The equation with Fourier transformation

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\mathbf{k}}(\vec{r})=E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$V(\vec{r})=V_{ext}(\vec{r})+V_H(\vec{r})+V_{xc}(\vec{r})$$

$$V_{ext}(\vec{r})=\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}$$

$$V_H(\vec{r})=\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'$$

$$V_{xc}(\vec{r})=V_{xc}[\rho(\vec{r})]$$

Fourier transformation of the potential

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\mathbf{k}}(\vec{r})=E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$V(\vec{r})=\sum_l V(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}} \quad , V(\vec{G})=\frac{1}{\Omega_{cell}}\int_{cell} V(\vec{r})e^{-i\vec{G}\cdot\vec{r}}d^3\vec{r}$$

Fourier transformation of the potential

$$\left(\frac{1}{2}(-i\nabla + \vec{k})^2 + V(\vec{r})\right)u_{n,\mathbf{k}}(\vec{r}) = E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r}) \quad , \quad u_{n,\mathbf{k}}(\vec{r}) = \sum_{p=1}^{\infty} C_p e^{i\vec{G}_p\cdot\vec{r}}$$

$$\begin{bmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \cdots \end{pmatrix} = E_n(\mathbf{k}) \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \cdots \end{pmatrix}$$

$\infty \times \infty$ matrix

The Hamiltonian matrix element

$$H_{m,n} = \left\langle e^{i\vec{G}_m\cdot\vec{r}} \left| \frac{1}{2}(-i\nabla + \vec{k})^2 \right| e^{i\vec{G}_n\cdot\vec{r}} \right\rangle_\infty = \frac{1}{2}(\vec{G}_n + \vec{k})^2 \delta_{m,n} + V(\vec{G}_m - \vec{G}_n)$$

The Hamiltonian matrix element

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}+\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'+V_{xc}[\rho(\vec{r})]\right)u_{n,\mathbf{k}}(\vec{r})=E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$H_{m,n}\rightarrow\left\langle e^{i\vec{G}_m\cdot\vec{r}}\left|\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}\right|e^{i\vec{G}_n\cdot\vec{r}}\right\rangle_\infty=\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\int_\infty e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}=\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}e^{i(\vec{G}_n-\vec{G}_m)\cdot(\vec{R}+\vec{\tau})}\int_\infty e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\frac{-Z_\tau}{\left|\vec{r}\right|}$$

$$=\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{\tau}}\int_\infty e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\frac{-Z_\tau}{\left|\vec{r}\right|}=N_{cell}\sum_{\tau=1}^{N_{basis}}e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{\tau}}\int_\infty e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\frac{-Z_\tau}{\left|\vec{r}\right|}$$

$$=-N_{cell}\sum_{\tau=1}^{N_{basis}}e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{\tau}}\frac{-Z_\tau 4\pi}{\left|\vec{G}_n-\vec{G}_m\right|^2}$$

The Hamiltonian matrix element

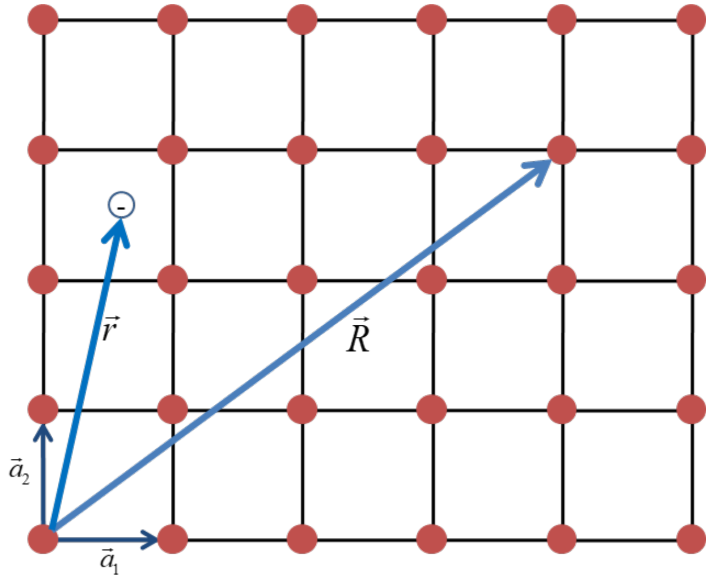
$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+\sum_{\mathbf{R}}^{\infty}\sum_{\tau=1}^{N_{basis}}\frac{-Z_\tau}{\left|\vec{r}-\vec{R}-\vec{\tau}\right|}+\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'+V_{xc}[\rho(\vec{r})]\right)u_{n,\mathbf{k}}(\vec{r})=E_n(\mathbf{k})u_{n,\mathbf{k}}(\vec{r})$$

