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

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

$$H = \sum_n \Big( \varepsilon_{\mathsf{A}} \, | \, \mathsf{A}_n \, \rangle\langle \, \mathsf{A}_n \, | + \varepsilon_{\mathsf{B}} \, | \, \mathsf{B}_n \, \rangle\langle \, \mathsf{B}_n \, | \\ - t \sum_n \Big( | \, \mathsf{A}_n \, \rangle\langle \, \mathsf{B}_n \, | + | \, \mathsf{B}_n \, \rangle\langle \, \mathsf{A}_{n+1} \, | + | \, \mathsf{B}_n \, \rangle\langle \, \mathsf{A}_n \, | + | \, \mathsf{A}_{n+1} \, \rangle\langle \, \mathsf{B}_n \, | \Big) \quad .$$

(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 $\varepsilon_{\mathsf{A}} = \varepsilon_{\mathsf{B}}$ 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

$$H = \sum_{\boldsymbol{R}} \Big( \varepsilon_{\mathsf{A}} \, | \, \mathsf{A}_{\boldsymbol{R}} \, \rangle\langle \, \mathsf{A}_{\boldsymbol{R}} \, | + \varepsilon_{\mathsf{B}} \, | \, \mathsf{B}_{\boldsymbol{R}} \, \rangle\langle \, \mathsf{B}_{\boldsymbol{R}} \, | \Big) \\ - t \sum_{\boldsymbol{R}} \Big( | \, \mathsf{A}_{\boldsymbol{R}} \, \rangle\langle \, \mathsf{B}_{\boldsymbol{R}} \, | + | \, \mathsf{A}_{\boldsymbol{R}} \, \rangle\langle \, \mathsf{B}_{\boldsymbol{R}+\boldsymbol{a}_1} \, | + | \, \mathsf{A}_{\boldsymbol{R}} \, \rangle\langle \, \mathsf{B}_{\boldsymbol{R}-\boldsymbol{a}_2} \, | + \text{H.c.} \Big) \quad .$$

(a) Find the $2 \times 2$ Hamiltonian matrix $\hat{H}(\boldsymbol{k})$. You may find it convenient to write $\boldsymbol{k} = \frac{\theta_1}{2\pi} \, \boldsymbol{b}_1 + \frac{\theta_2}{2\pi} \, \boldsymbol{b}_2$ 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) 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

$$t_{\mu\nu} = t_{\rm w} \, \delta_{\mu\nu} - (t_{\rm s} + t_{\rm w}) \, \hat{\eta}_\mu \, \hat{\eta}_\nu \quad ,$$

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

(a) Find the matrix $\hat{t}_{\mu\nu}(\boldsymbol{k})$. You may find it convenient to write $\boldsymbol{k} = \frac{\theta_1}{2\pi} \, \boldsymbol{b}_1 + \frac{\theta_2}{2\pi} \, \boldsymbol{b}_2$ 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 $t_{\rm s} = 1$ and $t_{\rm w} = \frac{1}{2}$, plot the dispersions $E_\pm(\boldsymbol{k})$ along the path $\Gamma$MK$\Gamma$.