Recap :- ① Why bands originate?

② Diametric POV for band theory

free e^- — tBM

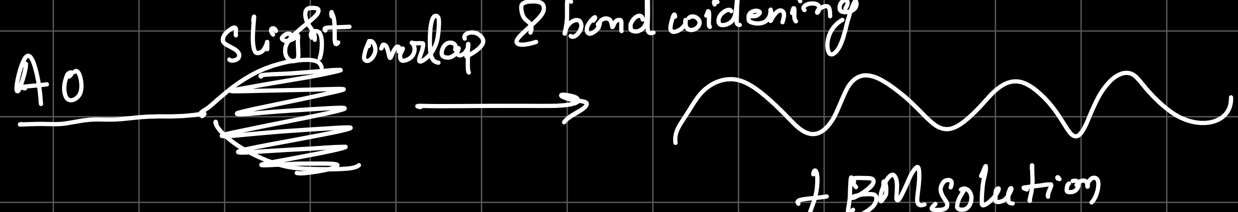
Localised orbitals + hopping

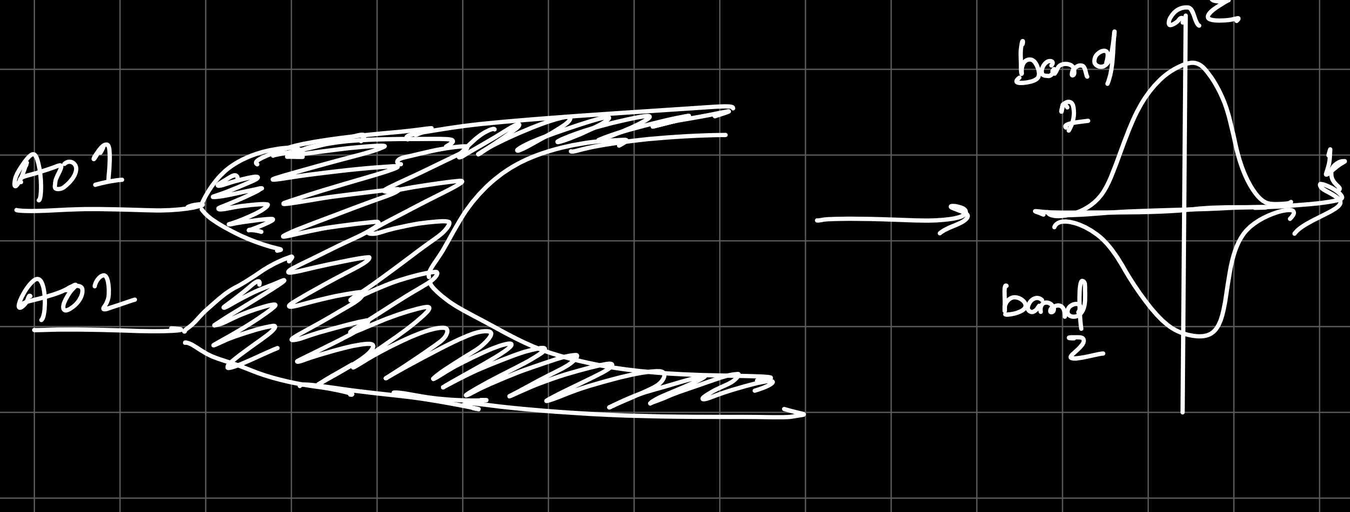
↓

Variational approach : LCAO to be tried.

