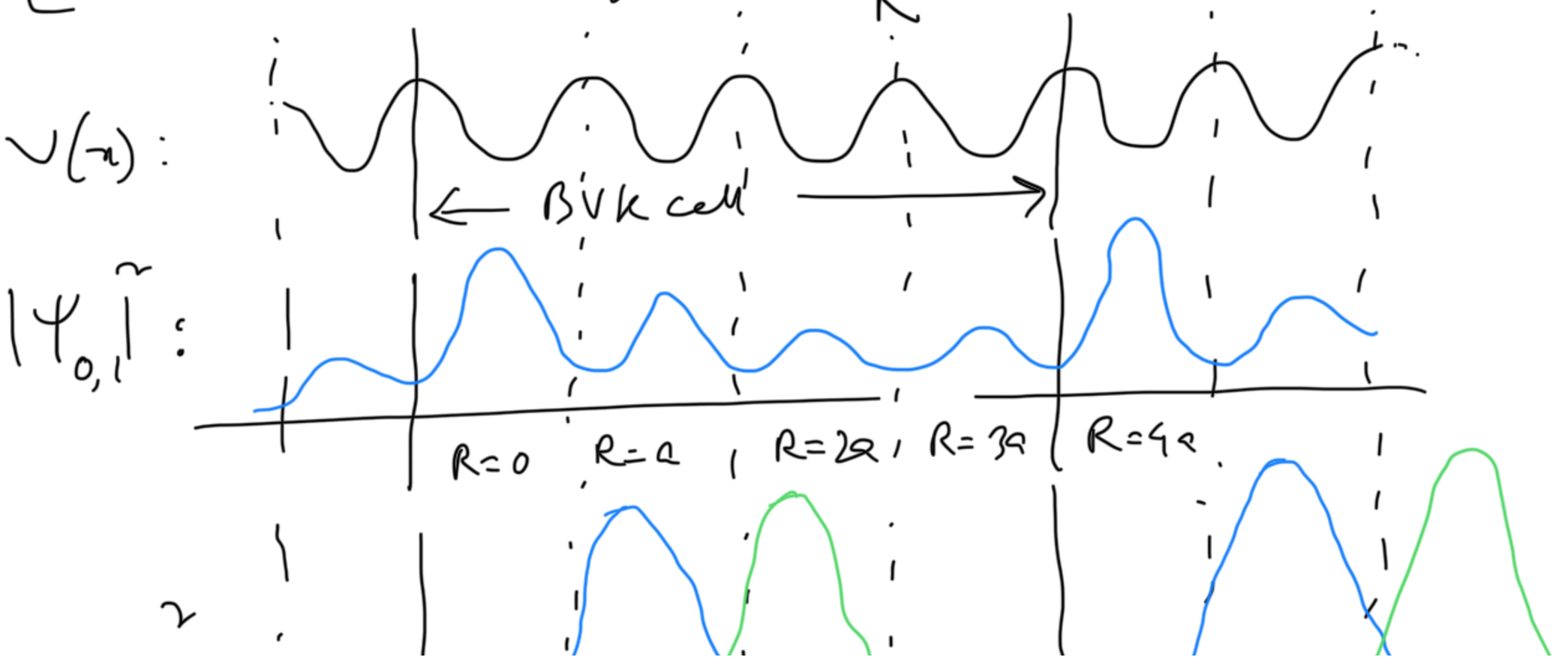
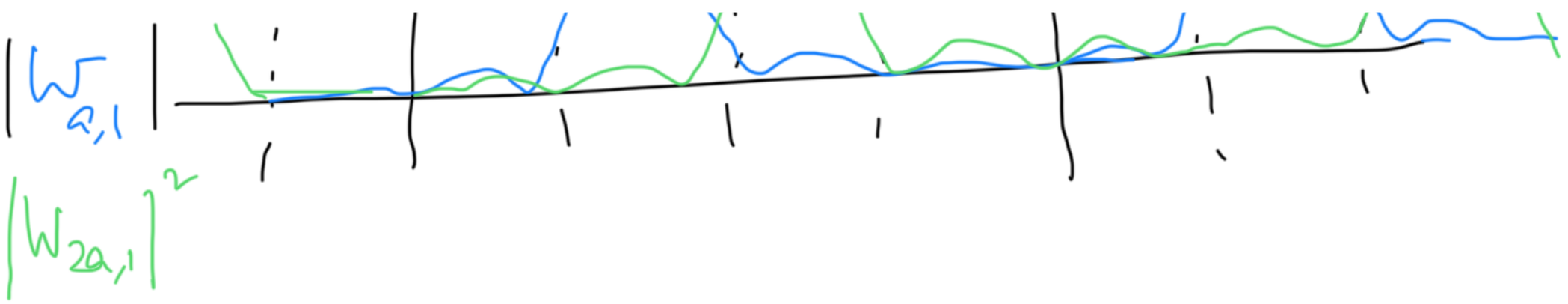
Tight binding Hamiltonian

