

## Bloch Theorem :

101

$$\psi_{\underline{k}}(\underline{r}) = u_{\underline{k}}(\underline{r}) \cdot e^{i\underline{k}\cdot\underline{r}} \quad [\text{see Kittel}]$$

with  $u_{\underline{k}}(\underline{r}) = u_{\underline{k}}(\underline{r} + \underline{T})$  and  $\underline{T}$  is a lattice vector.

Localized basis  $\varphi(\underline{r} - \underline{R}_i)$  ; i.e. localized around site  $\underline{R}_i$

construct  $\psi_{\underline{k}}(\underline{r})$  with

$$\psi_{\underline{k}}(\underline{r}) = \frac{1}{\sqrt{N}} \sum_{\underline{R}_i} e^{i\underline{k}\cdot\underline{R}_i} \varphi(\underline{r} - \underline{R}_i) \quad \text{with } \underline{k} \text{ being a reciprocal lattice vector.}$$

$N = \text{number of sites}$

We can show that this  $\psi_{\underline{k}}(\underline{r})$  is a Bloch function:

$$\begin{aligned} \psi_{\underline{k}}(\underline{r}) &= e^{i\underline{k}\cdot\underline{r}} \cdot e^{-i\underline{k}\cdot\underline{r}} \frac{1}{\sqrt{N}} \sum_{\underline{R}_i} e^{i\underline{k}\cdot\underline{R}_i} \varphi(\underline{r} - \underline{R}_i) \\ &= e^{i\underline{k}\cdot\underline{r}} \cdot \frac{1}{\sqrt{N}} \sum_{\underline{R}_i} e^{-i\underline{k}\cdot(\underline{r} - \underline{R}_i)} \varphi(\underline{r} - \underline{R}_i) \\ &\equiv e^{i\underline{k}\cdot\underline{r}} \cdot u_{\underline{k}}(\underline{r}) \quad \text{with} \end{aligned}$$

$$u_{\underline{k}}(\underline{r}) \equiv \frac{1}{\sqrt{N}} \sum_{\underline{R}_i} e^{-i\underline{k}\cdot(\underline{r} - \underline{R}_i)} \varphi(\underline{r} - \underline{R}_i)$$

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this is no longer a function of  $\underline{R}_i$   
and is insensitive to  $\underline{r} \rightarrow \underline{r} + \underline{T}$  substitution  
i.e.  $u_{\underline{k}}(\underline{r}) = u_{\underline{k}}(\underline{r} + \underline{T})$ .