1 orbital ⇒ 1 band

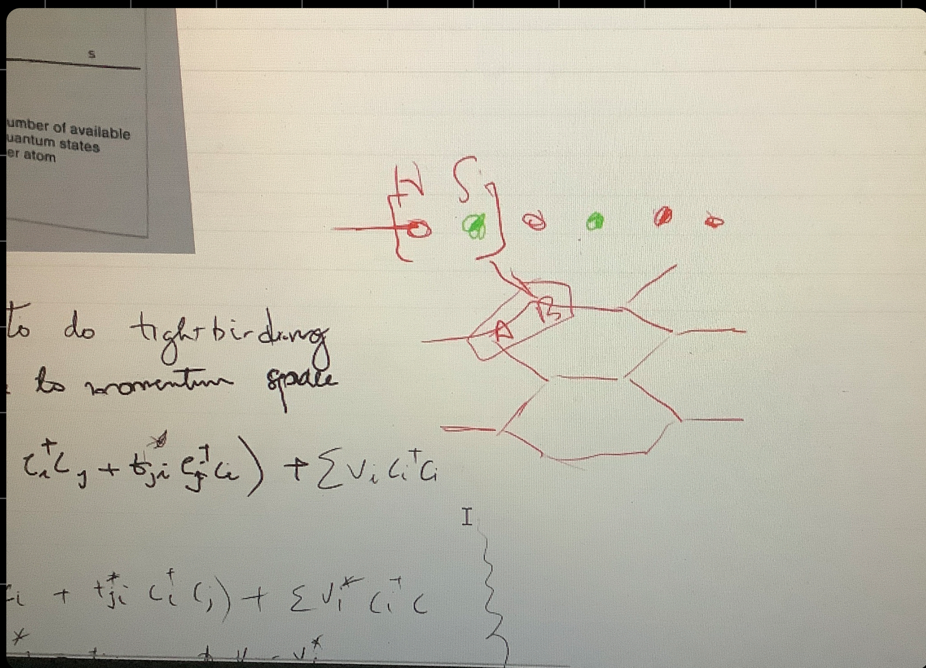
2 orbitals ⇒ 2 bands

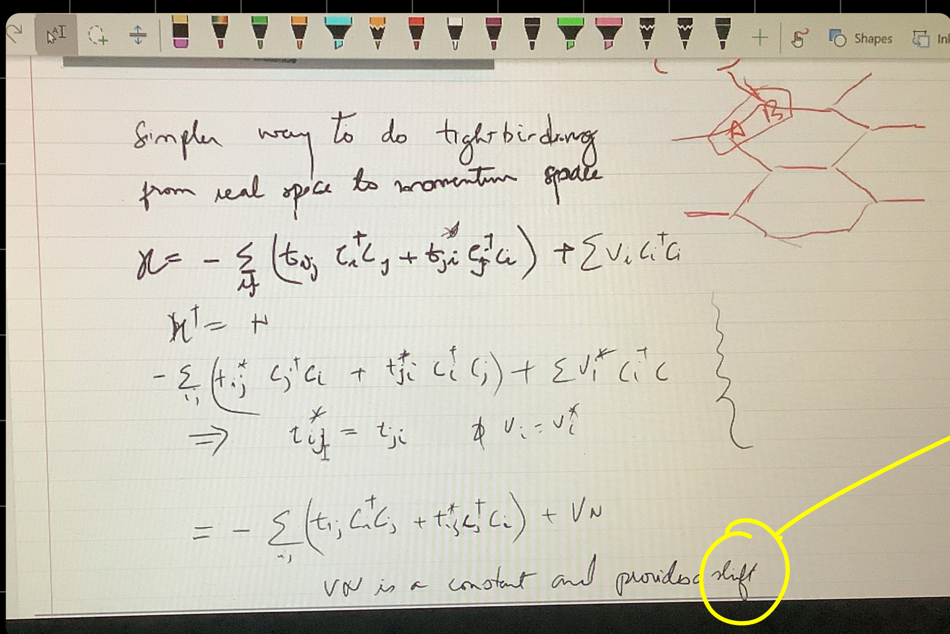




2 band models

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





Simpler way to do tightbinding
from real space to momentum space

$\mathcal{H} = -\sum_{ij}\left(t_{ij}\, c_i^\dagger c_j + t_{ji}^* c_j^\dagger c_i\right) + \sum V_i c_i^\dagger c_i$

$\mathcal{H}^\dagger = \mathcal{H}$

$-\sum_{ij}\left(t_{ij}^*\, c_j^\dagger c_i + t_{ji}^* c_i^\dagger c_j\right) + \sum V_i^* c_i^\dagger c$

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

$= -\sum_{ij}\left(t_{ij}\, c_i^\dagger c_j + t_{ij}^* c_j^\dagger c_i\right) + VN$

VN is a constant and provides shift

provides a shift

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

$$c_k = \sqrt{\frac{a}{2\pi}} \sum_j c_j e^{-ikj}$$

$\{c_i, c_j^\dagger\} = \delta_{ij}$ $\qquad \mathcal{H}(\vec{r}) \longrightarrow \mathcal{H}(\vec{k})$

exercise :-

show that $-t\sum_{ij} c_i^\dagger c_j = \sum_k (-2t\cos ka)\, \underline{c_k^\dagger c_k}$

