2D weak potential band structure – single square BL

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

$K = 2\pi/a$

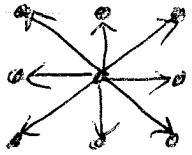
a = lattice constant BL

The smallest R.L. vectors are

$\vec{K}_0 = 0$

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

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



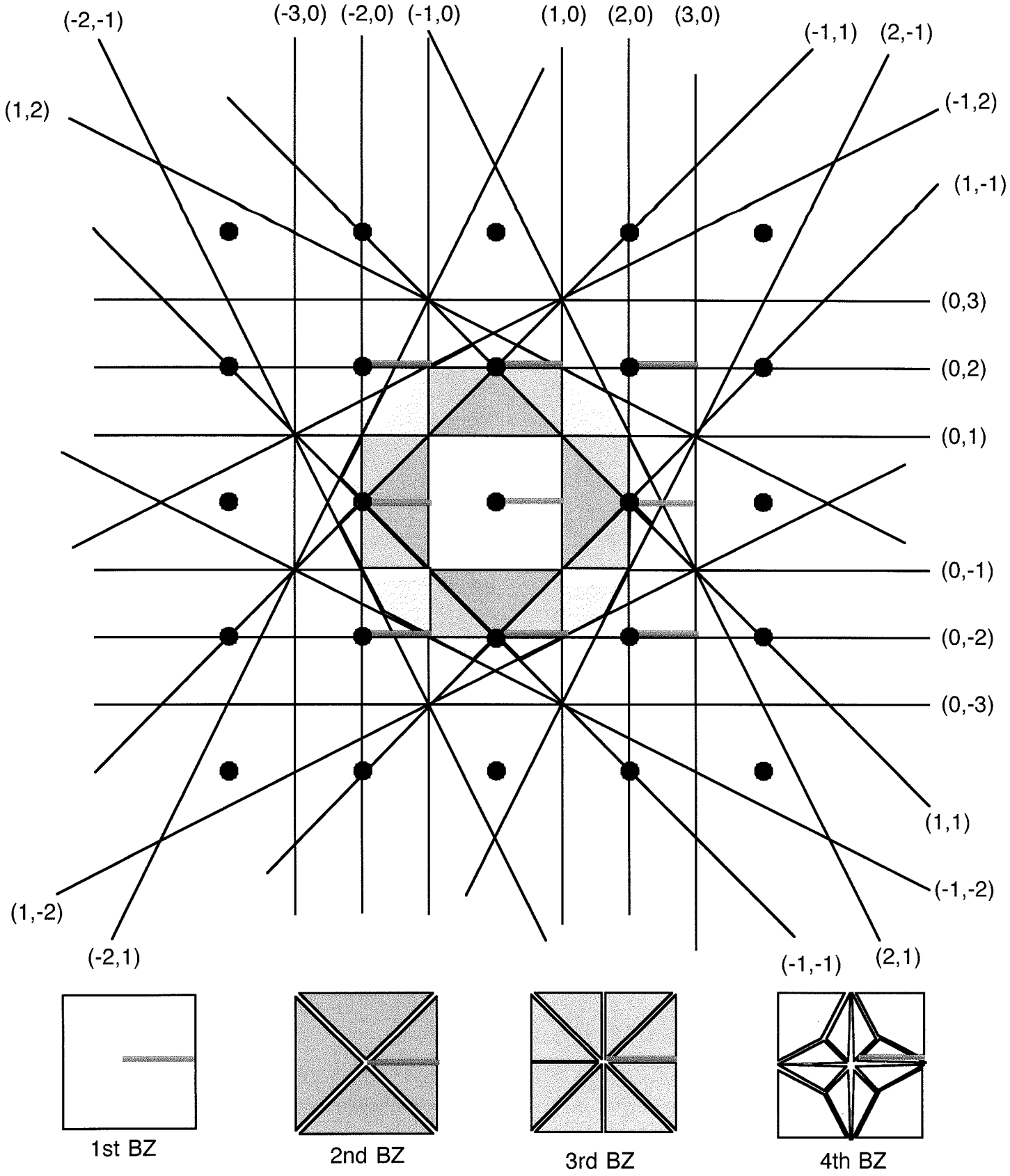
For $\vec{q} = q\hat{x}$ in 1st BZ, ie $0 \le q \le \frac{K}{2}$, we will plot the band structure, in the reduced zone scheme, for all bands corresponding the above 8 R.L. vectors.

