4.2 The Bloch-Theorem

The Eigenstate ψ of a one electron Hamiltonian

$$H = -\frac{\hbar^2 \Delta^2}{2m} + U(\vec{r}) \tag{4.1}$$

with $U(\vec{r}+\vec{R}) = U(\vec{r})$ for all $\vec{R}$ in the Bravais lattice can be chosen as

$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{nk}(\vec{r}) \qquad , \tag{4.2}$$

with $u_{n,k}$ being a function with the periodicity of the lattice:

$$u(\vec{r}+\vec{R}) = u(\vec{r}) \tag{4.3}$$

From Eq. (4.2) and (4.3) follows

$$\psi_{nk}(\vec{r}+\vec{R}) = e^{i\vec{k}\vec{R}} \psi_{nk}(\vec{r}) \qquad , \tag{4.4}$$

which allows to define the Bloch-Theorem in an alternative way:

One can always choose Eigenstates ψ of H so, that for each ψ we find a wave vector $\vec{k}$ with

$$\psi(\vec{r}+\vec{R}) = e^{i\vec{k}\vec{R}} \psi(\vec{r}) \qquad , \tag{4.5}$$

This may be rewritten as

$$\psi(\vec{r}+\vec{R}) = e^{i\vec{k}(\vec{r}+\vec{R})} e^{-i\vec{k}\vec{r}} \psi(\vec{r}) = e^{i\vec{k}(\vec{r}+\vec{R})} u(\vec{r}) \qquad , \tag{4.6}$$

with

$$u(\vec{r}) = e^{-i\vec{k}\vec{r}} \psi(\vec{r}) \tag{4.7}$$

being a (lattice) periodic function. Thus Eq. (4.2) and (4.5) are equivalent.