Fourier Transforms and Bloch's Theorem

Basics

- The potential for the electron in a crystal lattice is periodic with the lattice, i.e. $V(r + T) = V(r)$ with T = translation vector of the lattice. It is therefore always possible to develop $V(r)$ into a Fourier series in reciprocal space and we obtain

$$V(\underline{r}) = \Sigma_{\underline{G}} V_{\underline{G}} \cdot \exp(i \cdot \underline{G} \cdot \underline{r})$$

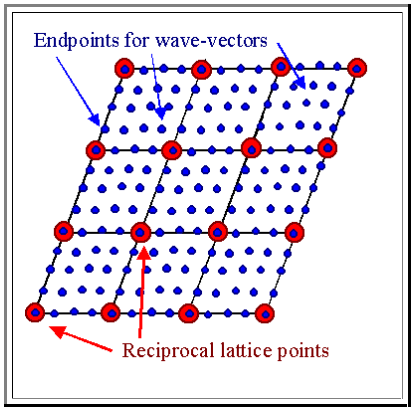
  - The V_G are the Fourier coefficients of the potential.
  - $\underline{G}$ is a reciprocal lattice vector; the sum must be taken over all reciprocal vectors and there are infinitely many. *We will, however, no longer use the underlining for vectors.*
  - In simple approximations it will be generally sufficient to consider only a few vectors of reciprocal space; i.e., most V_G are **0**.
- The wave function $\psi(r)$ can also be Fourier transformed. Without loss of generality it can be expressed as a sum of the plane waves which are the solutions of the free electron gas problem (with $V = 0$):

$$\psi(r) = \Sigma_k C_k \cdot \exp(ikr)$$

- The C_k are the Fourier coefficients of the wave function and k denotes the wave vector as obtained from the simple **free electron gas model** (e.g. $k_x = \pm n_x \cdot 2\pi / L_x$).
  - Since L_x must be a multiple of the lattice constant a, i.e. $L_x = N \cdot a$ (with $N = L_x/a$ = number of elementary cells in L_x), all k-vectors can be written as

$$k_x = \pm \frac{n_x \cdot 2\pi}{N \cdot a}$$

  - We know that $2\pi/a$ is simply the magnitude of the reciprocal lattice vector characterizing the set of planes perpenduclar to the direction of a (if taken as a unit vector of the elementary cell) with spacing a; i.e. for the **{100}** planes, $n_x \cdot 2\pi/a$ gives the whole set of reciprocal lattice vectors with the same direction, and $1/N$ intersperses N points between the reciprocal lattice points defined by n_x.
  - In other words and generalized for three dimensions: The allowed points for **k**-vectors are points in reciprocal space interspersed between the lattice points of the reciprocal lattice.
- We have the following picture, with (for reasons of clarity, very few) blue k-points between the red G-points:



  - The picture makes clear that any arbitrary wave vector k can be written as a sum of some reciprocal lattice vector G plus a suitable wave vector k'; i.e., we can always write $k = G + k'$ *and k' can always be confined to the **1.** Brillouin zone* (= the elementary cell of the reciprocal lattice).
  - Alternatively, any reciprocal lattice vector G can always be written as $G = k - k'$ This is a relation that should look familiar; we are going to use it a few lines further down.
- If we now pluck both expressions into the Schrödinger equation

$$-\frac{\hbar^2}{2m}\cdot\Delta\psi + V(r)\cdot\psi(r) = E\cdot\psi(r)$$

- and do the differentiations, we obtain

$$\Sigma_k \frac{(\hbar\cdot k)^2}{2m}\cdot C_k\cdot\exp(ikr) + \Sigma_{k'}\Sigma_G\ C_{k'}\cdot V_G\cdot\exp(i\cdot[k'+G]\cdot r) = E\cdot\Sigma_k C_k\cdot\exp(ikr)$$

- We have written **k'** in the double sum to indicate that it is not important how we sum up the components. That allows us to rename the summation indices and to replace **k'** as shown:

$$k' + G = k$$

$$k' = k - G$$

- Reshuffling the equation we obtain

$$\Sigma_k \exp(ik\cdot r)\cdot\left(\left(\frac{(\hbar\cdot k)^2}{2m} - E\right)\cdot C_k + \Sigma_G (C_{k-G}\cdot V_G)\right) = 0$$

- If this looks a bit like magic, you should consult the link.

Since this equation holds for any space vector **r**, the expression in the red brackets must be zero by itself and we obtain

$$\left(\frac{(\hbar\cdot k)^2}{2m} - E\right)\cdot C_k + \Sigma_G(C_{k-G}\cdot V_G) = 0$$

This is nothing but Schrödinger's equation for crystals written as a collection of algebraic equations. It couples the Fourier coefficients V_G of a periodic potential (which we know) to the Fourier coefficients C_k and C_{k-G} of the wave functions (which we want to calculate) in an unique way.

- If you have trouble visualizing this, write some parts of this infinite system of equations in a matrix as shown in the link for a slightly different situation.

The problem now is much simplified. While our original Fourier expansion of the wave function was a sum containing a large number of coefficients C_k because we have a large number of **k**'s, we now only have to consider a sum over **G**'s - of which we have far less (if still infinitely many).

- This is so because our system of equations from above only contains C_{k-G}. Solving it, gives a definite wavefunction for any chosen **k** as a sum over just C_{k-G} coefficients.
- Since we can express all **k** vectors outside the **1st** Brillouin zone as a sum of a **k**-vector in the first Brillouin zone and some **G**-vector (see above), we only have to consider **N** terms for the **k**-values.
- Since we have **N** **k**-vectors, we have **N** sets of equations, each one describing one wavefunction ψ_k of which we now know that it can be expressed as a Fourier series over points in reciprocal space positioned at **k – G** with **G** = any reciprocal wave vector. This means we have

$$\psi_k(r) = \Sigma_G C_{k-G}\cdot\exp(i\cdot[k-G]\cdot r)$$

- or, after rewriting the exponential

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} \cdot \exp(-i\mathbf{G}\mathbf{r}) \cdot \exp(i\mathbf{k}\mathbf{r})$$

The first term *shown in red*, upon inspection, is nothing but the Fourier series of some function $\mathbf{u_k(r)}$ that has the periodicity of the lattice; it is defined by:

$$u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} \cdot \exp(-i\mathbf{G}\mathbf{r})$$

- We thus obtain

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}) \cdot \exp(-i\mathbf{G}\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} \cdot \exp(-i\mathbf{G}\,\mathbf{r}) \cdot \exp(i\mathbf{k}\,\mathbf{r})$$

And this is Bloch's theorem that we endeavored to prove.