$\mathcal{E}_i(\vec{q}) = \frac{\hbar^2}{2m}(\vec{q} + \vec{K}_i)^2$ measure energy in units of $\mathcal{E}_x = \frac{\hbar^2}{2m}\left(\frac{K}{2}\right)^2$

R.L. vector		energy		degeneracy	
$\vec{K}_0 = 0$		$\mathcal{E} = \frac{\hbar^2 q^2}{2m}$	$\mathcal{E}/\mathcal{E}_x = 4(q/K)^2$	1	(a)
$\{\vec{K}_1\}$	$-K\hat{x}$	$\mathcal{E} = \frac{\hbar^2}{2m}(q-K)^2$	$\mathcal{E}/\mathcal{E}_x = 4\left(\frac{q}{K}-1\right)^2$	1	(b)
	$+K\hat{x}$	$\mathcal{E} = \frac{\hbar^2}{2m}(q+K)^2$	$\mathcal{E}/\mathcal{E}_x = 4\left(\frac{q}{K}+1\right)^2$	1	(c)
	$\pm K\hat{y}$	$\mathcal{E} = \frac{\hbar^2}{2m}(q^2+K^2)$	$\mathcal{E}/\mathcal{E}_x = 4\left(\left(\frac{q}{K}\right)^2+1\right)$	2	(d)
$\{\vec{K}_2\}$	$K(-\hat{x}\pm\hat{y})$	$\mathcal{E} = \frac{\hbar^2}{2m}\left[(q-K)^2+K^2\right]$	$\mathcal{E}/\mathcal{E}_x = 4\left[\left(\frac{q}{K}-1\right)^2+1\right]$	2	(e)
	$K(+\hat{x}\pm\hat{y})$	$\mathcal{E} = \frac{\hbar^2}{2m}\left[(q+K)^2+K^2\right]$	$\mathcal{E}/\mathcal{E}_x = 4\left[\left(\frac{q}{K}+1\right)^2+1\right]$	2	(f)

we plot the above curves of $\mathcal{E}/\mathcal{E}_x$ vs q/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, $\mathbf{K} = (2\pi/a)(n, m)$.



