

Recap :- ① why bands originate?

② Diagrammatic POV for band theory

free e⁻

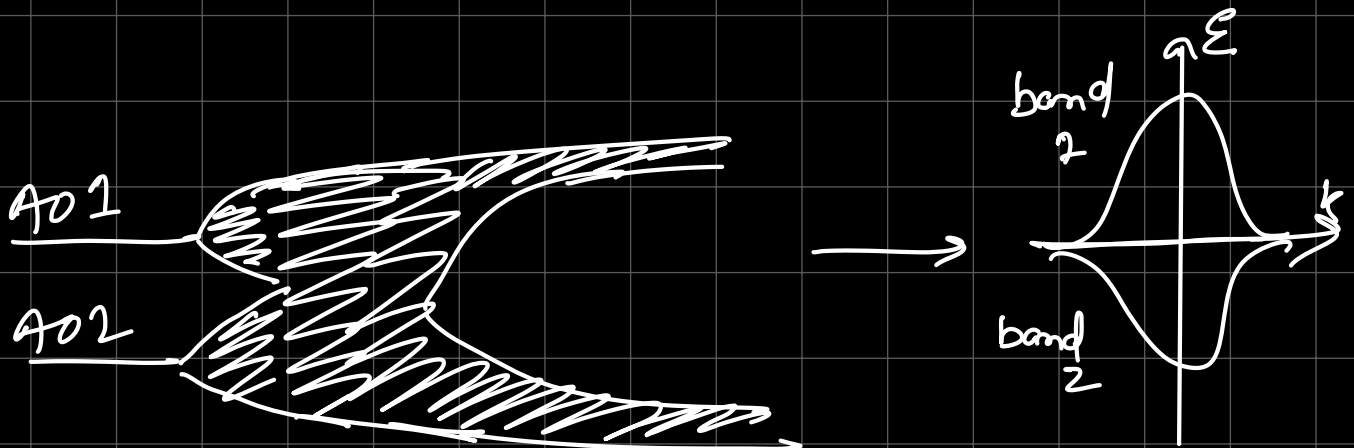
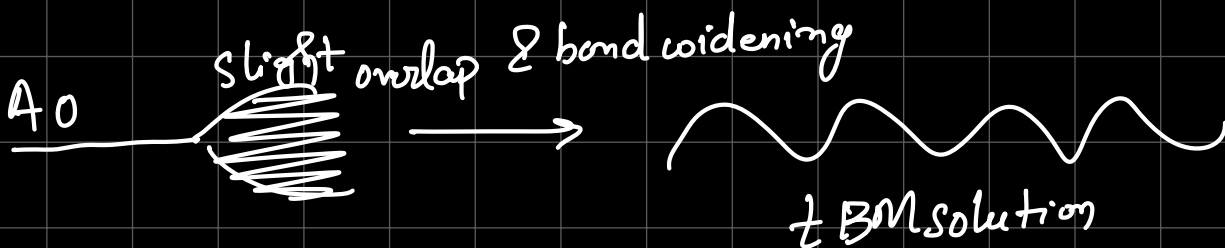
tBM

localised orbitals + hopping

Variational approach : LCAO
to be tried.

1 orbital $\Rightarrow$ 1 band

2 orbitals $\Rightarrow$ 2 bands

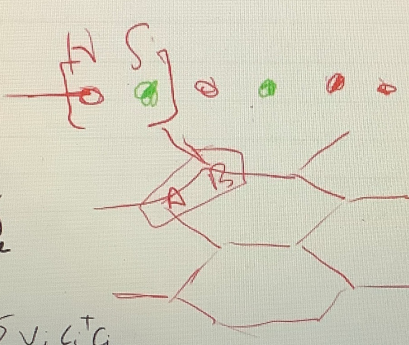


2 band models

$$H = - \sum_{ij} t_{ij} c_i^\dagger c_j + h.c. + \sum_i V_i c_i^\dagger c_i$$

number of available quantum states per atom

to do tight binding
to momentum space

$$H = - \sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ji}^* c_j^\dagger c_i) + \sum_i V_i c_i^\dagger c_i$$


I

Simpler way to do tight binding
from real space to momentum space

$$H = - \sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ji}^* c_j^\dagger c_i) + \sum_i V_i c_i^\dagger c_i$$

