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

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

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 variab

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

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

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 $\sum_i$ are now identical

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

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

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

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

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

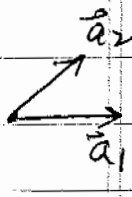
If S_K vanishes — we saw that there will be no diffraction peak in X-ray scattering at $\vec{K}$.

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

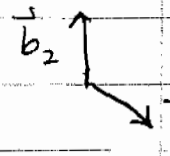


↑ lies in center of cells of triangular lattice in xy plane, and halfway between the two triangular layers

R.L.

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

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

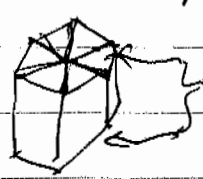


Then $S_K = e^{-i\vec{K}\cdot\vec{d}_1} + e^{-i\vec{K}\cdot\vec{d}_2}$

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

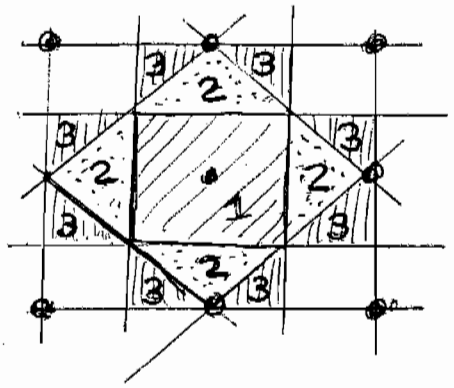
$$S_K = 1 + e^{-2\pi i\left(\frac{n_1}{3} + \frac{n_2}{3} + \frac{n_3}{2}\right)}$$

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.



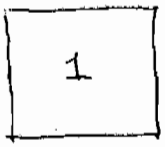
and Fermi Surface)

Zones in Two dimensions – single square BL

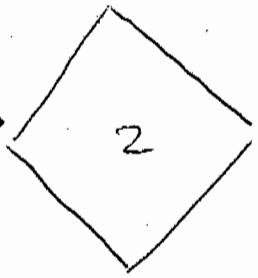


Draw in Bragg planes

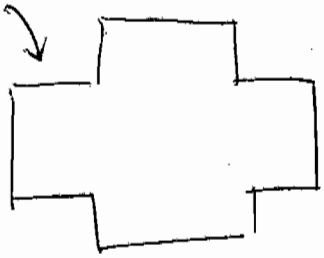
so outer surface 1st zone looks like



outer surface 2nd zone is →



outer surface 3rd zone is ↘



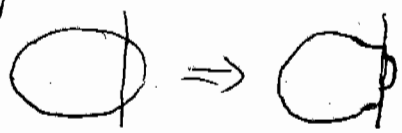
surface of nth zone gets more complicated as n increases

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

1) Draw free fermi sphere corresponding to desired energy

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

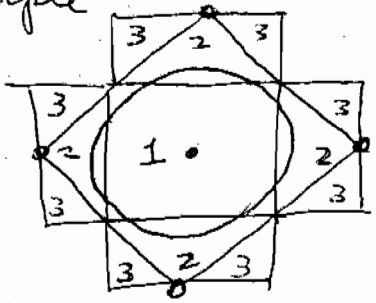
3) deform free energy sphere where it intersects zone boundary so that it is ⊥ to Bragg plane (HW prob #2)



(often ignore this step as 1st approx)

4) This gives constant energy surface in <u>extended</u> 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 <u>reduced</u> zone scheme. Or translate through all recip lattice vectors to get <u>repeated</u> zone scheme.

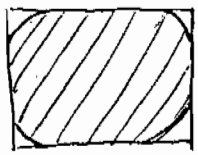
example



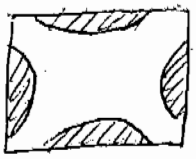
extended zone scheme

This free electron surface of energy ε_0 intersects 1st & 2nd zones only

Translate pieces of curves back to 1st BZ



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

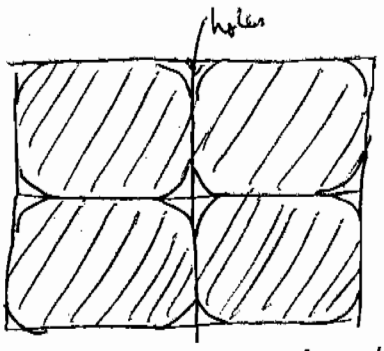


branches of surface in 2nd ~~band~~ translated back to <u>1st</u> BZ

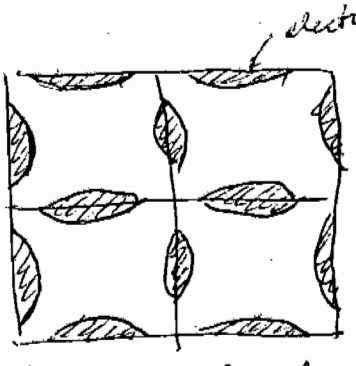
reduced zone scheme

Branches of curve in <u>reduced</u> zone scheme
Shaded areas are states of lower energy $\varepsilon < \varepsilon_0$.
Unshaded areas are states of greater energy $\varepsilon > \varepsilon_0$

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



branches in 1st zone



branches in 2nd zone

branches of fermi surface are closed curves

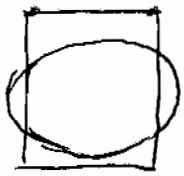
If surface we have drawn is Fermi surface, then shaded areas are filled states.

In 1st band we have small pockets of holes
In 2nd band we have small pockets of electrons

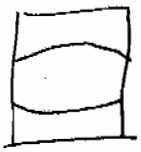
} more meaning to this when we get to dynamics

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

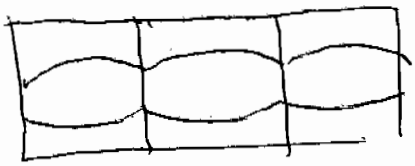
1st BZ



in this case, branches in 1st zone are



when we extend to repeated zone scheme we get



surface of constant energy is an <u>open</u> 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. ⇒ 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