1st BZ

2nd BZ

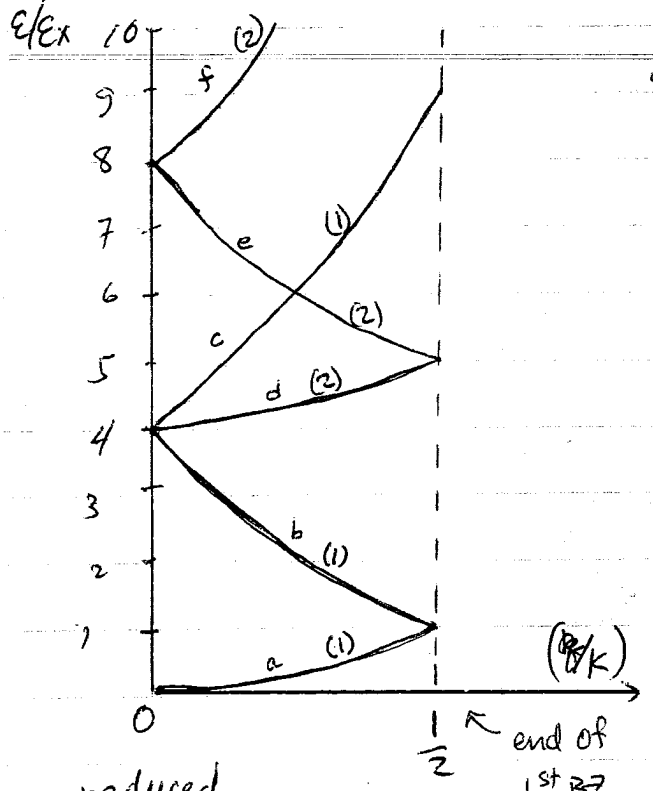
3rd BZ

4th BZ

Pieces of the nth Brillouin Zone translated back into the 1st BZ

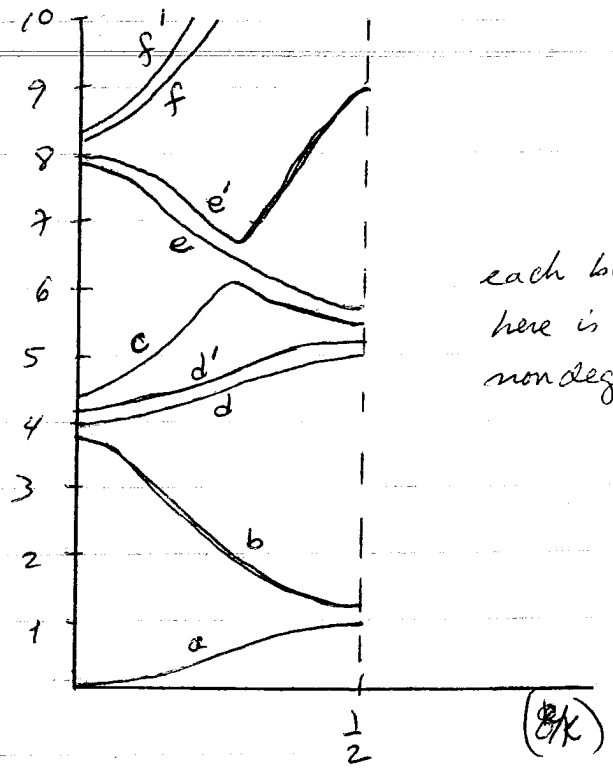
Red lines indicate values of $\vec{k}$ for free electron states giving rise to the band structure plotted in reduced ~~zone~~ zone scheme on preceding page.

free electrons



reduced zone scheme

weak potential



each band here is non degenerate

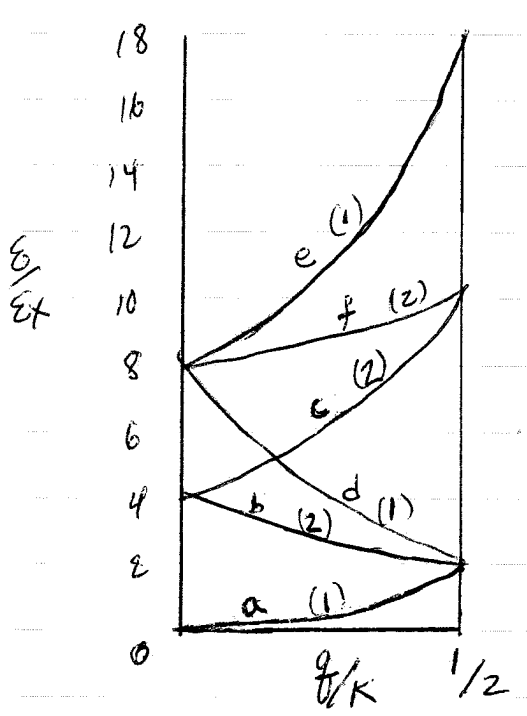
a) 1st BZ
b) 2nd BZ
d) 3rd + 4th BZs
c) 5th + 7th BZs
e) 5th, 6th + 7th BZs
f) 8th + 9th BZ + higher

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

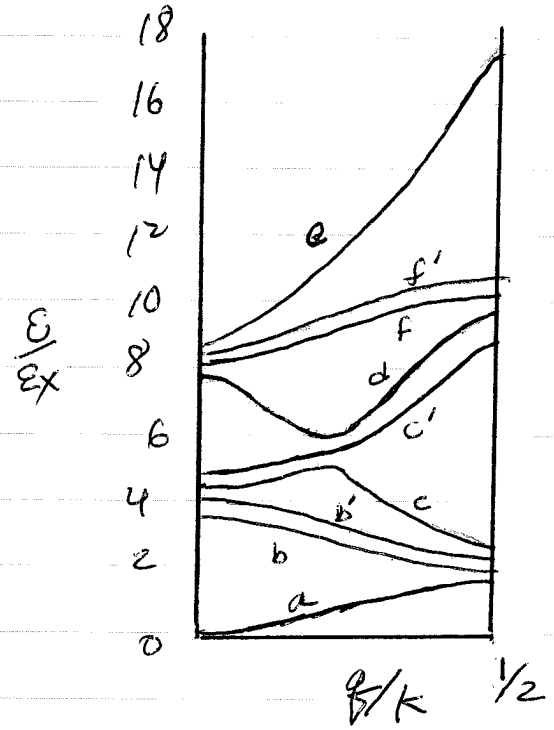
Weak potential splits degeneracies
More complicated band structure than in 1 dimension
Not necessarily true that $\max\left[\mathcal{E}_n(\vec{k})\right] \leq \min\left[\mathcal{E}_{n+1}(\vec{k})\right]$

