2.3 Brillouin Zone

We already discussed the idea that a periodic crystal potential can be expanded into a Fourier series with an expansion

\[ V(\mathbf{r}) = \sum \frac{A_{m}}{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r}) \]

Let us now consider what such a periodic potential will do to a free electron, represented by a plane wave with wave vector \( \mathbf{k} \)

\[ \psi(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) \]

From perturbation theory we know that the strength of the interaction depends on the matrix element

\[ M_{kk'} = \int d\mathbf{r} \, \psi^{*}(\mathbf{r}) V(\mathbf{r}) \psi(\mathbf{r}) \]

Now we plug in the definitions of \( V(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) from above and look for possible interactions (where \( M_{kk'} \neq 0 \)).
\[ u(k') = \sum_{\tilde{n}} \int \frac{d^3 k}{(2\pi)^3} \rho \left( \frac{\tilde{k} - \tilde{k}'}{\hbar} \right)^2 e^{i \tilde{k} \cdot \tilde{r}} \]

\[ = \sum_{\tilde{n}} A_{\tilde{n}} \int \frac{d^3 k}{(2\pi)^3} e^{i (\tilde{k} - \tilde{k}') \cdot \tilde{r}} \]

\[ = \sum_{\tilde{n}} A_{\tilde{n}} \delta(\tilde{k} - \tilde{k}') \tilde{G}_\tilde{n} \]

This will be non-zero only when the delta function is non-zero and that will happen when the condition \( \tilde{k} - \tilde{k}' = \tilde{G}_\tilde{n} \).

In other words: The moment am is conserved up to a reciprocal lattice vector \( \tilde{G}_\tilde{n} \).

In addition to momentum conservation, we also have to have energy conservation, which means \( |k'| = |k| \).

Combining together momentum + energy conservation gives us

\[ |k'|^2 = |k + \tilde{G}_n|^2 = |k|^2 + |\tilde{G}_n|^2 + 2 k \cdot \tilde{G}_n = |k|^2 \]
Subtracting $|k|^2$ from both sides gives us:

$$|G_h|^2 = -2k \cdot G_h$$

Dividing through by 4 gives:

$$-\frac{1}{2} \cdot \left( \frac{G_h}{2} \right) = \left| \frac{G_h}{2} \right|^2$$

This condition is often called Bragg's reflection and what it says is that waves will reflect off the crystal planes due to the periodic crystal potential. But it also gives us a set of points in reciprocal space which satisfy the condition of reflection and those points are on planes which bisect the reciprocal lattice vectors.
This set of planes which bisect the reciprocal lattice vectors enclose a particular primitive unit cell in reciprocal space: the Wigner-Seitz cell. The WSS cell in reciprocal space is called the Brillouin Zone.

Often the distinction is made between the 1st, 2nd, etc. Brillouin Zones which are constructed by bisecting the 1st, 2nd, etc. neighbor lattice points.

The Brillouin Zone is a very useful concept, so let us explore the BZs of a few important lattices. Most of the important and widely used semiconductors have the FCC (face centered cubic) structure. This includes Si, Ge, GaAs, InP, InSb, etc. The only exceptions are C and...
With ices which typically have hexagonal cells, the lattice vectors of the ice structure are
\[ \mathbf{a}_1 = \frac{a}{2} (1 + \mathbf{e}_3), \quad \mathbf{a}_2 = \frac{a}{2} (\mathbf{e}_1 + \mathbf{e}_3) \]
and \[ \mathbf{a}_3 = \frac{a}{2} (\mathbf{e}_1 + \mathbf{e}_2) \]

Let's do the volume first:

\[ V_{\text{ice}} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \]
\[ = \frac{a^3}{8} (1 + 2) \cdot \left[ (\mathbf{e}_1 + \mathbf{e}_3) \times (\mathbf{e}_1 + \mathbf{e}_2) \right] \]
\[ = \frac{a^3}{8} (3 - 2) \cdot (-\mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3) \]
\[ = \frac{a^3}{8} \]
\[ = \frac{a^3}{4} \]

We could have obtained the same result by noticing that there are
4 lattice points in a volume of \( a^3 \).

\[
\mathbf{b}_1 = \frac{2\pi}{(a^3/4)} \cdot \frac{a^2}{2} \left[ \left( \frac{a}{2} + \hat{x} \right) \times \left( \frac{a}{2} + \hat{y} \right) \right]
\]

\[
= \frac{2\pi}{a} \left( -\frac{a}{2} + \hat{y} + \hat{z} \right)
\]

\[
\mathbf{b}_2 = \frac{2\pi}{a} \left( \frac{a}{2} - \hat{y} + \hat{z} \right)
\]

\[
\mathbf{b}_3 = \frac{2\pi}{a} \left( \frac{a}{2} + \hat{y} - \hat{z} \right)
\]

The reciprocal lattice of a face centered cubic lattice is a bcc lattice.