PHYSICS 152B/232
Spring 2017
Homework Assignment #1 Solutions

[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.

Solution :

(a) There are two atoms per unit cell (one A and one B). The length of the Wigner-Seitz cell is $a = 2a_0$, where a_0 is the separation between neighboring A and B sites.

(b) From the Hamiltonian above, we read off the hopping matrix

$$H_{aa'}(n-n') = \begin{pmatrix} -\varepsilon_{\mathsf{A}} \, \delta_{n-n',0} & t \, (\delta_{n-n',0} + \delta_{n-n',1}) \\ t \, (\delta_{n-n',0} + \delta_{n-n',-1}) & -\varepsilon_{\mathsf{B}} \, \delta_{n-n',0} \end{pmatrix}$$

Thus,

$$\hat{H}_{aa'}(k) = \sum_j t_{aa'}(j) \, e^{-ikja} = \begin{pmatrix} \varepsilon_{\mathsf{A}} & -t \, (1 + e^{-ika}) \\ -t \, (1 + e^{ika}) & \varepsilon_{\mathsf{B}} \end{pmatrix}$$

The energy eigenvalues are then

$$E_\pm(k) = \tfrac{1}{2}(\varepsilon_{\mathsf{A}} + \varepsilon_{\mathsf{B}}) \pm \sqrt{\tfrac{1}{4}(\varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}})^2 + 4t^2 \cos^2(\tfrac{1}{2}ka)} \quad ,$$

where we've used $|1 + e^{-ika}|^2 = 2 + 2\cos(ka) = 4\cos^2(\frac{1}{2}ka)$.

(c) See the plots in Fig. 1.

