

$$H_{ij}(\vec{k}) = \langle i(\vec{k}) | H | j(\vec{k}) \rangle$$

$$= \sum_{\vec{R}_i, \vec{R}_j} \langle i | e^{-i\vec{k} \cdot \vec{R}_i} H e^{i\vec{k} \cdot \vec{R}_j} | j \rangle$$

Wannier

$$= \sum_{\vec{d}_i, \vec{d}_j} \langle i | e^{-i\vec{k} \cdot \vec{r}_i} | e^{-i\vec{k} \cdot \vec{d}_i} H e^{i\vec{k} \cdot \vec{d}_j} | e^{i\vec{k} \cdot \vec{r}_j} | j \rangle$$

position of orbital inside the cell
position of the cell

Bloch

$$= \sum_{\vec{d}_i, \vec{d}_j} \langle \dots | H | \dots \rangle e^{i\vec{k} \cdot (\vec{d}_j - \vec{d}_i)}$$

$$= \sum_{\vec{d}} t t e^{i\vec{k} \cdot \vec{d}}$$

⚠

$$\begin{cases} \vec{d} = d d^i \vec{a}_i \\ \vec{K} = k^i \vec{G}_i \\ \vec{G}_i \cdot \vec{a}_j = \delta_{ij} \end{cases} \quad \left( \text{i.e. } d d^i, k^i \text{ are DIMENSIONLESS} \right)$$

$$[ \quad i i \quad j j \quad t t \quad d d(t) \quad d d(t) \quad d d(t) ]$$