$$H_{m,n}\rightarrow\left\langle e^{i\vec{G}_m\cdot\vec{r}}\left|\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'\right|e^{i\vec{G}_n\cdot\vec{r}}\right\rangle_\infty=\int_\infty e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\int\frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'=\sum_{\vec{G}}\iint e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}\frac{\rho(\vec{G})e^{i\vec{G}\cdot\vec{r}'}}{\left|\vec{r}-\vec{r}'\right|}d^3\vec{r}'d^3\vec{r}$$

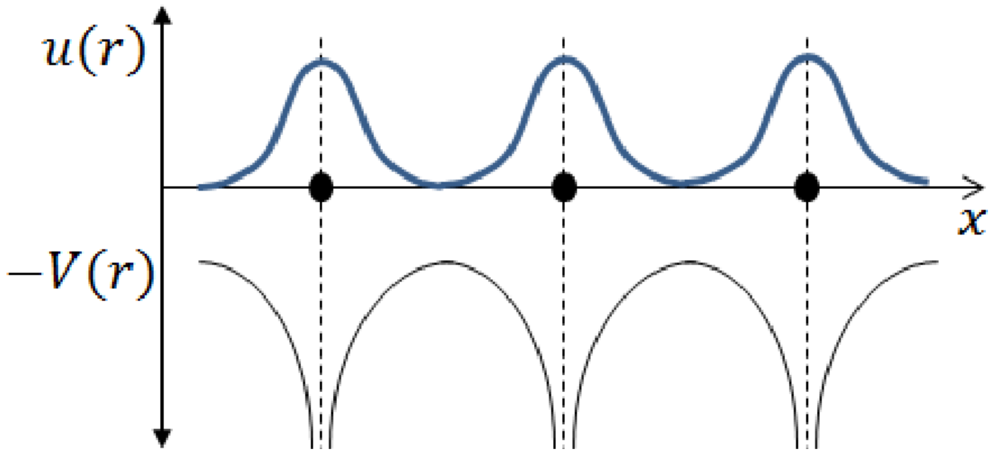
$$=\sum_{\vec{G}}\rho(\vec{G})\int d^3\vec{r}e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}e^{i\vec{G}\cdot\vec{r}}\int\frac{e^{i\vec{G}\cdot(\vec{r}'-\vec{r})}}{\left|\vec{r}'-\vec{r}\right|}d^3\vec{r}'$$

$$=\sum_{\vec{G}}\rho(\vec{G})\frac{4\pi}{G^2}\int d^3\vec{r}e^{i(\vec{G}_n-\vec{G}_m)\cdot\vec{r}}e^{i\vec{G}\cdot\vec{r}}=\sum_{\vec{G}}\rho(\vec{G})\frac{4\pi}{G^2}N_{cell}\delta_{\vec{G}_n-\vec{G}_m,\vec{G}}=N_{cell}\frac{4\pi\rho(\vec{G})}{\left|\vec{G}_n-\vec{G}_m\right|^2}$$

Hamiltonian with a translational symmetry



Translation Operator



- Now let us think of Hamiltonian with a periodic potential

$$V(\vec{r}+\vec{R}) = V(\vec{r})$$

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(\vec{r})$$

$$\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r})$$