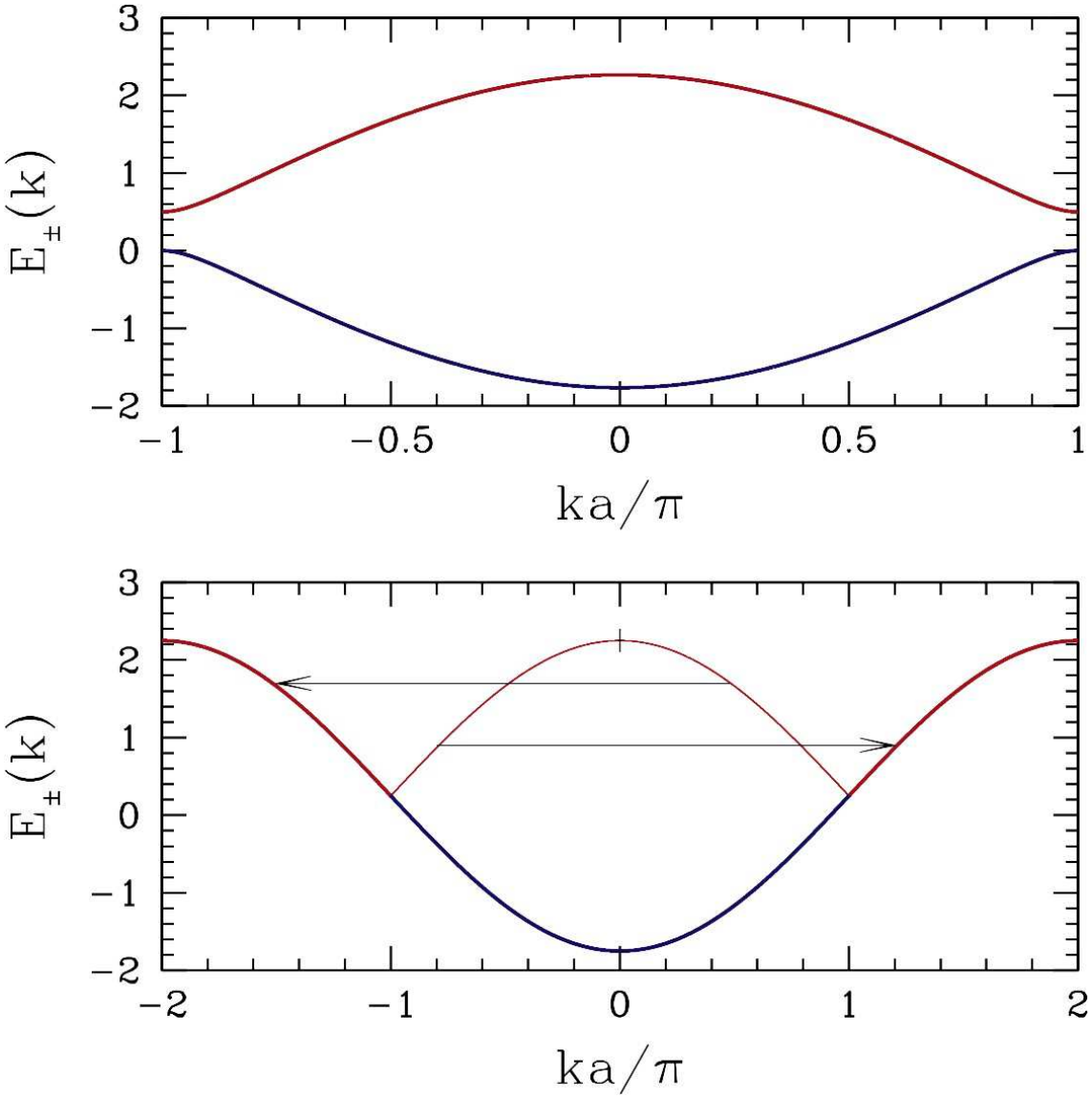

Figure 1: Energy bands $E_\pm(k)$ for problem 1. Top: $\varepsilon_\mathsf{A} = 0.5$, $\varepsilon_\mathsf{B} = 0.0$, $t = 1.0$. Bottom: $\varepsilon_\mathsf{A} = \varepsilon_\mathsf{B} = 0.5$, $t = 1$. The extended zone plot of the dispersion is shown for the latter case, in which the one-dimensional dispersion $E(k) = \varepsilon_0 - 2t\cos(ka')$ is recovered, with $a' = \frac{1}{2}a$ and $k \in \left[-\frac{\pi}{a'}, \frac{\pi}{a'}\right]$.

(d) Let $\varepsilon_\mathsf{A} = \varepsilon_\mathsf{B} = \varepsilon_0$. Then $E_\pm(k) = \varepsilon_0 \pm 2t\cos\left(\frac{1}{2}ka\right)$. If we translate the section of the + band on the interval $k \in \left[-\frac{\pi}{a}, 0\right]$ by $\frac{2\pi}{a}$, and the section on the interval $k \in \left[0, \frac{\pi}{a}\right]$ by $-\frac{2\pi}{a}$, we obtain the dispersion $E(k) = \varepsilon_0 - 2t\cos(ka')$ on the interval $k \in \left[-\frac{\pi}{a'}, \frac{\pi}{a'}\right]$, with $a' = \frac{1}{2}a$.

[**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 high symmetry points Γ, K, and M.

(c) Find an expression for the band gap Δ. Is the gap direct or indirect?

Solution :

(a) The Hamiltonian matrix is

$$\hat{H}(\boldsymbol{k}) = \begin{pmatrix} \varepsilon_{\mathsf{A}} & -t\,\gamma(\boldsymbol{k}) \\ -t\,\gamma^*(\boldsymbol{k}) & \varepsilon_{\mathsf{B}} \end{pmatrix} \quad ,$$

where

$$\gamma(\boldsymbol{k}) = 1 + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2} = 1 + e^{i\theta_1} + e^{-i\theta_2} \quad .$$

There are two bands:

$$E_\pm(\boldsymbol{k}) = \tfrac{1}{2}\big(\varepsilon_{\mathsf{A}} + \varepsilon_{\mathsf{B}}\big) \pm \sqrt{\tfrac{1}{4}\big(\varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}}\big)^2 + t^2 \big|\gamma(\boldsymbol{k})\big|^2} \quad .$$