Recall, $W_{Rn}(x) = \frac{1}{\sqrt{N}} \sum_q^{BZ} e^{-iqR} \psi_{qn}(x) = \frac{1}{\sqrt{N}} \sum_q e^{iq(x-R)} u_{qn}(x)$

$$\langle W_{Rn} | W_{R'n'} \rangle = \delta_{RR'} \delta_{nn'}$$

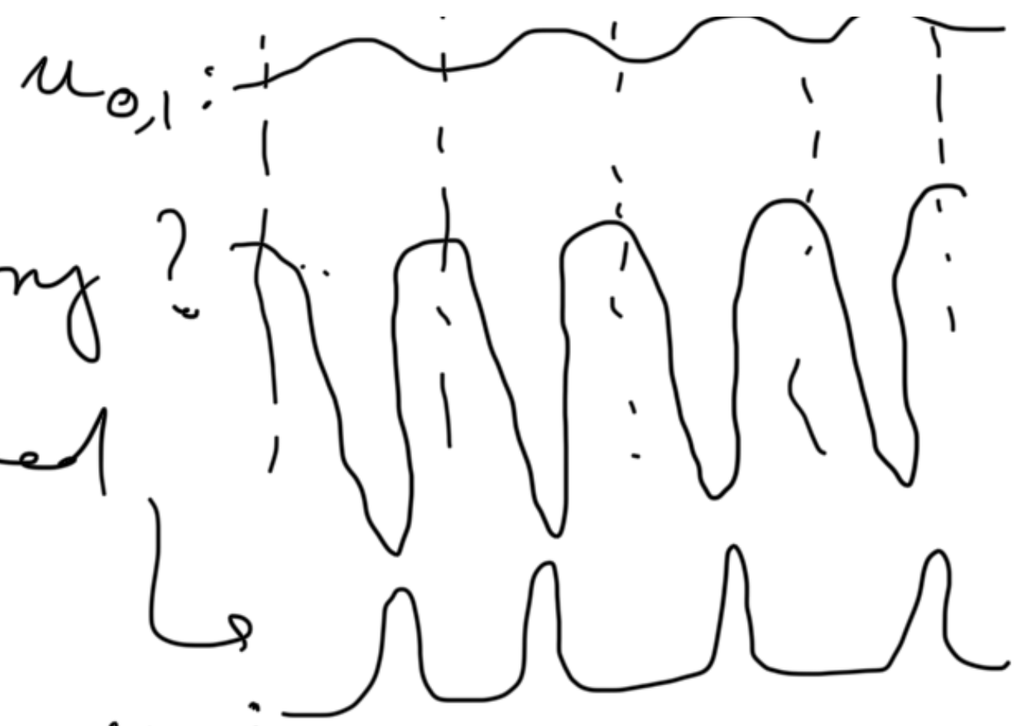
[Conversely: $\psi_{qn}(x) = \frac{1}{\sqrt{N}} \sum_R^{BVK} e^{iqR} W_{Rn}(x)$]





Given a periodic potential $V(x)$ which is smooth enough to be expressed in a small set of Fourier basis $\left\{ e^{iGx} : G = -M\frac{2\pi}{a}, \dots, +M\frac{2\pi}{a} \right\}$ then we now know that we can consider expanding u_{qn} in the same basis to solve for $\{E_{qn}\ \psi_{qn}\}$.

