4.3 Proof of the Bloch-Theorem

For each vector $\vec{R}$ of the Bravais lattice we define a translation operator T_R by

$$T_R f(\vec{r}) = f(\vec{r} + \vec{R}) \tag{4.8}$$

for an arbitrary function f.
Since the Hamiltonian is periodic, we find

$$T_R H\psi(\vec{r}) = H(\vec{r} + \vec{R})\psi(\vec{r} + \vec{R}) = H(\vec{r})\psi(\vec{r} + \vec{R}) = HT_R\psi(\vec{r}) \tag{4.9}$$

Eq. (4.9) holds for all state functions ψ; so we can write

$$T_R H = HT_R \qquad \text{or} \qquad [T_R, H] = 0 \qquad . \tag{4.10}$$

Successively applying the translation leads to

$$T_R T_{R'}\psi(\vec{r}) = T_{R'}T_R\psi(\vec{r}) = \psi\left(\vec{r} + \vec{R} + \vec{R}'\right) \qquad , \tag{4.11}$$

i.e.

$$T_R T_{R'} = T_{R'} T_R = T_{R+R'} \qquad . \tag{4.12}$$

Following Eq. (4.10) we can choose the Eigenvectorsystem of H to be simultaneously a Eigenvectorsystem of T_R:

$$\begin{aligned} H\psi &= E\psi \\ T_R\psi &= c(\vec{R})\psi \end{aligned} \tag{4.13}$$

Following Eq. (4.12) the Eigenvalues $c(\vec{R})$ of the translation operator obey

$$T_R T_{R'}\psi(\vec{r}) = c(\vec{R}')T_R\psi(\vec{r}) = c(\vec{R}')c(\vec{R})\psi(\vec{r}) \qquad . \tag{4.14}$$

Thus for the Eigenvalues we find

$$c(\vec{R} + \vec{R}') = c(\vec{R})c(\vec{R}') \qquad . \tag{4.15}$$

Let's have a closer look on the primitive translation vectors of the Bravais lattice $\vec{a}_i$. For adequate variables x_i we can write

$$c(\vec{a}_i) = e^{i2\pi x_i} \qquad . \tag{4.16}$$

Thus for a general translation vector

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \tag{4.17}$$

we find by successively applying Eq. (4.15)

$$c(\vec{R}) = c(\vec{a}_1)^{n_1} * c(\vec{a}_2)^{n_2} * c(\vec{a}_3)^{n_3} \tag{4.18}$$

which may be rewritten as

$$c(\vec{R}) = e^{i\vec{k}\vec{R}} \tag{4.19}$$

using Eq. (4.16) and the following definitions:

$$\vec{k} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3 \tag{4.20}$$

and

$$\vec{a}_i\vec{b}_j = 2\pi\delta_{i,j} \qquad . \tag{4.21}$$

The above defined vectors $\vec{b}$ are the basic vectors of the reciprocal lattice.
Summing up, we have shown that for every vector of the real space the Eigenvectors ψ of H can be chosen to fulfill the following relation:

$$T_R\psi(\vec{r}) = \psi(\vec{r} + \vec{R}) = c(\vec{R})\psi(\vec{r}) = e^{i\vec{k}\vec{R}}\psi(\vec{r}) \qquad . \tag{4.22}$$

This is the definition of the Bloch theorem according to Eq. (4.5). Additional illustrative information you can find in the MaWi II script.