(b) Recall $\boldsymbol{k}_\Gamma = 0$, $\boldsymbol{k}_{\mathrm{K}} = \frac{1}{3}\boldsymbol{B}_1 + \frac{1}{3}\boldsymbol{B}_2$, and $\boldsymbol{k}_{\mathrm{M}} = \frac{1}{2}\boldsymbol{b}_1$. Thus,

$$\gamma(\Gamma) = 3 \qquad , \qquad \gamma(\mathrm{K}) = 0 \qquad , \qquad \gamma(\mathrm{M}) = 1$$

and

$$E_\pm(\Gamma) = \tfrac{1}{2}\big(\varepsilon_{\mathsf{A}} + \varepsilon_{\mathsf{B}}\big) \pm \sqrt{\tfrac{1}{4}\big(\varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}}\big)^2 + 9t^2}$$
$$E_\pm(\mathrm{K}) = \varepsilon_{\mathsf{A}} \ , \ \varepsilon_{\mathsf{B}}$$
$$E_\pm(\mathrm{M}) = \tfrac{1}{2}\big(\varepsilon_{\mathsf{A}} + \varepsilon_{\mathsf{B}}\big) \pm \sqrt{\tfrac{1}{4}\big(\varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}}\big)^2 + t^2} \quad .$$

(c) Since nitrogen has a greater nuclear charge, we expect $\varepsilon_{\mathsf{B}} < \varepsilon_{\mathsf{A}}$. The maximum valence ($-$) band energy is then ε_{B}, at K. The minimum conduction band energy is ε_{A}, also at K. Thus, the gap is direct and equal to $\Delta = \varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}}$. The direct gap at wavevector $\boldsymbol{k}$ is

$$\Delta(\boldsymbol{k}) \equiv E_+(\boldsymbol{k}) - E_-(\boldsymbol{k}) = \sqrt{\big(\varepsilon_{\mathsf{A}} - \varepsilon_{\mathsf{B}}\big)^2 + 4t^2\big|\gamma(\boldsymbol{k})\big|^2} \quad .$$

[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

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

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

Solution :

$\hat{\boldsymbol{\eta}}$	$\hat{\eta}_j^x\hat{\eta}_j^x$	$\hat{\eta}_j^x\hat{\eta}_j^y$	$\hat{\eta}_j^y\hat{\eta}_j^y$
$\pm\hat{\boldsymbol{a}}_1$	$\frac{1}{4}$	$-\frac{\sqrt{3}}{4}$	$\frac{3}{4}$
$\pm\hat{\boldsymbol{a}}_2$	$\frac{1}{4}$	$\frac{\sqrt{3}}{4}$	$\frac{3}{4}$
$\pm\hat{\boldsymbol{a}}_3$	1	0	0

Table 1: Values of $\eta_j^\mu\eta_j^\nu$ for the six nearest neighbor vectors.

(a) On the triangular lattice, there are six nearest neighbors. Defining the primitive direct lattice vectors $\boldsymbol{a}_1 = a\,(\frac{1}{2}\hat{\boldsymbol{x}} - \frac{\sqrt{3}}{2}\hat{\boldsymbol{y}})$ and $\boldsymbol{a}_2 = a\,(\frac{1}{2}\hat{\boldsymbol{x}} + \frac{\sqrt{3}}{2}\hat{\boldsymbol{y}})$, the six nearest neighbor vectors are $\pm\boldsymbol{a}_1$, $\pm\boldsymbol{a}_2$, and $\pm\boldsymbol{a}_3$, where $\boldsymbol{a}_3 \equiv -\boldsymbol{a}_1 - \boldsymbol{a}_2 = -a\,\hat{\boldsymbol{x}}$. From the entries in Tab. 1, we have

