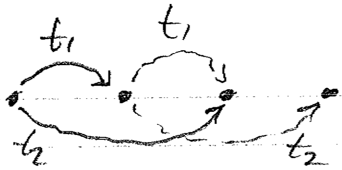
PHY 240A HW7 solutions

1. $\varepsilon_0 \equiv 0.$



(a) $\varepsilon_k = t_1\left(e^{ika} + e^{-ika}\right) + t_2\left(e^{ik2a} + e^{-ik2a}\right) = 2t_1\cos ka + 2t_2\cos 2ka$

(b) $h_k = \varepsilon_k S_k$: $2t_1\cos ka = \varepsilon_k(1+2s_1\cos ka) \Rightarrow \varepsilon_k = \dfrac{2t_1\cos ka}{1+2s_1\cos ka}$

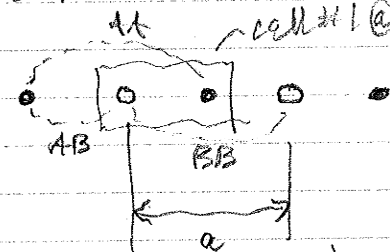
$t_1 \equiv 1$ Suppose t_2 and s_2 are reasonably small.

$$\varepsilon_k^{(a)} = 2(\cos ka + t_2\cos 2ka) \Longleftrightarrow \varepsilon_k^{(b)} \cong 2\cos ka\,(1 - s_1\cos ka + \dots)$$
$$= 2\cos ka + 2t_2\cos 2ka \qquad\qquad = 2\cos ka - 2s_1\cos^2 ka + \dots$$
$$= 2\cos ka - s_1(\underbrace{1}+\cos 2ka) + \dots$$

Each brings in the same 2^{nd} wavelength [2ka vs. ka]. Overlap form shifts energy in this case and also small bits of higher wavevectors $[(s_1\cos ka)^2, (s_1\cos ka)^3, \dots]$

PLOT ....

2.



$h_{AA} = \varepsilon_A + t_{AA}\left(e^{ika} + e^{-ika}\right) = \varepsilon_A + 2t_{AA}\cos ka$

$h_{BB} = \varepsilon_B + 2t_{BB}\cos ka$

(a) $h_{AB} = t_{AB}\left(1 + e^{-ika}\right) = t_{AB}\, e^{-ika/2}\, 2\cos\frac{ka}{2}$ if you want to write it this way.

(b) let $c = a/2$ be the lattice constant when all atoms are identical. In this case, $t_{AB} \to t_1$, $t_{AA} = t_2 = t_{BB}$

Now $h_{AA} \to h_{11} = \varepsilon_0 + 2t_2\cos 2kc$
$h_{BB} \to h_{22} = \varepsilon_0 + 2t_2\cos 2kc$
$h_{AB} \to h_{12} = 2t_1\cos kc\; e^{-ikc}$

The phase factor will not affect eigvals (bands). H has 2 bands but k goes only to $\pi/a = \frac{1}{2}\frac{\pi}{c}$.

Zone has been folded back. 2 bands but half as many k values (or distance to BZ boundary)

(c) $\hat{h}_k = \underset{\sim}{v}_k \cdot \underset{\sim}{\sigma}$; $\underset{\sim}{v}_k$ "looks like" a vector.

Go to next page.

2. (cont.) generalized: $\hat{h}_k = v_0(k)\underset{\approx}{1} + \underset{\sim}{v}(k)\cdot\underset{\sim}{\sigma}$

Every 2×2 matrix can be expanded in this way. $\hat{h}_k$ being Hermitian means v_0 and $\underset{\sim}{v}$ are real.

Using $\begin{bmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{bmatrix}$ and the expressions from above,

$$\boxed{\begin{aligned} v_0 &= (H_{AA}+H_{BB})/2 = \frac{\varepsilon_A+\varepsilon_B}{2} + 2\,\frac{t_{AA}+t_{BB}}{2}\cos ka \\ v_3 &= \frac{H_{AA}-H_{BB}}{2} = \frac{\varepsilon_A-\varepsilon_B}{2} + 2\,\frac{t_{AA}-t_{BB}}{2}\cos ka \\ v_1 &= \operatorname{Re} H_{AB} = 2t_{AB}\cos^2\frac{ka}{2} \\ v_2 &= -\operatorname{Im} H_{AB} = 2t_{AB}\cos\frac{ka}{2}\sin\frac{ka}{2} \end{aligned}}$$

Then $v_0\underset{\approx}{1} + \vec{v}\cdot\vec{\underset{\approx}{\sigma}}$ should reproduce $\underset{\approx}{H}(k)$

Interesting fact: diagonaliz'n gives eigvals

$$\begin{aligned} \varepsilon_{k,\pm} &= v_0(k) \pm |\vec{v}_k| \\ &= v_0(k) \pm \sqrt{v_{k,x}^2 + v_{k,y}^2 + v_{k,z}^2}\,. \end{aligned}$$

3. "GaAs": 2 atoms in zincblende structure.
near neighbor hopping.
atom 1: 2 orbitals a, b
at origin (0,0,0) + fcc related sites
atom 2: 1 orbital
located at $(\frac{1}{4},\frac{1}{4},\frac{1}{4})a$ + fcc related sites

Let origin + $(\frac{1}{4}\frac{1}{4}\frac{1}{4})a$ be in unit cell $R=0$
atom 2 will be connected to atom 1 in unit cells:
$\underset{\sim}{R}_1=(0,0,0)$, $R_2=(0,\frac{1}{2},\frac{1}{2})a$, $R_3=(\frac{1}{2},0,\frac{1}{2})a$, $R_4=(\frac{1}{2},\frac{1}{2},0)a$.

$H_{1,1}$: ε_1 no near neighbor of type 1
$H_{2a,2a}$: ε_{2a} " " " " " 2
$H_{2b,2b}$: ε_{2b} " " " " " 2

$$H_{1,2a}: \sum_R t_a(R)\, e^{ik\cdot R} = t_a\left[1+e^{i(k_y+k_z)a/2}+e^{i(k_x+k_z)\frac{a}{2}}+e^{i(k_x+k_y)\frac{a}{2}}\right]$$
$$\equiv T_a(k)$$

orbital 2b is just another like 2a so

$H_{1,2b} = T_b(k)$, ← like $T_a(k)$ but with $t_a \to t_b$

$H_{2a,2b} = 0$. No on-site (off-diag. matrix elements, no 1^{st} neighbor).

so

$$H = \begin{array}{c|ccc} & 1 & 2a & 2b \\ \hline 1 & \varepsilon_1 & T_a(k) & T_b(k) \\ 2a & T_a^*(k) & \varepsilon_{2a} & 0 \\ 2b & T_b^*(k) & 0 & \varepsilon_{2b} \end{array}$$

is the TB Hamiltonian matrix.