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

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



Free electrons



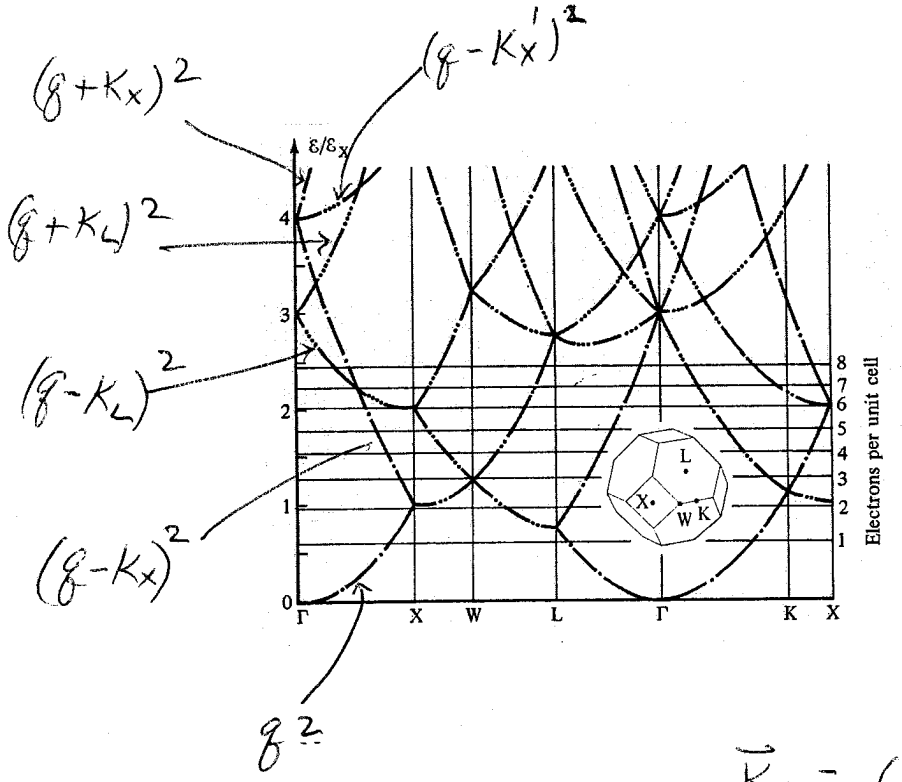
Weak potential

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 $\varepsilon_n(\vec{q})$ vs $|\vec{q}|$ along these directions, as done above.]

3 Dimensional free electron band structure



A+M

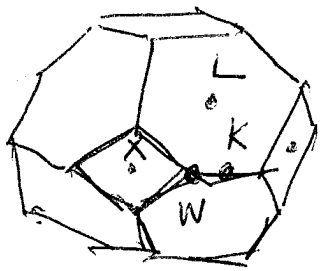
Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = \mathbf{0})$, K, L, W, and X. ε_x is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for 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 $\varepsilon^0_{\vec{q}-\vec{K}}$ for $\vec{q}$ in special directions for all $\vec{K}$ in R.L.

$\vec{K}_X = (1,0,0)$

$\vec{K}_L = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$

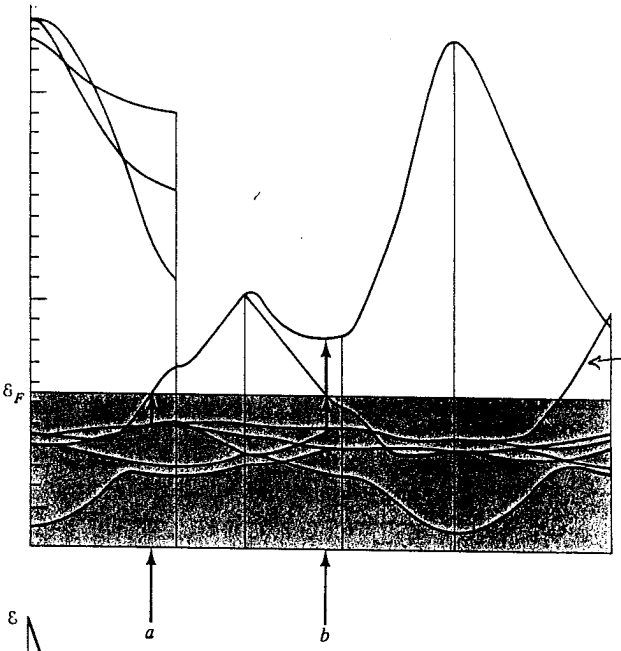
$\vec{q}_X = \left(\frac{1}{2},0,0\right)$