$$\begin{aligned}
\hat{t}_{xx}(\boldsymbol{k}) &= 2t_{\rm w}(c_1 + c_2 + c_3) - (t_{\rm s} + t_{\rm w})(\tfrac{1}{2}c_1 + \tfrac{1}{2}c_2 + 2c_3) \\
\hat{t}_{yy}(\boldsymbol{k}) &= 2t_{\rm w}(c_1 + c_2 + c_3) - (t_{\rm s} + t_{\rm w})(\tfrac{3}{2}c_1 + \tfrac{3}{2}c_2) \\
\hat{t}_{xy}(\boldsymbol{k}) = \hat{t}_{yx}(\boldsymbol{k}) &= \tfrac{\sqrt{3}}{2}\,(t_{\rm s} + t_{\rm w})(c_1 - c_2) \quad ,
\end{aligned}$$

$\boldsymbol{k}$	θ_1	θ_2	θ_3	c_1	c_2	c_3	$E_+(\boldsymbol{k})$	$E_-(\boldsymbol{k})$
Γ	0	0	0	1	1	1	$3(t_\mathrm{s}-t_\mathrm{w})$	$3(t_\mathrm{s}-t_\mathrm{w})$
K	$\frac{2\pi}{3}$	$\frac{2\pi}{3}$	$-\frac{4\pi}{3}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}(t_\mathrm{s}-t_\mathrm{w})$	$-\frac{3}{2}(t_\mathrm{s}-t_\mathrm{w})$
M	π	0	$-\pi$	-1	1	-1	$3t_\mathrm{s}+t_\mathrm{w}$	$-t_\mathrm{w}-3t_\mathrm{s}$

Table 2: Dispersion at high symmetry points.

where $\theta_3 \equiv -(\theta_1+\theta_2)$ and where $c_j = \cos\theta_j$. Thus,

$$\hat{t}_{\nu\nu}(\boldsymbol{k}) = \begin{pmatrix} \frac{1}{2}(3t_\mathrm{w}-t_\mathrm{s})(c_1+c_2)-2t_\mathrm{s}c_3 & \frac{\sqrt{3}}{2}(t_\mathrm{s}+t_\mathrm{w})(c_1-c_2) \\ \frac{\sqrt{3}}{2}(t_\mathrm{s}+t_\mathrm{w})(c_1-c_2) & \frac{1}{2}(t_\mathrm{w}-3t_\mathrm{s})(c_1+c_2)+2t_\mathrm{w}c_3 \end{pmatrix}$$
$$= (t_\mathrm{w}-t_\mathrm{s})(c_1+c_2+c_3) + \tfrac{1}{2}(t_\mathrm{w}+t_\mathrm{s})(c_1+c_2-2c_3)\,\sigma^z + \tfrac{\sqrt{3}}{2}(t_\mathrm{s}+t_\mathrm{w})(c_1-c_2)\,\sigma^x$$

The eigenvalues of $\hat{H}_{\mu\nu}(\boldsymbol{k}) = -\hat{t}_{\mu\nu}(\boldsymbol{k})$ are then

$$E_\pm(\boldsymbol{k}) = (t_\mathrm{s}-t_\mathrm{w})(c_1+c_2+c_3) \pm (t_\mathrm{s}+t_\mathrm{w})\sqrt{c_1^2+c_2^2+c_3^2-c_1c_2-c_2c_3-c_1c_3} \quad .$$

Note that under a 60° rotation, $\boldsymbol{a}_1 \to -\boldsymbol{a}_3$, $\boldsymbol{a}_2 \to -\boldsymbol{a}_1$, and $\boldsymbol{a}_3 \to -\boldsymbol{a}_2$, so $(\theta_1,\theta_2,\theta_3) \to (-\theta_3,-\theta_1,-\theta_2)$. This symmetry is manifestly preserved by the above dispersions.

(b) See the results in Tab. 2. Note that the bands are degenerate at both Γ and K.

(c) See the plot in Fig. 2.