Note that this works well if M can be taken to be a finite small number; which means that we have already assumed that $\{u_{qn}\}$ (and thus $\{\psi_{qn}\}$) are all quite smooth functions in real space since $V(x)$ is smooth $\Rightarrow$ Nearly free electron model:

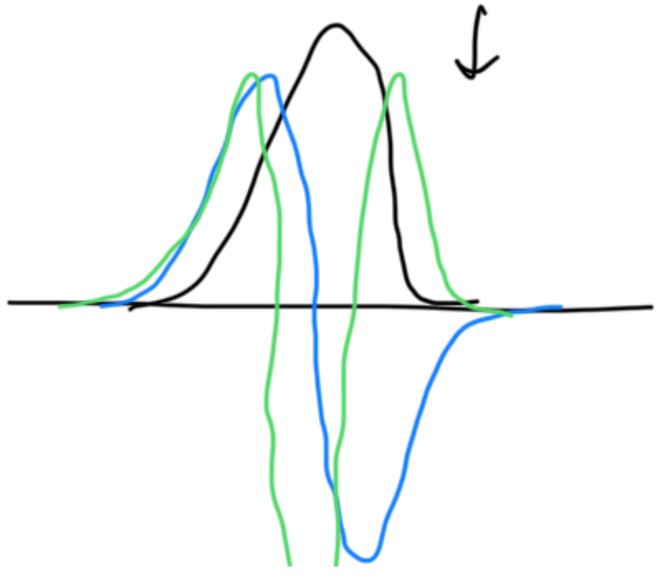


But what if $V(x)$ is strong? $\{u_{qm}\}$ will be highly localized

$\Rightarrow$ Need lot large M.

$\Rightarrow$ large matrix $\rightarrow$ heavy computation.

In such scenarios, instead of expanding $\psi_{qn}(x)$ in term of fourier basis, we can expand $\psi_{Rn}(x)$ in some orthonormal set of localized fns $\{\phi_{Rl}\}$



$$\therefore \quad \psi_{Rn}(x) = \sum_{m}^{N_b} C_m^n \phi_{Rm}(x)$$

$N_b \rightarrow$ number of basis orbitals used

$$\therefore \psi_{qn}(r) = \sum_{R}^{Bvk} e^{iqR} \sum_{m}^{N_b} C_m^n \phi_{Rm}(r)$$

$$\boxed{\langle \phi_{Rn} | \phi_{R'n'} \rangle = \delta_{RR'} \delta_{nn'}}$$

$$\therefore \hat{H} |\psi_{qn}\rangle = E_{qn} |\psi_{qn}\rangle$$

$$\Rightarrow \hat{H} \sum_{R} e^{iqR} \sum_{m} C_m^n |\phi_{Rm}\rangle = E_{qn} \sum_{R'} e^{iqR'} \sum_{\ell} C_\ell^n |\phi_{R'\ell}\rangle$$

Contract with $\langle \phi_{R''j} |$:

$$\sum_{R} e^{iqR} \sum_{m} \langle \phi_{R''j} | \hat{H} | \phi_{Rm} \rangle C_m^n = E_{qn} \sum_{R'} e^{iqR'} \sum_{\ell} C_\ell^n \langle \phi_{R''j} | \phi_{R'\ell} \rangle$$

$$\Rightarrow \sum_{R} e^{iqR} \sum_{m} H_{R''-R,jm} C_m^n = E_{qn} \sum_{R'} e^{iqR'} \sum_{\ell} C_\ell^n \delta_{R''R'} \delta_{j\ell}$$

$$= E_{qn} e^{iqR''} C_j^n$$

$$\therefore e^{iq(R-R'')} \sum_{m}^{N_b}$$

$$\Rightarrow \sum_R e^{i\mathbf{q}\cdot\mathbf{R}} \sum_m H_{R'j,Rm}\, C^n_m = E_{qn}\, C^n_j$$

Set $R'=0$ owing to translational symmetry.

$$\Rightarrow \sum_R^{N_b} e^{i\mathbf{q}\cdot\mathbf{R}} \sum_m^{N_b} H_{0j,Rm}\, C_m = E_q\, C_j$$

dropping n since it is just the order of the eigenstate and eigenvalue

N_b number of simultaneous equations for each q.