← 1st BZ of fcc

A+M

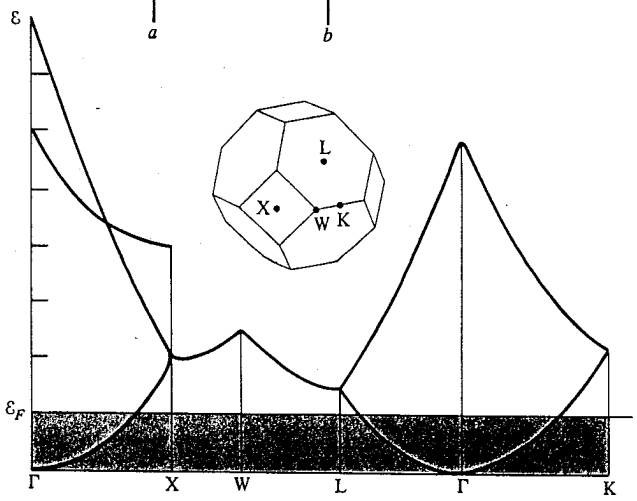
Figure 15.11
Burdick's calculated bands for copper, illustrating that the absorption threshold for transitions up from the conduction band is about 4 eV, while the threshold for transitions from the *d*-band to the conduction band is only about 2 eV. (The energy scale is in tenths of a rydberg (0.1 Ry = 1.36 eV).) Note the resemblance of the bands other than the *d*-bands to the free electron bands plotted below.



s band - free electron like

} d bands - tight binding like

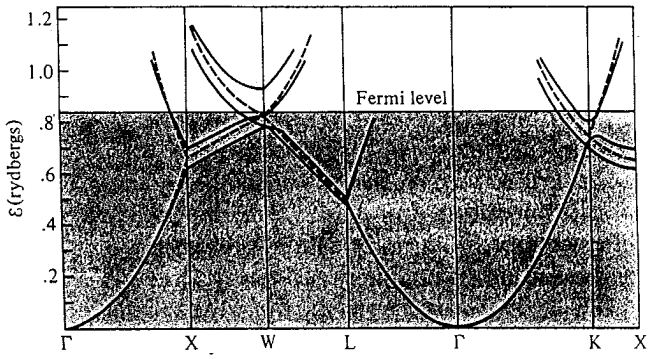
$Cu = [Ar]\, 3d^{10} 4s^1$



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).)



$AL = [Ne]\, 3s^2 3p^1$

$Z = 3$

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:

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

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

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

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

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

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

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 $\sum_c$ are now identical

$$U_K = \frac{1}{v} \int_{\substack{\text{all} \\ \text{space}}} d^3r \; e^{-i\vec{K}\cdot\vec{r}} \sum_j \phi(\vec{r} - \vec{d}_j) \qquad \text{as } v \equiv \frac{V}{N}$$

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

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

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

$$U_K = \frac{1}{v} \phi_K S_K \qquad \text{proportional to geometric structure factor } S_K$$

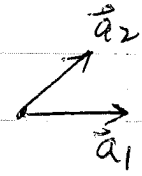
If S_K vanishes — we saw that there will be no diffraction peak in X-ray scattering at $\vec{K}$.

Now we see the analogous result, when $S_K = 0$ then $U_K = 0$, and there will be no energy gap opening up for electron states with 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 $\vec{d}_1 = 0$, $\vec{d}_2 = \frac{1}{3}(\vec{a}_1 + \vec{a}_2) + \frac{1}{2}\vec{a}_3$

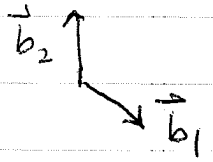


↑ lies in center of cells of triangular lattice in xy plane, and halfway between the two triangular layers

R.L.

$$\vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$$

$$\begin{cases} \vec{b}_1 = \frac{4\pi}{\sqrt{3}a}\left(\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\right) \\ \vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{c}\hat{z} \end{cases}$$

