in 2nd ~~band~~ translated back to 1st BZ

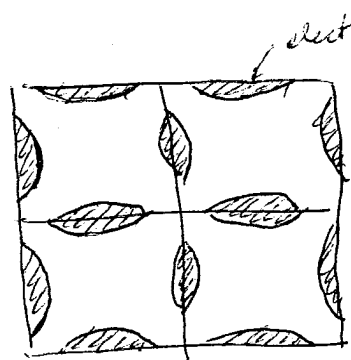
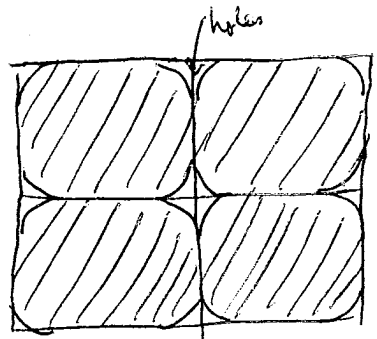
reduced zone scheme

Branches of curve in reduced zone scheme

shaded areas are states of lower energy $E < E_0$.
 unshaded areas are states of greater energy $E > E_0$

In repeated zone scheme, branches look like

zones in 1st zone



branches in 2nd zone

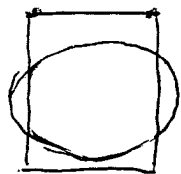
branches of Fermi surface are closed curves

If surface we have drawn is Fermi surface, then shaded areas are filled states.

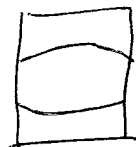
In 1st band we have small pockets of holes } more meaning
 In 2nd band we have small pockets of electrons } to this when
 we get to dynamics

In both cases, the constant energy surface in the repeated zone scheme is a closed curve. This need not be the case for a less symmetric crystal

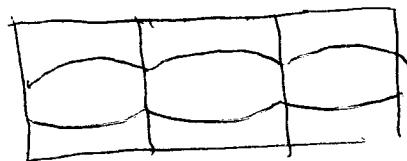
1st BZ



in this case, branches in 1st zone are



when we extend to repeated zone scheme we get



surface of constant energy is an open curve

The distinction between open and closed surfaces will be very important when we consider the dynamics (motion in magnetic field - energy conserved - electron moves on const energy surface)

See text for pictures in 3-D.

Note that in 2 + 3 dimensions, one always has partially full bands. \Rightarrow weak potential method does not give insulators or semiconductors.