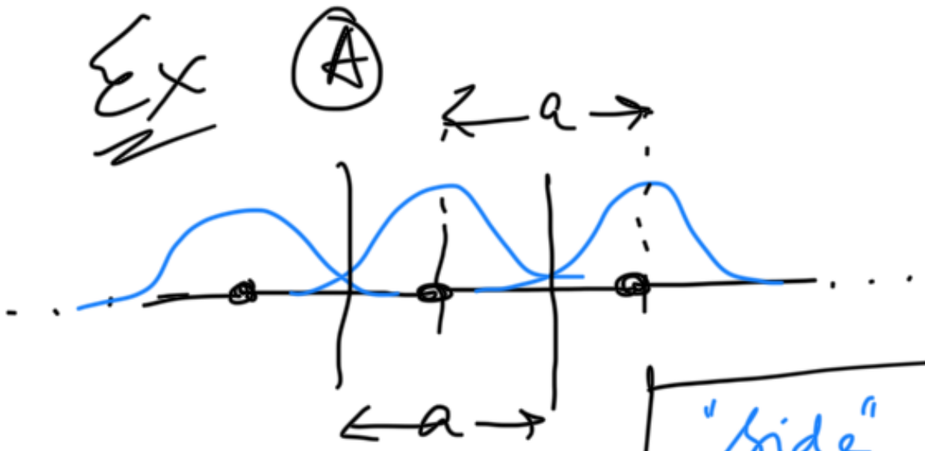
Note (R,m) denotes a single basis orbital.
$(0,j)$ may be same (if $R=0, j=m$) or different basis orbitals.

If $R=0, m=j$ the $(0,j)$ and (R,m) are same basis orbitals
$H_{0j,0j}$ → onsite term. → traditionally E_0

If $(0,j)$ and (R,m) are different basis orbitals
then $H_{0j,Rm}$ → hopping term → traditionally "t"

Ex

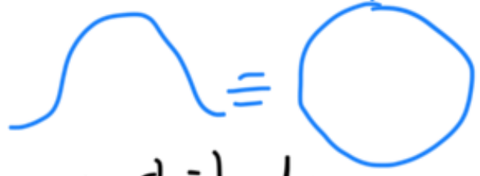
A



m = 1 to 1

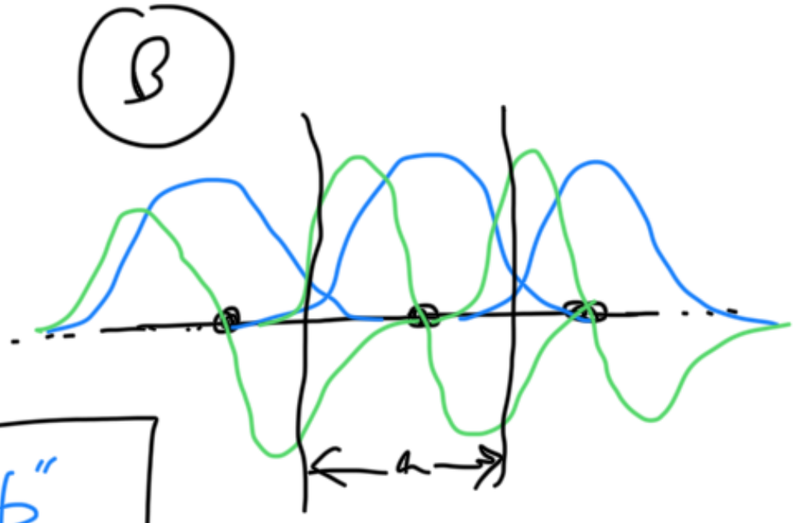
N_b = 1

"side" "top"



