4. RECIPROCAL LATTICE.

Aim: To become familiar with the concept of the reciprocal lattice. It is very important and frequently used in the rest of the course to develop models and describe the physical properties of solids.

Lattices are periodic structures and position-dependent physical properties that depend on the structural arrangement of the atoms are also periodic. For example the electron density in a solid is a function of position vector **r**, and its periodicity can be expressed as $n(\mathbf{r}+\mathbf{T})=n(\mathbf{r})$, where **T** is a translation vector of the lattice.

The periodicity means that the lattice and physical properties associated with it can be Fourier transformed. Since space is three dimensional, the Fourier analysis transforms it to a three-dimensional **reciprocal space**. Physical properties are commonly described not as a function of **r**, but instead as a function of wave vector ("spatial frequency" or k-vector) **k**. This is analogous to the familiar Fourier transformation of a time-dependent function into a dependence on (temporal) frequency. The lattice structure of real space implies that there is a lattice structure, the **reciprocal lattice**, also in the reciprocal space.

A. Fourier transformation (K p. 27-29).

We start with a repetition of the basics of the Fourier transformation in one and three dimensions.

B. Reciprocal lattice vectors (K p. 29-30).

The reciprocal lattice points are described by the reciprocal lattice vectors, starting from the origin.

$\mathbf{G} = v_1\, \mathbf{b_1} + v_2\, \mathbf{b_2} + v_3\, \mathbf{b_3}$, where v_i are integers and the $\mathbf{b_i}$ are the primitive translation vectors of the reciprocal lattice. From the definition of the $\mathbf{b_i}$ (K p. 29), it can be shown that $\exp(i\mathbf{GT}) = 1$. This implies that the Fourier series of a function with the periodicity of the lattice can only contain the lattice vectors (spatial frequencies) **G**.

Since the Miller indices of sets of parallel lattice planes in real space are integers, we can interpret the coefficients v_i as Miller indices (hkl). This leads to a physical relation between sets of planes in real space and reciprocal lattice vectors. Hence we write $\mathbf{G} = h\, \mathbf{b_1} + k\, \mathbf{b_2} + l\, \mathbf{b_3}$. The reciprocal lattice vectors are labelled with Miller indices $\mathbf{G_{hkl}}$. Each point in reciprocal space comes from a set of crystal planes in real space (with some exceptions, for example (n00), (nn0) and (nnn) with n>1 in cubic systems; nevertheless they occur in the Fourier series and are necessary for a correct physical description).

Consider the (hkl) plane closest to the origin. It cuts the coordinate axes in $\mathbf{a_1}/h$, $\mathbf{a_2}/k$ and $\mathbf{a_3}/l$. A triangular section of the plane has these points in the corners. The sides of the triangle are given by the vectors $(\mathbf{a_1}/h) - (\mathbf{a_2}/k)$ and analogously for the other two sides. Now the scalar product of $\mathbf{G_{hkl}}$ with any of these sides is easily seen to be zero. Hence the vector $\mathbf{G_{hkl}}$ is directed normal to the (hkl) planes. The distance between two lattice planes is given by the projection of for example $\mathbf{a_1}/h$ onto the unit vector normal to the planes, i.e. $d_{hkl} = (\mathbf{a_1}/h)\bullet\mathbf{n_{hkl}}$, where d_{hkl} is the interplanar distance between two (hkl)-planes. The unit normal is just $\mathbf{G_{hkl}}$ divided by its length. Hence the magnitude of the reciprocal lattice vector is given by $2\pi/ d_{hkl}$.

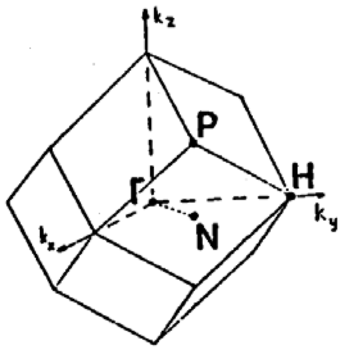
C. Brillouin zones (K p. 33-38).

The (first) Brillouin zone is defined as the Wigner-Seitz cell of the reciprocal lattice. It is also customary to define higher Brillouin zones. The zone boundaries are planes normal to each **G** at its midpoint. They partition reciprocal space into a number of fragments (K fig. 9b). These fragments are labelled with the number of a higher Brillouin zone. Each of these zones (the second, the third and so on) consists of several fragments, but the volume of all the Brillouin zones are the same.

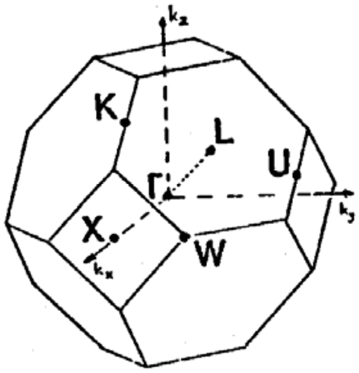
Examples: Brillouin zones in one dimension (K fig 11, p. 35) and two dimensions (K fig. 9b).
Reciprocal lattices to: a) simple cubic lattice
b) fcc lattice, c) bcc lattice, d) hexagonal lattice.

Brillouin zones of the three latter structures are illustrated below and can also be found in Physics Handbook.

bcc-gitter



fcc-gitter



hexagonalt gitter