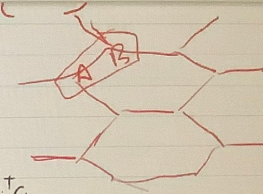
$$H^\dagger = H$$

$$- \sum_{ij} (t_{ij}^* c_j^\dagger c_i + t_{ji} c_i^\dagger c_j) + \sum_i V_i^* c_i^\dagger c_i$$

$$\Rightarrow t_{ij}^* = t_{ji} \quad \& \quad V_i = V_i^*$$

$$= - \sum_{ij} (t_{ij} c_i^\dagger c_j + t_{ji}^* c_j^\dagger c_i) + V_N$$

V_N is a constant and provides shift



provides a shift

now, change basis to $\vec{k}$ space

$$c_{\vec{k}} = \frac{1}{\sqrt{2\pi}} \sum_j c_j e^{-i\vec{k} \cdot \vec{r}_j}$$

$$\{C_i, C_j^\dagger\} = \delta_{ij} \quad \mathcal{H}(\vec{r}) \rightarrow \mathcal{H}(\vec{k})$$

exercise:-

show that $\sum_{ij} C_i^\dagger C_j = \sum_k (-2t \cos ka) \underline{C_k^\dagger C_k}$
for nearest
nbr

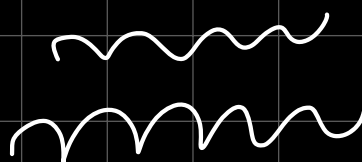
$\hat{H}(k) = (-2t \cos ka)$ with a k -mode for each.
↳ 1x1 matrix

Suman Saurav, Vysakh → DTP

Discovering or how to get 2x2 matrix for 2 band model.

The screenshot shows a handwritten derivation in OneNote for Windows 10. At the top, a diagram shows a 1D chain of sites with hopping parameter t and lattice constant a . The derivation starts with the expression for the wavefunction χ in terms of creation and annihilation operators a_k and b_k . It then simplifies this expression using the identity $e^{iKa/2} = \cos(ka/2) + i \sin(ka/2)$ to arrive at the 2x2 matrix $X(k)$. The matrix is defined as $X(k) = \begin{pmatrix} V_a & -2t \cos(ka/2) \\ -2t \cos(ka/2) & V_b \end{pmatrix}$. A note states that the eigenvalues of $X(k)$ tell us about dispersion. Finally, the energy bands $\epsilon_{\pm}$ are given by $\epsilon_{\pm} = \frac{V_a + V_b}{2} \pm \frac{1}{2} \sqrt{(V_a - V_b)^2 + 4t^2 \cos^2(ka/2)}$.

SSH intuition



when site
energies
are diff

$$\begin{pmatrix} a_k \\ b_k \end{pmatrix} = U_k \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

$$(c_k^\dagger \ d_k^\dagger) = (a_k^\dagger \ b_k^\dagger) U_k$$

$$U_k^\dagger = U_k^{-1}$$

$$H = \sum_k (c_k^\dagger \ d_k^\dagger) U_k^\dagger H U_k \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

$$U_k H U_k^\dagger = \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix}$$

$$H = \sum_k (c_k^\dagger \ d_k^\dagger) \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

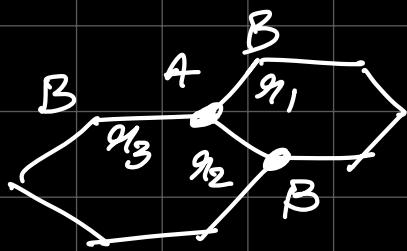
Because the AOs

have different energies,
so when we do tBM, it'll
have spaced bands.

→ structure of eigenvector
gives info abt topological
character of the system.

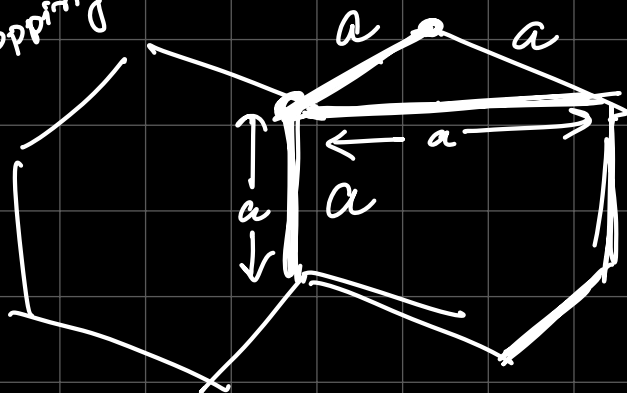
Spoiler: Eigenvectors are important → tBA why.

tBM of honeycomb lattice



$$H(k) = \begin{pmatrix} 0 & -t(e^{-ikr_1} + e^{-ikr_2} + e^{-ikr_3}) \\ \epsilon^* & 0 \end{pmatrix}$$

honeycomb with
NNN hopping



wed morning → honeycomb

wed afternoon → SSH

Inversion symmetry

⇒ Orbitals have inversion symmetry

↙
site ≠ orbitals

e.g. → hex BN → it has alternate B2N

↘
but is an insulator

↓
as a pair is isoelectronic with C