orbitals

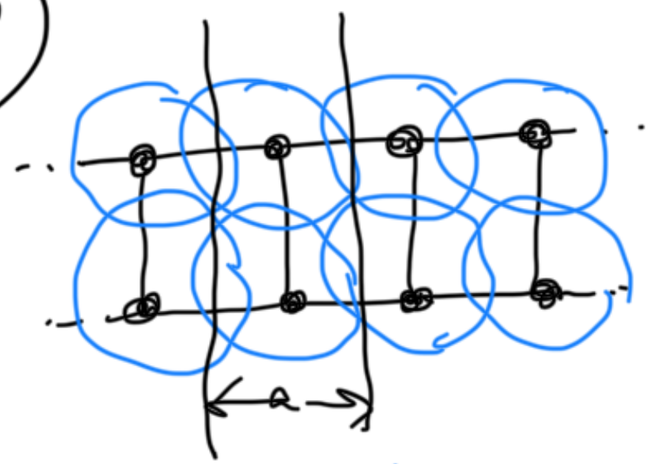
B



m = 1 to 2

N_b = 2

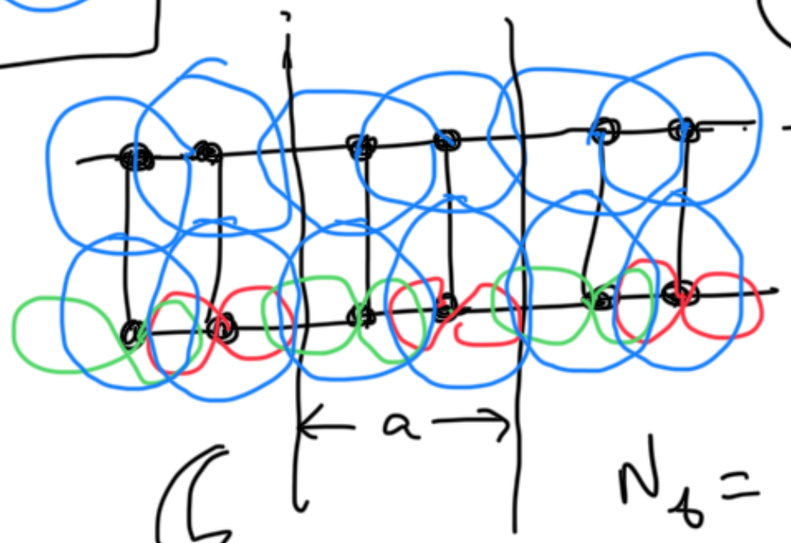
C



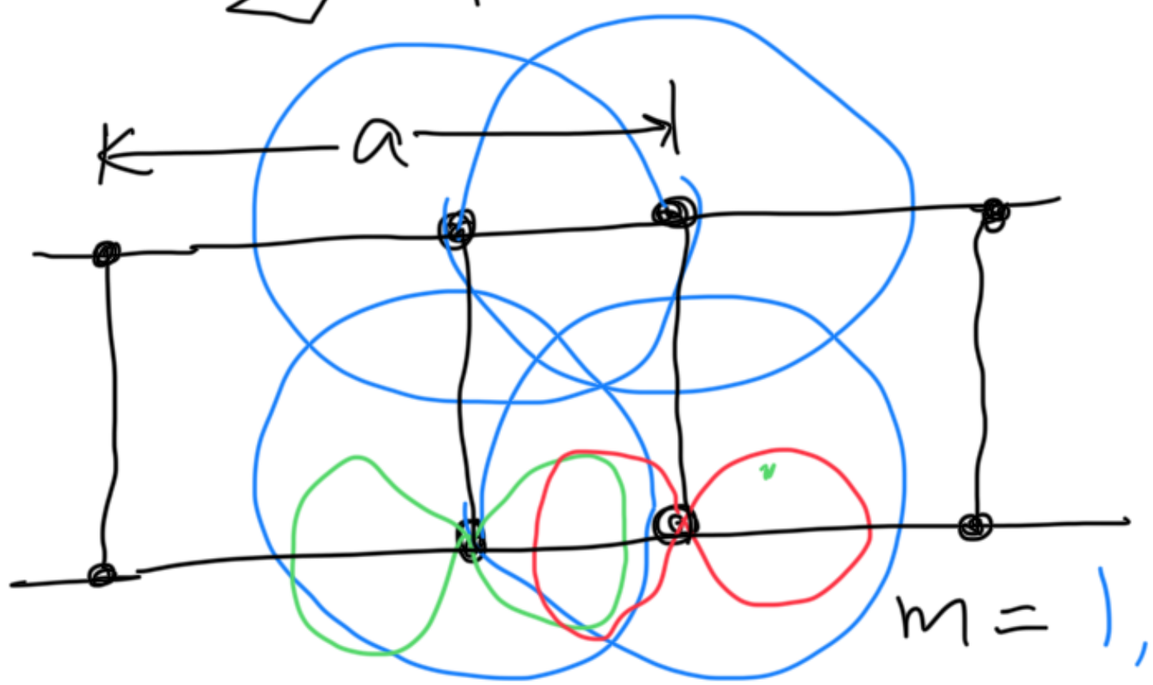
m = 1 to 2

N_b = 2

D

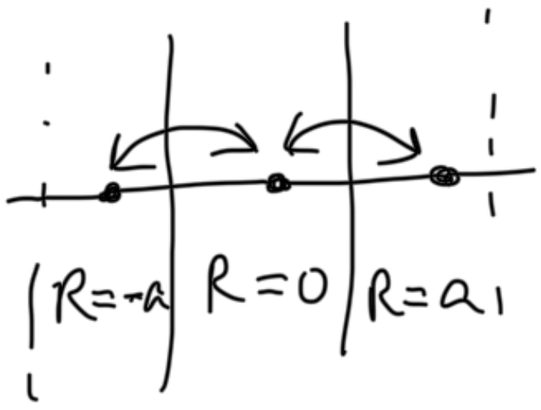


N_b = 6



m = 1, 2, 3, 4, 5, 6

For (A) : Orbital overlaps only between nearest neighbours. H



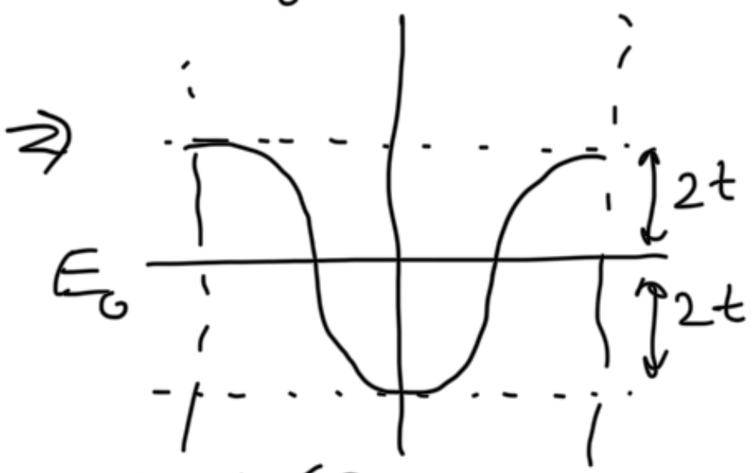
$$\begin{bmatrix} e^{-iaq} H_{01,-a1} + e^{0} H_{01,01} + e^{+iaq} H_{01,a1} \end{bmatrix} C_1 = E_q C_1$$

$H_{01,-a1}$: t ; $H_{01,01}$: E_0 ; $H_{01,a1}$: t

$N_b = 1$

$m = 1 \; t_{01}$

$$E_q = E_0 + 2t \cos qa \Rightarrow$$



for $E_{q=0;1} < E_{q=\pm\pi/a;1}$; t must < 0

Recall $H = \begin{bmatrix} E_0 & t \\ t & E_0 \end{bmatrix}$ → would not give nodeless state as ground state if not $t<0$.
(test it)