Sheet 6

A2

2.1

$V_{KS}(r+R) = V_{KS}(r)$

$\Psi = u_k(r)\exp(ikr)$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{KS}(r)\right)\Psi_i = E_i(r)\Psi_i(r)$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{KS}(r)\right) u_{i,k}\, e^{-i\vec{k}\vec{r}} = \epsilon_{i,k}(r) u_{i,k}(r)$$

$$\nabla^2 u_{ik} e^{-i\vec{k}\vec{r}} = \nabla \cdot \nabla\left(u_{ik} e^{i\vec{k}\vec{r}}\right)$$

$$= \nabla \cdot \left(-ik\, u_{ik}\, e^{i\vec{k}\vec{r}} + e^{ikr}\nabla u_{ik}\right)$$

$$= \left(k^2 u_{ik} e^{i\vec{k}\vec{r}} + ik e^{ikr}\nabla u_{ik} + ik e^{ikr}\nabla u_{ik} + e^{-ikr}\nabla^2 u_{ik}\right)$$

$$= \left(k^2 e^{-ikr} + 2ik\, e^{ikr}\nabla u_{ik} + e^{ikr}\nabla^2 u_{ik}\right)$$

$$= e^{ikr}\left(k^2 + 2ik + \nabla^2\right) u_{ik}$$

$$= e^{-ikr}(k+\nabla)^2 u_{ik}$$

$$\Rightarrow \left[\frac{\hbar^2}{2m}\nabla^2 + V_{KS}(r)\right] u_{ik} e^{ikr}$$

$$= -\frac{\hbar^2}{2m} e^{ikr}(k+\nabla)^2 u_{ik}(r) + V_{KS}(r) e^{ikr} u_{ik} = E_i u_{ik} e^{ikr}$$

$$\Rightarrow \left[-\frac{\hbar^2}{2m}(k+\nabla)^2 + V_{KS}\right] u_{ik}(r) = E_i u_{ik}(r)$$

A2.2

$$u_{i,k}(r) = \sum_{\vec{G}} C_{i,k,G}\, e^{i\vec{G}\vec{r}}$$

$$\left[-\frac{\hbar^2}{2m}(\nabla + ik)^2 + V_{KS}(r)\right] \sum_{G} C_{i,k,G}\, e^{i\vec{G}\vec{r}}$$

$$(\nabla + ik)^2 e^{i\vec{G}\cdot\vec{r}} = -G^2 - 2k\cdot G - k^2 = -|G+k|^2$$

$$\left[\frac{\hbar^2}{2m}|G+k|^2 + V_{KS}(r)\right] \sum_{G} C_{ikG}\, e^{i\vec{G}\vec{r}} = \epsilon_{ik} \sum_{G} C_{ikG}\, e^{i\vec{G}\vec{r}}$$

$$\sum_{G} \int e^{-i\vec{G}'\vec{r}} \left[\frac{\hbar^2}{2m}|G+k|^2 + V_{KS}(r)\right] C_{ikG}\, e^{i\vec{G}\cdot\vec{r}} = \epsilon_{ik} \sum_{G} C_{ikG} \overbrace{\int_{\Omega} e^{i\vec{G}\cdot\vec{r}}\, e^{-i\vec{G}'\cdot\vec{r}}\, d^3r}^{\Omega\,\delta_{\vec{G}\vec{G}'}}$$

$$\sum_{G} \int e^{-i\vec{G}'\vec{r}} \left(\frac{\hbar^2}{2m}|G+k|^2 + V_{KS}(r)\right] C_{ikG}\, e^{i\vec{G}\cdot\vec{r}} = \epsilon_{ik} \sum_{G} C_{ikG}\, \delta_{\vec{G}\vec{G}'} = \Omega\, \epsilon_{ik}\, C_{ik\vec{G}'}$$

$$LHS = \sum_{G} \int e^{i(\vec{G}-\vec{G}')r} \left(\frac{\hbar^2}{2m}|G+k|^2\right) C_{ikG}\, d^3r + \sum_{G} \int e^{-i\vec{G}'\vec{r}}\, V_{KS}(r)\, C_{ikG}\, e^{i\vec{G}\vec{r}}\, d^3r$$

$$= \sum_{G} \Omega\, \delta_{GG'} \left(\frac{\hbar^2}{2m}|G+k|^2\right) C_{ikG} + \sum_{G} C_{ikG} \overbrace{\int e^{i(\vec{G}-\vec{G}')r}\, V_{KS}(r)\, d^3r}^{\text{Fourier-Trafo: } V(G-G')}$$

$$= \sum_{G} \Omega\, \delta_{GG'} \left(\frac{\hbar^2}{m}|G+k|^2\right) C_{ikG} + \sum_{G} C_{ikG}\, V(G-G') \cdot \Omega$$

$$\Rightarrow \sum_{G} \left[\delta_{GG'} \left(\frac{\hbar^2}{2m}|G+k|^2\right) + V(G-G')\right] C_{ikG} = \epsilon_{ik}\, C_{ikG'}$$

$G \leftrightarrow G'$

$$\hookrightarrow \sum_{G'} \left[\delta_{GG'} \frac{\hbar^2}{2m}|G+k|^2 + V(G'-G)\right] C_{ikG'} = \epsilon_{ik}\, C_{ikG}$$

sollte ok sein weil $\sum_{G'}$ über alle G' geht