

# Fourier Transforms and Bloch's Theorem

## Basics

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

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} \cdot \exp(i \cdot \mathbf{G} \cdot \mathbf{r})$$

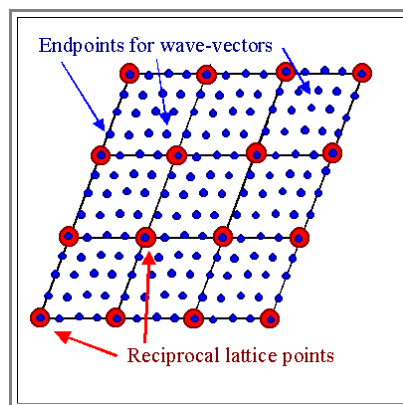
- The  $V_{\mathbf{G}}$  are the Fourier coefficients of the potential.
  - $\mathbf{G}$  is a reciprocal lattice vector; the sum must be taken over all reciprocal vectors and there are infinitely many. *We will, however, no longer use the underlining for vectors.*
  - In simple approximations it will be generally sufficient to consider only a few vectors of reciprocal space; i.e., most  $V_{\mathbf{G}}$  are 0.
- The wave function  $\psi(\mathbf{r})$  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  $\mathbf{V} = 0$ ):

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} \cdot \exp(i \mathbf{k} \mathbf{r})$$

- The  $C_{\mathbf{k}}$  are the Fourier coefficients of the wave function and  $\mathbf{k}$  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  $\mathbf{k}$ -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 perpendicular to the direction of  $\mathbf{a}$  (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  $\mathbf{k}$ -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**  $\mathbf{k}$ -points between the **red**  $\mathbf{G}$ -points:



- The picture makes clear that any arbitrary wave vector  $\mathbf{k}$  can be written as a sum of some reciprocal lattice vector  $\mathbf{G}$  plus a suitable wave vector  $\mathbf{k}'$ ; i.e., we can always write  $\mathbf{k} = \mathbf{G} + \mathbf{k}'$  and  $\mathbf{k}'$  can always be confined to the **1. Brillouin zone** (= the elementary cell of the reciprocal lattice).
  - Alternatively, any reciprocal lattice vector  $\mathbf{G}$  can always be written as  $\mathbf{G} = \mathbf{k} - \mathbf{k}'$ . 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

$$\sum_{\mathbf{k}} \frac{(\hbar \cdot \mathbf{k})^2}{2m} \cdot C_{\mathbf{k}} \cdot \exp(i \mathbf{k} \cdot \mathbf{r}) + \sum_{\mathbf{k}'} \sum_{\mathbf{G}} C_{\mathbf{k}'} \cdot V_{\mathbf{G}} \cdot \exp(i \cdot [\mathbf{k}' + \mathbf{G}] \cdot \mathbf{r}) = E \cdot \sum_{\mathbf{k}} C_{\mathbf{k}} \cdot \exp(i \mathbf{k} \cdot \mathbf{r})$$

- We have written  $\mathbf{k}'$  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  $\mathbf{k}'$  as shown:

$$\mathbf{k}' + \mathbf{G} = \mathbf{k}$$

$$\mathbf{k}' = \mathbf{k} - \mathbf{G}$$

- Reshuffling the equation we obtain

$$\sum_{\mathbf{k}} \exp(i \mathbf{k} \cdot \mathbf{r}) \cdot \left( \left( \frac{(\hbar \cdot \mathbf{k})^2}{2m} - E \right) \cdot C_{\mathbf{k}} + \sum_{\mathbf{G}} (C_{\mathbf{k} - \mathbf{G}} \cdot V_{\mathbf{G}}) \right) = 0$$

- If this looks a bit like magic, you should consult the [link](#).

Since this equation holds for any space vector  $\mathbf{r}$ , the expression in the red brackets must be zero by itself and we obtain

$$\left( \frac{(\hbar \cdot \mathbf{k})^2}{2m} - E \right) \cdot C_{\mathbf{k}} + \sum_{\mathbf{G}} (C_{\mathbf{k} - \mathbf{G}} \cdot V_{\mathbf{G}}) = 0$$

This is nothing but Schrödinger's equation for crystals written as a collection of algebraic equations. It couples the Fourier coefficients  $V_{\mathbf{G}}$  of a periodic potential (which we know) to the Fourier coefficients  $C_{\mathbf{k}}$  and  $C_{\mathbf{k} - \mathbf{G}}$  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  $C_{\mathbf{k}}$  because we have a large number of  $\mathbf{k}$ 's, we now only have to consider a sum over  $\mathbf{G}$ 's - of which we have far less (if still infinitely many).

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

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

- 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  $u_{\mathbf{k}}(\mathbf{r})$  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.