Ring-Hamiltonian

1 electron on a ring of protons at sites $R_1, R_2, \dots R_N$
- equivalent intersite interval a
- length $L = N.a$
- define quantum number $k \equiv \frac{2\pi}{L} . n$ with $n = 1, \dots, N$ or $n = -\frac{N}{2}+1, \dots 0, \dots, \frac{N}{2}$
- define wavefunction:

$$\psi_k(r) \equiv \frac{1}{\sqrt{N}} \sum_{R_i} e^{ikR_i} \varphi(r - R_i)$$

with

$\langle \varphi(r-R_i) | H | \varphi(r-R_i) \rangle = E_0$ or $\langle \varphi(r) | H | \varphi(r) \rangle = E_0$
$\langle \varphi(r-R_i) | H | \varphi(r-R_{i+1}) \rangle = t$ or $\langle \varphi(r) | H | \varphi(r+a) \rangle = t$
$\langle \varphi(r-R_i) | H | \varphi(r-R_{i-1}) \rangle = t$ or $\langle \varphi(r) | H | \varphi(r-a) \rangle = t$
and 0 otherwise

$$* \quad \langle \psi_k(r) | H | \psi_k(r) \rangle = \left\langle \frac{1}{\sqrt{N}} \sum_{R_i} e^{ikR_i} \varphi(r-R_i) \,\middle|\, H \,\middle|\, \frac{1}{\sqrt{N}} \sum_{R_j} e^{ikR_j} \varphi(r-R_j) \right\rangle$$

$$= \frac{1}{N} \sum_{R_i} \sum_{R_j} e^{ik(R_j - R_i)} \langle \varphi(r-R_i) | H | \varphi(r-R_j) \rangle$$

$R \equiv R_j - R_i$

$$= \frac{1}{N} \cdot N \cdot \sum_R e^{ikR} \langle \varphi(r) | H | \varphi(r-R) \rangle$$

$R = 0$ $\quad = 1 . E_0$
$R = a$ $\quad e^{ika} . t$
$R = -a$ $\quad e^{-ika} . t$ $+$

$$= E_0 + t(e^{ika} + e^{-ika})$$
$$= E_0 + 2t \cos ka$$
$$= E_0 + 2t \cos\left(\frac{2\pi}{N} . n\right)$$

$k \neq k'$:

$$\langle \psi_k(r) | H | \psi_{k'}(r) \rangle = \langle \frac{1}{\sqrt{N}} \sum_{R_i} e^{ikR_i} \varphi(r-R_i) | H | \frac{1}{\sqrt{N}} \sum_{R_j} e^{ik'R_j} \varphi(r-R_j) \rangle$$

$$= \frac{1}{N} \sum_{R_i} \sum_{R_j} e^{-ikR_i} \cdot e^{ik'R_j} \langle \varphi(r-R_i) | H | \varphi(r-R_j) \rangle$$

$e^{ik'R_i} \cdot e^{-ik'R_i} = 1 \rightarrow$

$$= \frac{1}{N} \sum_{R_i} \sum_{R_j} e^{i(k'-k)R_i} \cdot e^{ik'(R_j - R_i)} \langle \dots \rangle$$

$$= \frac{1}{N} \sum_{R_i} e^{i(k'-k)R_i} \cdot \sum_{R_j} e^{ik'(R_j-R_i)} \langle \quad \rangle$$

$$* \quad = \frac{1}{N} \sum_{R_i} e^{i(k'-k)R_i} \cdot \sum_{R_j} e^{ik'(R_j-R_i)} \cdot f(R_j - R_i)$$

$$** \quad = \frac{1}{N} \sum_{R_i} e^{i(k'-k)R_i} \cdot F(k')$$

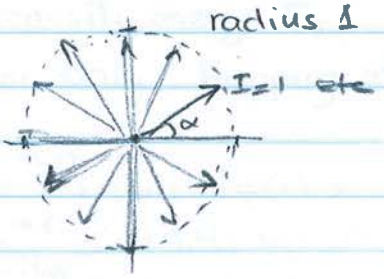
$$= \frac{F(k')}{N} \cdot \sum_{R_i} e^{i(k'-k) \cdot R_i}$$

$k' = \frac{2\pi}{L} n'$, $k = \frac{2\pi}{L} n$, $L = aN$, $m \equiv n' - n$, $R_i = a \cdot I$

$$= \frac{F(k')}{N} \cdot \sum_{I} e^{i \frac{2\pi}{N} \cdot m \cdot I}$$

$$= 0 \quad \rightarrow \text{ wavefunctions with different k-values do not couple !}$$

Angle $\alpha \equiv \frac{2\pi m}{N} \rightarrow$



The sum of all vectors $e^{i\frac{2\pi m}{N} \cdot I}$ in the complex plane is zero.

