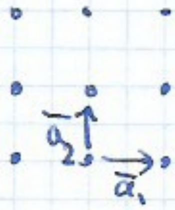
HUBBARD MODEL AND ITS EXTENSIONS

§ 1. WANNIER FUNCTIONS

$$\vec{R}_n = \sum_{i=1}^{d} c_i \vec{a}_i$$



primitive vectors

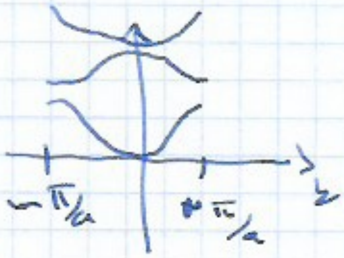
$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r})$$

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

Bloch theorem $\qquad \psi_{\vec{k}m}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}m}(\vec{r})$

$$u_{\vec{k}m}(\vec{r} + \vec{R}_n) = u_{\vec{k}m}(\vec{r})$$

$$\vec{k} \to \vec{k} + \vec{G}$$



1st Brillouin zone

consider a single band $m = 1$, e.g. 1s orbitals

Df. Wannier functions

$$W_i(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in BZ} e^{-i\vec{k}\cdot\vec{R}_i}\, \psi_{\vec{k}}(\vec{r})$$

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{i} e^{i\vec{k}\cdot\vec{R}_i}\, W_i(\vec{r})$$

discrete Fourier transforms.

Orthogonality

$$\int W_i(\bar r)^* W_j(\bar r)\, d_3 r = \frac{1}{N}\sum_{\bar k \bar k'} e^{i(\bar k\cdot \bar R_i - \bar k' \bar R_j)} \underbrace{\int \psi_{\bar k}^*(\bar r)\,\psi_{\bar k'}(\bar r)\, d_3 r}_{\delta_{\bar k \bar k'}} =$$

$$= \frac{1}{N}\sum_{\bar k} e^{i\bar k(\bar R_i - \bar R_j)} = \delta_{ij}$$

Completeness

$$\sum_i W_i^*(\bar r)\, W_i(\bar r') = \frac{1}{N} \sum_{\bar k\bar k'} \underbrace{\sum_i e^{i(\bar k-\bar k')\bar R_i}}_{\delta_{\bar k\bar k'}} \psi^*_{\bar k}(\bar r)\,\psi_{\bar k'}(\bar r') =$$

$$= \sum_{\bar k}\psi^*_{\bar k}(\bar r)\,\psi_{\bar k}(\bar r') = \delta(\bar r - \bar r')$$

Observation

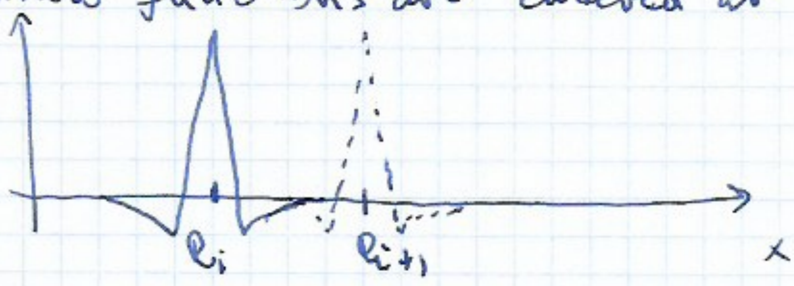
$$W_i(\bar r) = \frac{1}{\sqrt N}\sum_{\bar k} e^{-i\bar k\cdot(\bar R_i - \bar r)}\, u_{\bar k}(\bar r) =$$

$$= \frac{1}{\sqrt N}\sum_{\bar k} e^{+i\bar k(\bar r - \bar R_i)}\, u_{\bar k}(\bar r - \bar R_i + \bar R_i) =$$

$$= \frac{1}{\sqrt N}\sum_{\bar k} e^{i\bar k(\bar r - \bar R_i)}\, u_{\bar k}(\bar r - \bar R_i) =$$

$$= W(\bar r - \bar R_i)$$

Wannier functions are centered at lattice sites.



negative values are necessary for orthogonality.

Remarks

1. If we write

$$\begin{pmatrix} w_1(\bar r)\\ \vdots \\ w_N(\bar r)\end{pmatrix} = \frac{1}{\sqrt N}\underbrace{\begin{pmatrix} e^{-i\bar k_1\bar R_1} & \cdots & e^{-i\bar k_N \bar R_1}\\ \vdots & & \\ e^{-i\bar k_1 \bar R_N} & \cdots & e^{-i\bar k_N\bar R_N}\end{pmatrix}}_{\hat U} \begin{pmatrix}\psi_{\bar k_1}(\bar r)\\ \vdots\\ \psi_{\bar k_N}(\bar r)\end{pmatrix}$$

$\hat U$ – a unitary matrix

$$\hat U^{+} \hat U = 1, \quad \hat U^{-1} = \hat U^{+}$$

$$\{\psi_{\bar k}(\bar r)\} \longleftrightarrow \{w_i(\bar r)\}$$

two equivalent basis – complementary description

$$\Delta x \sim V^{1/3} \longleftrightarrow \Delta p \sim V^{-1/3}$$

2. Including more bands, $n = 1, 2, \dots$, the Wannier functions are not unique. They are connected via gauge transformation

→ novel interesting topological view on crystals