The matrix equation

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

$$\left|u_{n,\mathbf{k}}(\vec{r})\right\rangle=\sum_{l=1}^{\infty}C(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}} \quad , \quad V(\vec{r})=V_{ext}(\vec{r})+V_{Hxc}[\rho(\vec{r})]=\sum_{l=1}^{\infty}V(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}}$$

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

- We don’t want to play with the $\infty \times \infty$ dimension of the matrix.

The matrix equation, finite dimension

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

$$\left|u_{n,\mathbf{k}}(\vec{r})\right\rangle = \sum_{l=1}^{N_G} C(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}} \quad , \quad V(\vec{r}) = V_{ext}(\vec{r}) + V_{Hxc}[\rho(\vec{r})] = \sum_{l=1}^{2N_G} V(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}}$$

$$\boxed{\begin{bmatrix} H_{11} & H_{12} & H_{13} & \ldots H_{1N} \\ H_{21} & H_{22} & H_{23} & \ldots H_{2N} \\ H_{31} & H_{32} & H_{33} & \ldots H_{3N} \\ \ldots & \ldots & \ldots & \ldots \\ H_{N1} & H_{N2} & H_{N2} & H_{NN} \end{bmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \ldots \\ C_N \end{pmatrix} = E_n(\mathbf{k}) \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \ldots \\ C_N \end{pmatrix}}$$

- How can we make the matrix finite ?.

The matrix equation, finite dimension

$$\left|u_{n,\mathbf{k}}(\vec{r})\right\rangle = \sum_{l=1}^{N_G} C(\vec{G}_l) e^{i\vec{G}_l\cdot\vec{r}} \quad , \quad V(\vec{r}) = V_{ext}(\vec{r}) + V_{Hxc}[\rho(\vec{r})] = \sum_{l=1}^{2N_G} V(\vec{G}_l) e^{i\vec{G}_l\cdot\vec{r}}$$

- The Fourier basis waves are generated/provided within the energy cutoff, E_{cut}

$$\frac{\hbar^2}{2m}\left|\vec{G}\right|^2 \le E_{cut} \quad , \quad G_{\max} = \sqrt{2E_{cut}}$$

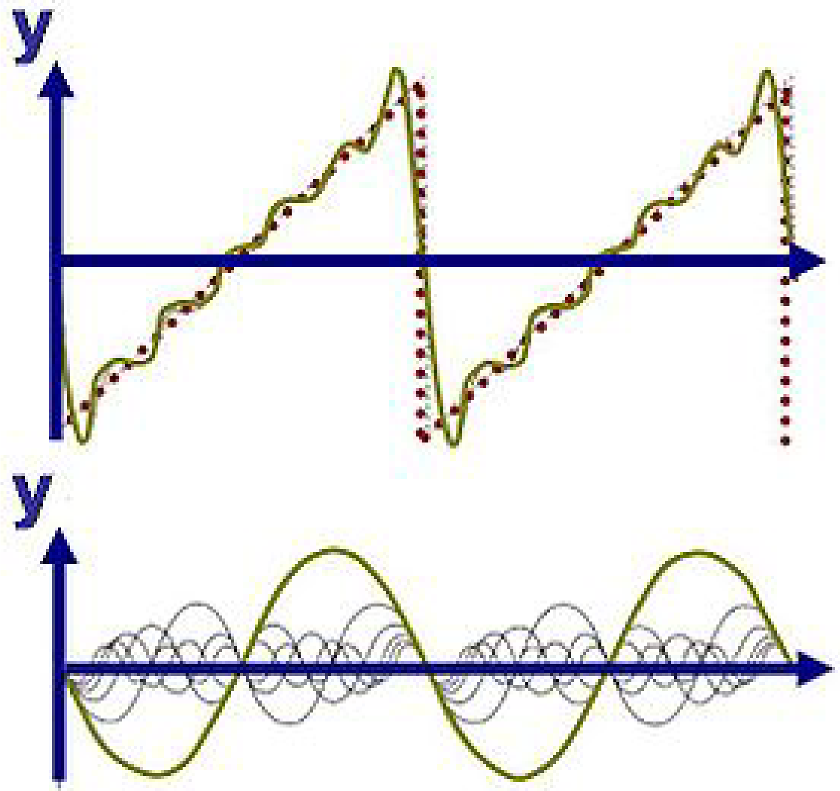
- Which factor of the system determine E_{cut} or G_{max} ??

Convergence of Fourier series

$$\left|u_{n,\mathbf{k}}(\vec{r})\right\rangle = \sum_{l=1}^{N_G} C(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}} \quad , \quad V(\vec{r}) = V_{ext}(\vec{r}) + V_{Hxc}[\rho(\vec{r})] = \sum_{l=1}^{2N_G} V(\vec{G}_l)e^{i\vec{G}_l\cdot\vec{r}}$$

- Low-G component ➔ Long-range behavior, overall shape. For example, the component $G = 0$?

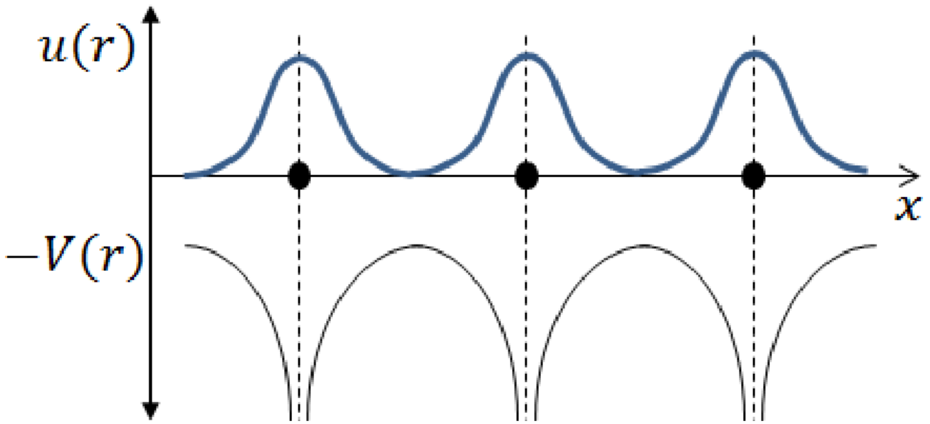
- High-G component➔ For the kink, sink of the potential



The matrix equation, finite dimension

$$\left|u_{n,\mathbf{k}}(\vec{r})\right\rangle = \sum_{l=1}^{N_G} C(\vec{G}_l) e^{i\vec{G}_l\cdot\vec{r}} \quad , \quad V(\vec{r}) = V_{ext}(\vec{r}) + V_{Hxc}[\rho(\vec{r})] = \sum_{l=1}^{2N_G} V(\vec{G}_l) e^{i\vec{G}_l\cdot\vec{r}}$$

- Which factor of the system determine E_{cut} or G_{max} ??



- How to do with the infinite depth of the potential ???