* $\langle \varphi(r-R_i) | H | \varphi(r-R_j) \rangle$ depends only on $(R_i - R_j)$, not on the absolute positions R_i or R_j

** $\sum_{R_j} e^{ik'(R_j - R_i)} \cdot f(R_j - R_i)$ does not depend on R_i due to periodicity.

Ring Hamiltonian in 1, 2, and 3 dimensions
(or an infinitely large lattice in 1,2,3 dimensions)

- assume only one basis function $\varphi(r)$ per site
- define Wannier function $\psi_{\underline{k}}(r) = \frac{1}{\sqrt{N}} \sum_{\underline{R}} e^{i\underline{k}\cdot\underline{R}} \varphi(\underline{r}-\underline{R})$

$\underline{R}$ covers all lattice sites
$\underline{k}$ covers all points in the Brillouin zone.

1 dim: $\underline{k}=k$ 2 dim: $\underline{k} = \begin{pmatrix} k_x \\ k_y \end{pmatrix}$ 3 dim: $\underline{k} = \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}$

- for each $\underline{k}$ one can calculate:

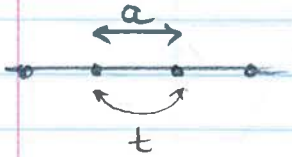
$$\langle \psi_k(r)|H|\psi_k(r)\rangle = \langle \frac{1}{\sqrt{N}} \sum_{\underline{R}_1} e^{i\underline{k}\underline{R}_1} \varphi(\underline{r}-\underline{R}_1)\,|H|\,\frac{1}{\sqrt{N}} \sum_{\underline{R}_2} e^{i\underline{k}\underline{R}_2} \varphi(\underline{r}-\underline{R}_2)\rangle$$

$$= \frac{1}{N} \sum_{\underline{R}_1}\sum_{\underline{R}_2} e^{ik(\underline{R}_2-\underline{R}_1)} \langle \varphi(\underline{r}-\underline{R}_1)|H|\varphi(\underline{r}-\underline{R}_2)\rangle$$

$$= \sum_{\underline{R}} e^{i\underline{k}\cdot\underline{R}} \langle \varphi(\underline{r})|H|\varphi(\underline{r}-\underline{R})\rangle$$

with $\underline{R}_1$ and $\underline{R}_2$ covering the same lattice sites
and with $\underline{R} \equiv \underline{R}_2 - \underline{R}_1$

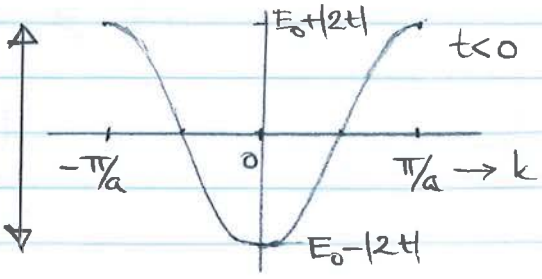
Example 1: 1 dimensional, on-site energy E_0,
nearest neighbor only: hopping integral t



$R=0 \rightarrow e^{ik\cdot 0} \langle \varphi(r)|H|\varphi(r)\rangle = E_0$
$R=a \rightarrow e^{ika} \langle \varphi(r)|H|\varphi(r-a)\rangle = e^{ika}\cdot t$
$R=-a \rightarrow e^{-ika} \langle \varphi(r)|H|\varphi(r+a)\rangle = e^{-ika}\cdot t$

$$\langle \psi_k(r)|H|\psi_k(r)\rangle = E_0 + 2t\cos(ka)$$

$ka = \frac{2\pi}{N}\cdot n$ bandwidth $= |4t|$
$= \frac{2\pi}{a}\cdot\frac{n}{N}$