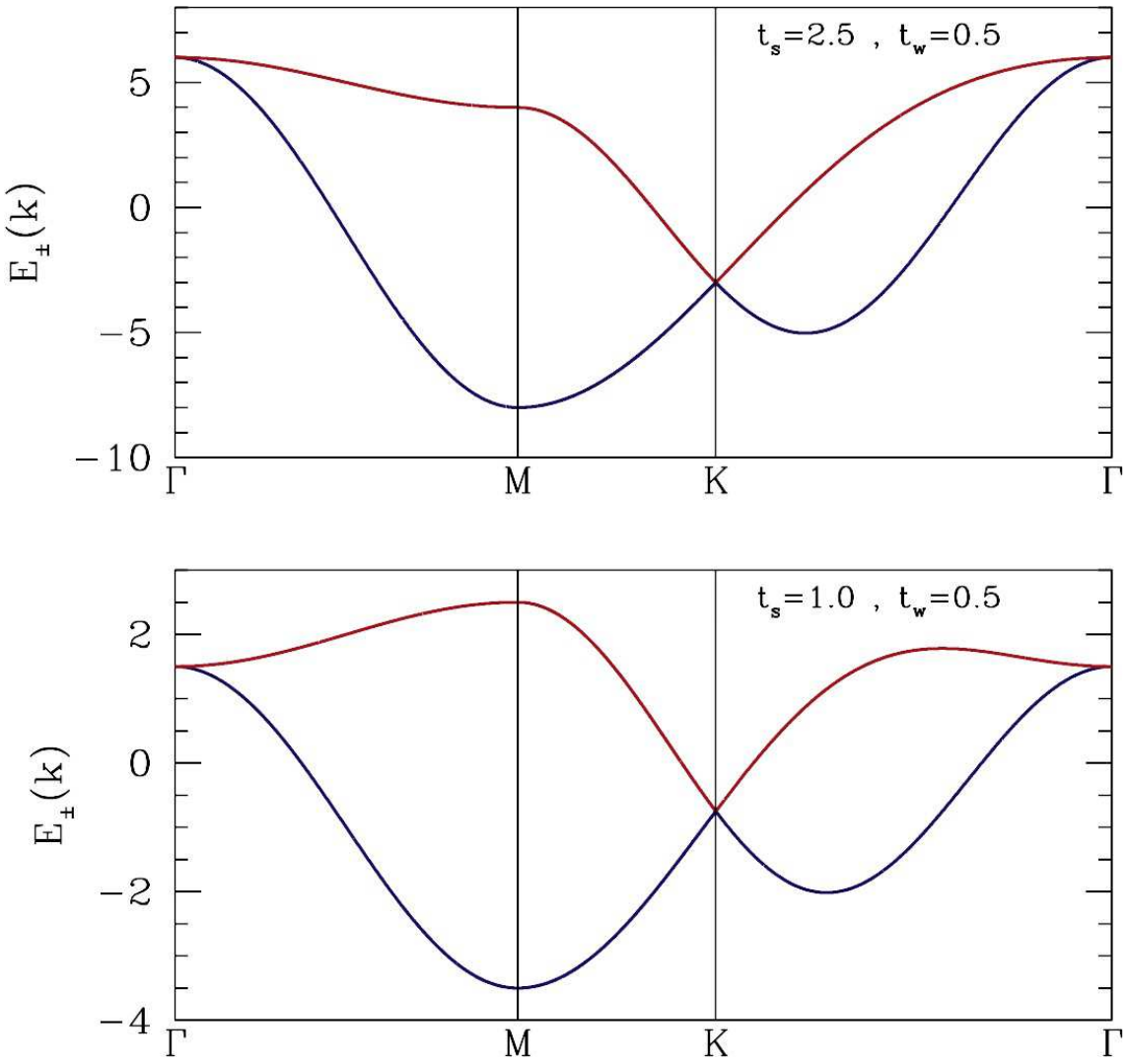

Figure 2: Energy bands $E_{\pm}(\boldsymbol{k})$ along high symmetry directions for problem 3. Top: $t_{\rm s} = 2.5$ and $t_{\rm w} = 0.5$. Bottom: $t_{\rm s} = 1.0$ and $t_{\rm w} = 0.5$.