for nearest nbr

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

↳ 1×1 matrix

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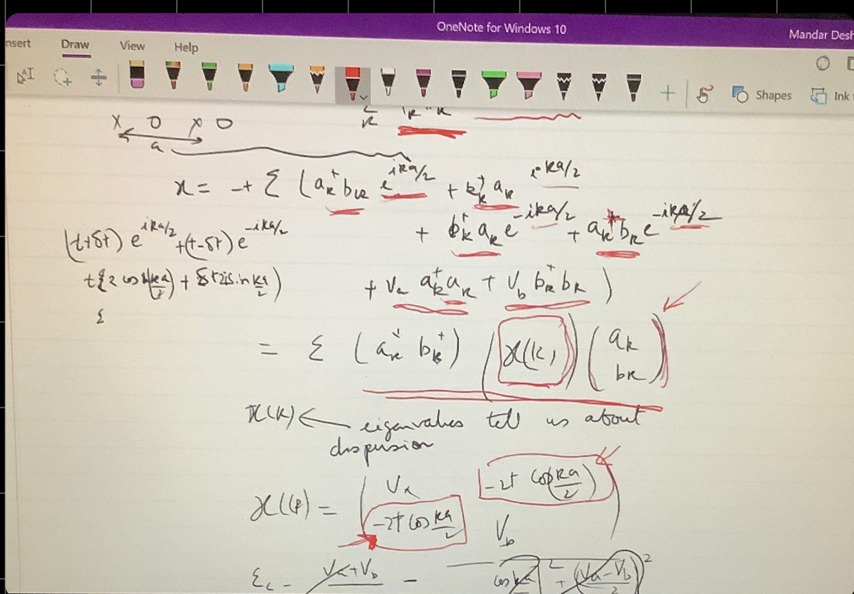
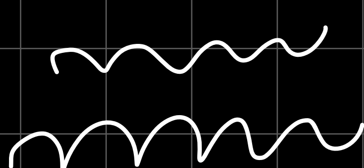
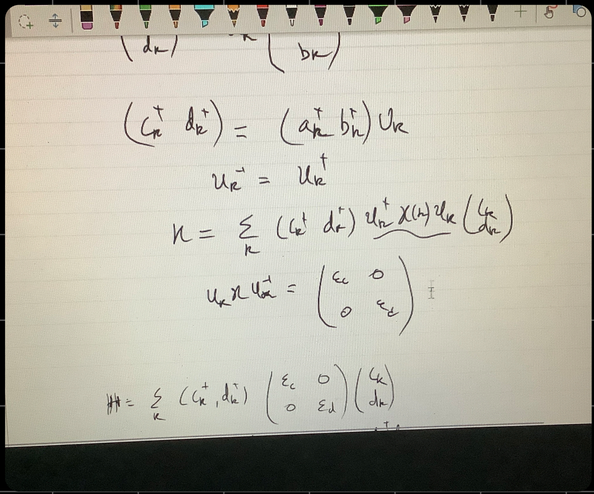
Discussion on how to get 2×2 matrix for 2 band model.



SSH intuition



when site energies are diff

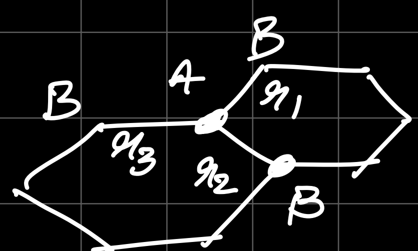


Because the AOs have different energies, so when we do tbm, it'll have spaced bands.

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

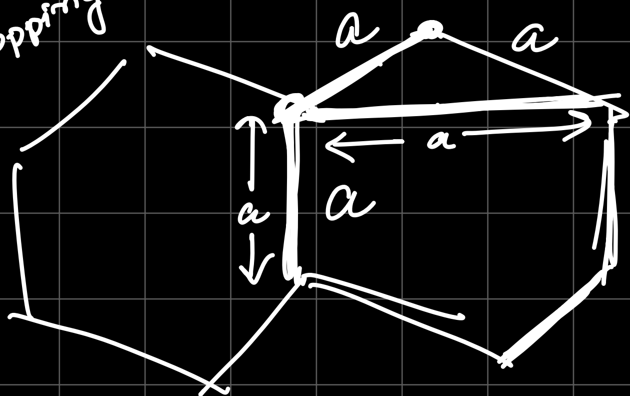
Spoiler: Eigenvectors are important → tBA why.

tBM of honeycomb lattice



$$H(k) = \begin{pmatrix} 0 & \underbrace{-t\left(e^{-ikr_1}+e^{-ikr_2}+e^{-ikr_3}\right)}_{\varepsilon} \\ \varepsilon^* & 0 \end{pmatrix}$$

honeycomb with NN hopping



Wed morning → honeycomb

Wed afternoon → SSH

Inversion symmetry $\Rightarrow$ Orbitals have inversion symmetry

site ≠ orbitals

e.g. → hex BN → it has alternate B & N

&

as a pair is isoelectronic with C

but is an insulator