example 2 : 2 dimensional square lattice
on-site energy E_0, nearest neighbor hopping t

$$\underline{R} = \begin{pmatrix}0\\0\end{pmatrix} + a\begin{pmatrix}n_x\\n_y\end{pmatrix} \qquad n_x, n_y = \text{Integer}$$

$$\underline{k} = \begin{pmatrix}k_x\\k_y\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix} + \frac{2\pi}{a}\cdot\frac{1}{N}\begin{pmatrix}n_x\\n_y\end{pmatrix}$$

$$\underline{R}=\underline{0} \rightarrow e^{i\underline{k}\cdot\underline{0}} \langle \varphi(\underline{r}) | H | \varphi(\underline{r}) \rangle = E_0$$

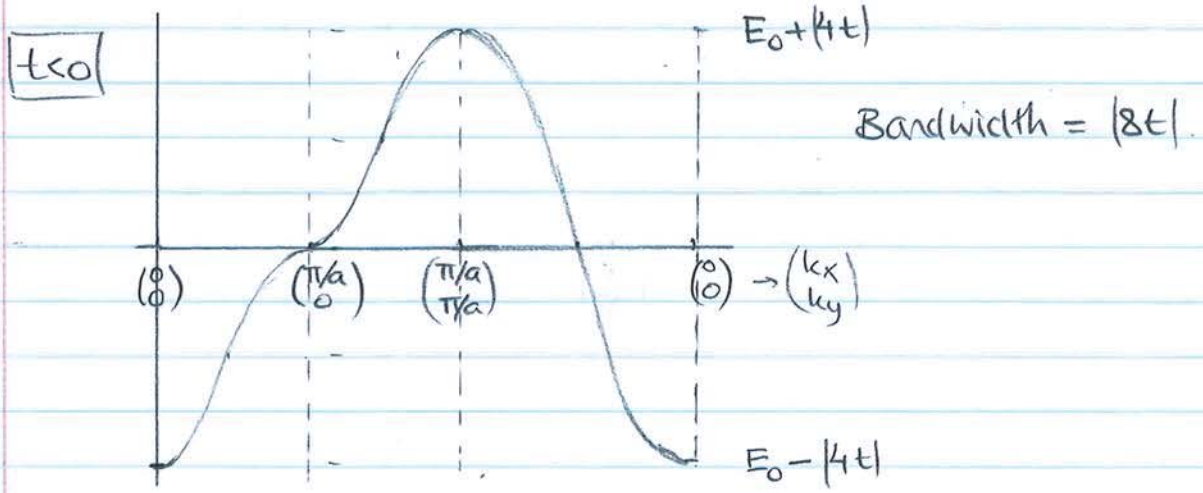
$$\underline{R}=\begin{pmatrix}a\\0\end{pmatrix} \rightarrow e^{ik_x a} \langle \varphi(\underline{r}) | H | \varphi(\underline{r}-\begin{pmatrix}a\\0\end{pmatrix}) \rangle = e^{ik_x a}\cdot t$$

$$\underline{R}=\begin{pmatrix}-a\\0\end{pmatrix} \rightarrow e^{-ik_x a} \langle \qquad\qquad \rangle = e^{-ik_x a}\cdot t$$

$$\underline{R}=\begin{pmatrix}0\\a\end{pmatrix} \rightarrow e^{ik_y a} \langle \varphi(\underline{r}) | H | \varphi(\underline{r}-\begin{pmatrix}0\\a\end{pmatrix}) \rangle = e^{ik_y a}\cdot t$$

$$\underline{R}=\begin{pmatrix}0\\-a\end{pmatrix} \rightarrow e^{-ik_y a} \langle \qquad\qquad \rangle = e^{-ik_y a}\cdot t$$

$$\langle \psi_{\underline{k}}(\underline{r}) | H | \psi_{\underline{k}}(\underline{r}) \rangle = E_0 + 2t\{\cos(k_x a) + \cos(k_y a)\}$$



<u>example 3</u>: 3 dimensional simple cubic lattice
on-site energy E_0, nearest neighbor hopping t

$$\langle \psi_{\underline{k}}(1) | H | \psi_{\underline{k}} \rangle = E_0 + 2t \{ \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \}$$