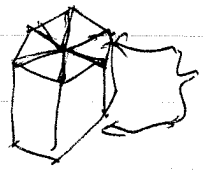


Then $S_K = e^{-i\vec{K}\cdot\vec{d}_1} + e^{-i\vec{K}\cdot\vec{d}_2}$

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

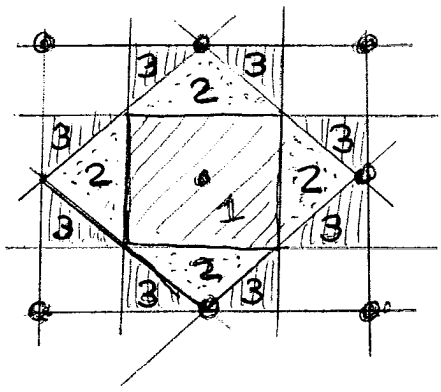
$$S_K = 1 + e^{-2\pi i\left(\frac{n_1}{3} + \frac{n_2}{3} + \frac{n_3}{2}\right)}$$

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



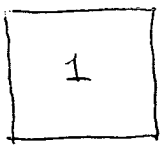
and Fermi Surface)

Zones in Two dimensions – single square BL

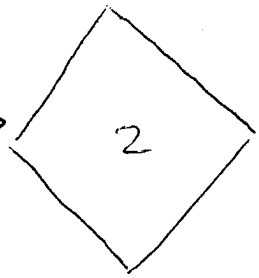


Draw in Bragg planes

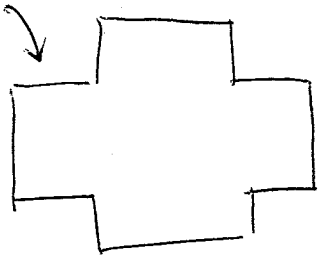
So outer surface 1st zone looks like



outer surface 2nd zone is →



outer surface 3rd zone is →



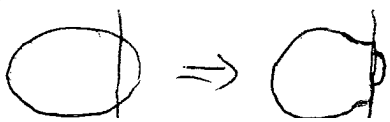
surface of nth zone gets more complicated as n increases

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

1) Draw free fermi sphere corresponding to desired energy

2) See ~~where~~ which zones surface of sphere intersects
There will be branches of surface in each ~~zone~~ band corresponding to the zones

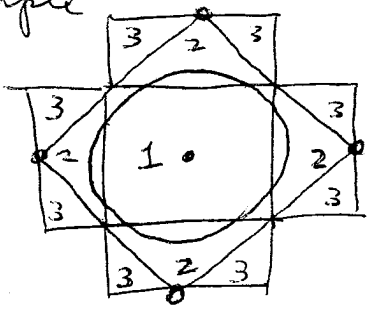
3) deform free energy sphere where it intersects zone boundary so that it is ⊥ to Bragg plane (HW prob #2)



(often ignore this step as 1st approx)

4) This gives constant energy surface in extended zone scheme. Translate branches of surface in nth 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.

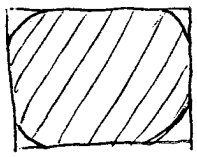
example



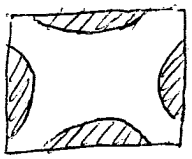
extended zone scheme

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.

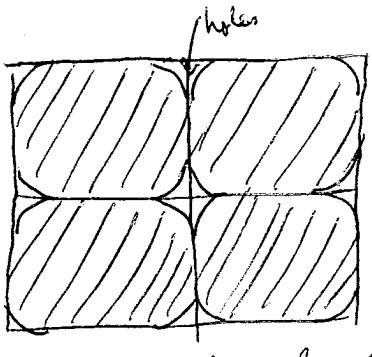


branches of surface in 2nd ~~zone~~ band translated back to 1st BZ

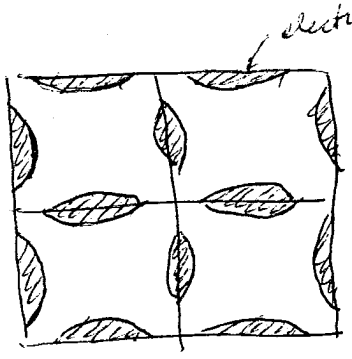
reduced zone scheme

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 ~~extended~~ repeated zone scheme, branches look like



branches in 1st zone



branches in 2nd zone

branches of ferm surface are closed curves