PHYSICS 152B/232
Spring 2017
Homework Assignment #1

[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 2×2 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 Γ, K, and M.

(c) Find an expression for the band gap Δ. 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 Γ, K, and M.

(c) For $t_{\mathrm{s}} = 1$ and $t_{\mathrm{w}} = \frac{1}{2}$, plot the dispersions $E_{\pm}(\boldsymbol{k})$ along the path ΓMKΓ.