

## (2) of Bandstructure

Fourier transform general form:  $x \rightarrow x-na \rightarrow \vec{r}$ ?

$$\psi(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d\vec{r} \psi(\vec{r}) e^{-i\vec{k}\cdot\vec{r}}$$

Applied to (1):

$$\psi_{k,l}(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \phi_l(x-na)$$

↓  
because of result of summation by  $n$

(4) substituting  $|\psi_{k,l}\rangle$  will change  $l \rightarrow m$

$$\begin{aligned} (14) \quad \langle \psi_{k,l} | \hat{H} | \psi_{k,m} \rangle &= \sum_n e^{ikna} \langle \phi_l(0) | \hat{H} | \phi_m(na) \rangle \quad \text{from (12)} \\ &= \frac{\sum_n e^{ikna} (\epsilon_s \delta_{n,0} - t \delta_{n,\pm 1})}{A} \end{aligned}$$

$$\begin{aligned} \langle \psi_{k,l} | \psi_{k,m} \rangle &= \frac{\sum_n e^{ikna} \langle \phi_l(0) | \phi_m(na) \rangle}{B} \quad \text{from (11)} \\ &= \frac{\sum_n e^{ikna} \delta_{n,0}}{B} \end{aligned}$$

$$\sum_k [\langle \psi_{k,m} | \hat{H} | \psi_{k,l} \rangle - \epsilon_k \langle \psi_{k,m} | \psi_{k,l} \rangle] c_{k,l} = 0 \quad \text{from (7)}$$

$$A = B$$

$$\sum_n e^{ikna} (\epsilon_s \delta_{n,0} - t \delta_{n,\pm 1}) = \epsilon_k \sum_n e^{ikna} \delta_{n,0}$$