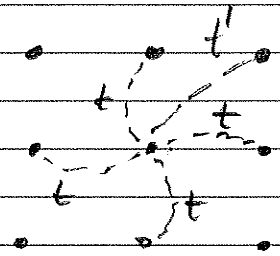
Tight Binding Example 1

s orbital on a square lattice. Nearest neighbor; 2nd neighbor



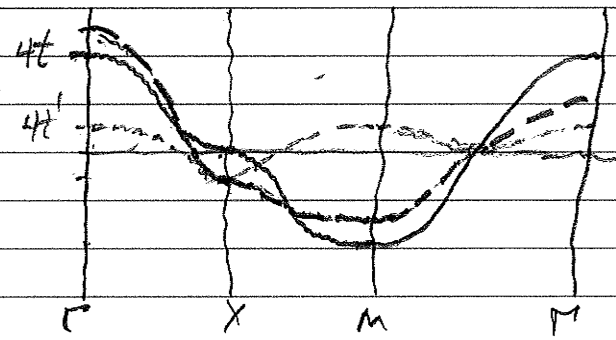
set $\varepsilon_s = 0$

(1st): $t\left[e^{ik\cdot(1,0)a} + e^{ik\cdot(0,1)a} + e^{ik\cdot(-1,0)a} + e^{ik\cdot(0,-1)a}\right]$

$= 2t\left(\cos k_x a + \cos k_y a\right)$

a=1

$\Gamma = (0,0)$
$X = (\pi,0) = (0,\pi)$
$M = (\pi,\pi)$



s band
band
on square
lattice

(2nd) $t'\left[e^{ik\cdot(1,1)a} + e^{ik\cdot(-1,1)a} + e^{ik\cdot(-1,-1)a} + e^{ik\cdot(1,-1)a}\right]$

$= t'\left[2\cos k_x a\, e^{ik_y a} + 2\cos k_x a\, e^{-ik_y a}\right] = 4t' \cos k_x a \cos k_y a$

At Γ: $4t'$. At X: $4t'(-1)(1)$. At M: $4t'(-1)(-1)$

This is a 1-band model, 1st & 2nd neighbors

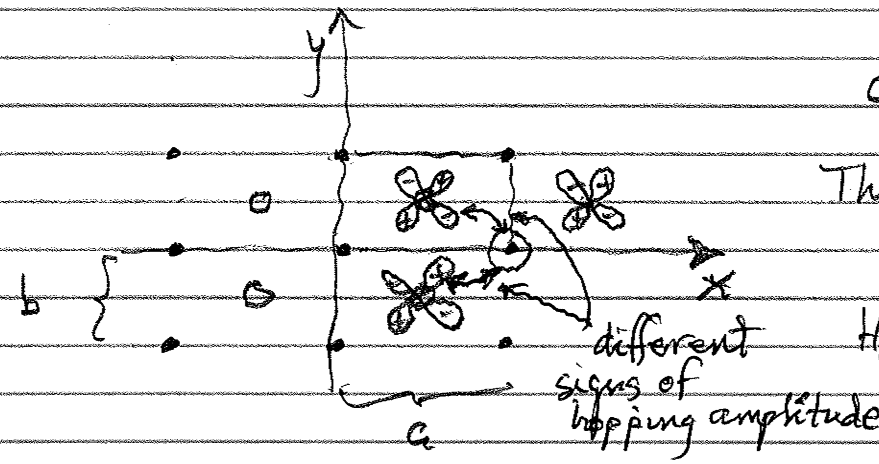
$t' \approx t/4$.

$H^{TB} = 2t(\cos k_x a + \cos k_y a) + 4t' \cos k_x a \cos k_y a$

(a 1×1 Hamiltonian matrix: single band)

Tight Binding Example 2

Rectangular lattice, 2 atoms. S state at origin, d_{xy} at center



On-site: ε_s; ε_d

This is a **2-band** model

$$H_{on\text{-}site} = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & \varepsilon_d \end{pmatrix}$$

s-s hopping $\quad 2t_{ss}(\cos k_x a + \cos k_y b) \equiv H_{1,1}(k)$

d-d hopping $\quad t_{dd}\left(e^{ik\cdot(a,0)} + e^{ik\cdot(0,b)} + e^{ik\cdot(-a,0)} + e^{ik\cdot(0,-b)}\right)$

$$= 2t_{dd}(\cos k_x a + \cos k_y b) \equiv H_{2,2}(k)$$

s-d hopping: $\quad t_{sd}\left(e^{ik(0,0)} + (-1)e^{ik\cdot(-a,0)} + e^{ik\cdot(-a,-b)} + (-1)e^{ik\cdot(0,-b)}\right)$

$$= t_{sd}\left(1 - e^{ik_y b} - e^{-ik_x a}(1 - e^{ik_y b})\right)$$

Note the minus signs

$$= t_{sd}(1 - e^{ik_y b})(1 - e^{-ik_x a})$$

$$= t_{sd}\, e^{ik_y b/2}\left(e^{-ik_y b/2} - e^{+ik_y b/2}\right) \times (\text{analogous for } k_x a)$$

$$= t_{sd}\, e^{ik_x a/2} e^{ik_y b/2}(-2i \sin k_y b/2)(-2i \sin k_x a/2)$$

$$= -4t_{sd} \sin(\xi/2)\sin(\eta/2)\, e^{i(\xi+\eta)/2} \equiv H_{1,2}(k)$$

$$H^{TB} = \begin{bmatrix} H_{1,1}(k) & H_{1,2}(k) \\ H_{1,2}^{*}(k) & H_{2,2}(k) \end{bmatrix}$$

2 band model.

H^{TB}, the 2×2 Hamiltonian on the previous page, has a complex $H_{1,2}(k)$ matrix element. That's OK, but since the model has inversion symmetry, it is possible to have a real TB matrix w/ the same eigvals.

Transform H^{TB} w/ the unitary transformation

$$\mathcal{U}_{ij}(k) = e^{-ik\cdot\tau_j}\,\delta_{ij} \;;\quad \tau_1 = (0,0) \text{ for s-function}, \quad \tau_2 = \tfrac{1}{2}(a,b) \text{ for d-fn}.$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & u \end{bmatrix}, \quad u \equiv e^{-i(\xi+\eta)/2}.$$

Then $\mathcal{U} H^{TB} \mathcal{U}^{+}$ becomes

$$\begin{bmatrix} H_{1,2}(k) & \tilde{H}_{1,2}(k) \\ \tilde{H}_{2,1}(k) & H_{2,2}(k) \end{bmatrix}$$

where $\tilde{H}_{1,2}(k) = \tilde{H}_{2,1}(k) = -4t_{sd}\sin\frac{\xi}{2}\sin\frac{\eta}{2}$ are real.

the phase factor $e^{\pm i(\xi+\eta)/2}$ has been transformed away