

**PHYSICS 239.c : CONDENSED MATTER PHYSICS**  
**HW ASSIGNMENT #3**

[1] Consider a one-dimensional chain of  $s$ -orbitals

$$H = \sum_n \left( \varepsilon_A |A_n\rangle\langle A_n| + \varepsilon_B |B_n\rangle\langle B_n| \right. \\ \left. - t \sum_n \left( |A_n\rangle\langle B_n| + |B_n\rangle\langle A_{n+1}| + |B_n\rangle\langle A_n| + |A_{n+1}\rangle\langle B_n| \right) \right) .$$

- (a) How many atoms are there per unit cell? What is the length of the Wigner-Seitz cell?
- (b) Find the dispersions  $E_a(k)$  of the energy bands.
- (c) Sketch the band structure over the one-dimensional Brillouin zone.
- (d) Show that for  $\varepsilon_A = \varepsilon_B$  that you recover the correct energy band for the uniform one-dimensional nearest-neighbor chain.

[2] Hexagonal boron nitride, BN, has a honeycomb lattice structure, with boron atoms at A sites and nitrogen atoms at B sites. The tight binding Hamiltonian is

$$H = \sum_{\mathbf{R}} \left( \varepsilon_A |A_{\mathbf{R}}\rangle\langle A_{\mathbf{R}}| + \varepsilon_B |B_{\mathbf{R}}\rangle\langle B_{\mathbf{R}}| \right) \\ - t \sum_{\mathbf{R}} \left( |A_{\mathbf{R}}\rangle\langle B_{\mathbf{R}}| + |A_{\mathbf{R}}\rangle\langle B_{\mathbf{R}+a_1}| + |A_{\mathbf{R}}\rangle\langle B_{\mathbf{R}-a_2}| + \text{H.c.} \right) .$$

- (a) Find the  $2 \times 2$  Hamiltonian matrix  $\hat{H}(\mathbf{k})$ . You may find it convenient to write  $\mathbf{k} = \frac{\theta_1}{2\pi} \mathbf{b}_1 + \frac{\theta_2}{2\pi} \mathbf{b}_2$  and express your answer in terms of  $\theta_{1,2}$ .
- (b) Find expressions for the band energies at high symmetry points  $\Gamma$ , K, and M.
- (c) Find an expression for the band gap  $\Delta$ . Is the gap direct or indirect?

[3] Consider a tight binding model of  $(p_x, p_y)$  orbitals on a triangular lattice. The hopping is restricted to nearest neighbor links. Recall that the hopping matrix elements are given by

$$t_{\mu\nu}(\hat{\boldsymbol{\eta}}) = t_w \delta_{\mu\nu} - (t_s + t_w) \hat{\eta}_\mu \hat{\eta}_\nu ,$$

where the link direction is  $\hat{\boldsymbol{\eta}}$ .

- (a) Find the matrix  $\hat{t}_{\mu\nu}(\mathbf{k})$ . You may find it convenient to write  $\mathbf{k} = \frac{\theta_1}{2\pi} \mathbf{b}_1 + \frac{\theta_2}{2\pi} \mathbf{b}_2$  and express your answer in terms of  $\theta_{1,2}$ .
- (b) Find expressions for the band energies at the high symmetry points  $\Gamma$ , K, and M.
- (c) For  $t_s = 1$  and  $t_w = \frac{1}{2}$ , plot the dispersions  $E_{\pm}(\mathbf{k})$  along the path  $\Gamma\text{MK}\Gamma$ .