Brownian lattice with a basis

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

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

since ions are located at positions \( \vec{R}_i + \vec{d}_j \).

Fourier transform is:

\[
U_k = \frac{1}{V} \int d^3r \ e^{-i \vec{k} \cdot \vec{R}} \sum_{i,j} \phi(r - \vec{R}_i - \vec{d}_j)
\]

primitive cell

\[
= \frac{1}{V} \int d^3r \ e^{-i \vec{k} \cdot \vec{r}} \sum_{i,j} \phi(r - \vec{R}_i - \vec{d}_j)
\]

all space

\[
= \sum_i \frac{1}{V} \int d^3r \ e^{-i \vec{k} \cdot \vec{R}_i} \sum_j \phi(r - \vec{R}_i - \vec{d}_j)
\]

all space

Let \( \vec{r}' = \vec{r} - \vec{R}_i \) and do change of integration variables

\[
U_k = \frac{1}{V} \int d^3r' \ e^{-i \vec{k} \cdot (\vec{r}' + \vec{R}_i)} \sum_j \phi(r' - \vec{d}_j)
\]

all space

\[
= \sum_i \frac{1}{V} \int d^3r' \ e^{-i \vec{k} \cdot \vec{R}_i} \sum_j \phi(r' - \vec{d}_j)
\]

all space, since \( \vec{R}_i \cdot \vec{R}_i = 2r_i^2 \)

\[
= \frac{N}{V} \int d^3r' \ e^{-i \vec{k} \cdot \vec{r}'} \sum_j \phi(r' - \vec{d}_j)
\]

all space
Since all the terms in the $\Xi$ are now identical

$$U_k = \frac{1}{N} \sum \int d^3r \ e^{-i\vec{R} \cdot \vec{r}} \ e^{i\vec{k} \cdot (\vec{r} - \vec{d}_j)} \ 	ext{as} \ \nu = \frac{V}{N}$$

Substitute in F.T. of $\phi(r)$

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

So

$$U_k = \frac{1}{V} \int d^3k' \ \phi_k \ \int \frac{d^3r}{(2\pi)^3} e^{i\vec{k}' \cdot \vec{r}} \ e^{-i\vec{k}' \cdot \vec{d}_j} \ \sum_j \ e^{i\vec{k} \cdot \vec{d}_j}$$

$$= \frac{1}{V} \ \phi_k \ \Xi_j \ e^{-i\vec{k} \cdot \vec{d}_j}$$

$$U_k = \frac{1}{V} \ \phi_k \ \xi_k \ \propto \ \text{geometric structure factor} \ \xi_k$$

If $\xi_k$ vanishes, we see that there will be no diffraction peak in X-ray scattering at $\vec{R}$.

Now we see the analogous result, when $\xi_k = 0$ then $U_k = 0$, and there will be no energy gap opening up for electron states with $\vec{k}$ that lie on the bragg plane $b_{i10}$.
An important case where this happens is for hcp crystals.

For hcp, \( \mathbf{a}_1 = a \hat{x}, \mathbf{a}_2 = \frac{a}{2} \hat{x} + \frac{\sqrt{3} a}{2} \hat{y}, \mathbf{a}_3 = c \hat{z} \).

Two point basis: \( \mathbf{d}_1 = 0, \mathbf{d}_2 = \frac{1}{2} (\mathbf{a}_1 + \mathbf{a}_2) + \frac{1}{2} \mathbf{a}_3 \).

\[ \mathbf{b}_1 = \frac{4\pi}{\sqrt{3} a} \left( \frac{1}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y} \right) \]
\[ \mathbf{b}_2 = \frac{4\pi}{\sqrt{3} a} \hat{y} \]
\[ \mathbf{b}_3 = \frac{2\pi}{c} \hat{z} \]

Then \( S_K = e^{-i K \cdot \mathbf{a}_1} + e^{-i K \cdot \mathbf{a}_2} \)

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

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

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 \( R = \pm 2\pi \frac{c}{3} \hat{z} \), i.e., the top and bottom surfaces of the 1st Bragg zone.

1st Bragg zone: no gap on these Bragg planes!
Zones in Two dimensions

- single square Brillouin zone

Draw in Bragg planes

So 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 (femil surface) in weak potential apply:

1) Draw free femil sphere corresponding to cleared energy

2) See which zones surface of sphere intersects
   There will be branches of surface in each zone

3) Deform free energy sphere where it intersects zone boundary so that it is \( \perp \) to Bragg plane (HW problem #2)

\[ \bigcirc \Rightarrow \bigcirc \]

(often ignore this step as 1st order)
4) This gives constant energy surface in extended zone scheme.
   Translate branches of surface in 1st zone back to 1st zone (by adding appropriate reciprocal lattice vector) to get branches of surface in reduced zone scheme.
   Or translate through all reciprocal lattice vectors to get repeated zone scheme.

*Example*

![Diagram of extended zone scheme]

Thin free electron surface intersects
1st + 2nd zones only

Translate pieces of curves back to 1st BZ

Branches of surface in reduced zone scheme
- Shaded areas are states of lower energy \( \varepsilon < \varepsilon_0 \)
- Unshaded areas are states of greater energy \( \varepsilon > \varepsilon_0 \)

In extended zone scheme, branches look like

Branches of Fermi surface are closed curves
If surface we have drawn in 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.

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.

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. 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.