See Ashcroft + Mermin Figs 9.8 and 9.9 for BZ's and Fermi surface branches in 3D

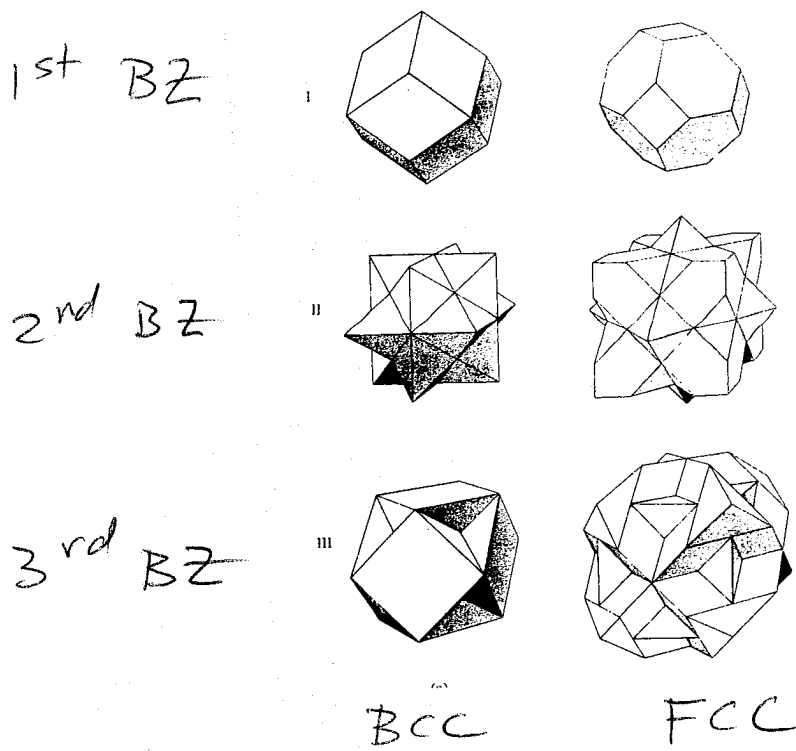


Figure 9.8 Surfaces of the first, second, and third Brillouin zones for (a) body-centered cubic and (b) face-centered cubic crystals. (Only the exterior surfaces are shown. It follows from the definition on page 163 that the interior surface of the n th zone is identical to the exterior surface of the $(n - 1)$ 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 (such as those described in Problem 4) that avoid making use of the explicit form of the Brillouin zones. (After R. Lück, doctoral dissertation, Technische Hochschule, Stuttgart, 1965.)

Free electron Fermi surface FCC

$$Z = 4$$

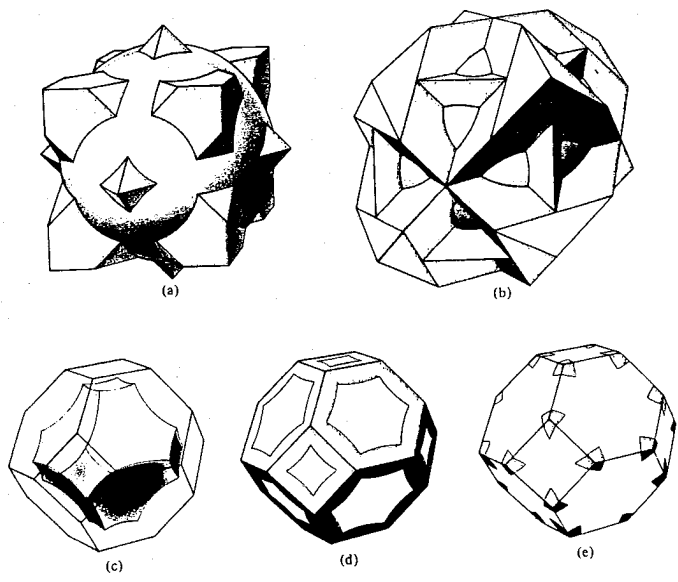


Figure 9.9 The free electron Fermi sphere for a face-centered cubic metal of valence 4. The first zone lies entirely within the interior of the sphere, and the sphere does not extend beyond the fourth zone. Thus the only zone surfaces intersected by the surface of the sphere are the (exterior) surfaces of the second and third zones (cf. Figure 9.8b). The second-zone Fermi surface consists of those parts of the surface of the sphere lying entirely within the polyhedron bounding the second zone (i.e., all of the sphere except the parts extending beyond the polyhedron in (a)). When translated through reciprocal lattice vectors into the first zone, the pieces of the second-zone surface give the simply connected figure shown in (c). (It is known as a "hole surface"; the levels it encloses have higher energies than those outside). The third-zone Fermi surface consists of those parts of the surface of the sphere lying outside of the second zone (i.e., the parts extending beyond the polyhedron in (a)) that do not lie outside the third zone (i.e., that are contained within the polyhedron shown in (b)). When translated through reciprocal lattice vectors into the first zone, these pieces of sphere give the multiply connected structure shown in (d). The fourth-zone Fermi surface consists of the remaining parts of the surface of the sphere that lie outside the third zone (as shown in (b)). When translated through reciprocal lattice vectors into the first zone they form the "pockets of electrons" shown in (e). For clarity (d) and (e) show only the intersection of the third and fourth zone Fermi surfaces with the surface of the first zone. (From R. Lück, *op. cit.*)