PHY 555: Solid-state Physics I

Homework #5

Due: 10/31/2022

Homework is due by the end of the due date specified above. ***Late homework will be subject to 3 points off per day past the deadline, please contact me if you anticipate an issue making the deadline.*** *It should be turned in via blackboard. For the conceptual and analytical parts, turn in a scan or picture of your answers (please ensure that they are legible) or an electronic copy if done with, e.g., LaTeX. For the computational part, turn in your source code and a short description of your results (including plots). The description can be separate (e.g., in LaTeX or word), or combined (e.g., in a jupyter notebook). Let me know if you are not sure about the format.*

Conceptual

1. ***5 points*** What are the approximations made to go from the expression for the fully general tight-binding matrix elements and secular equation:

$$\begin{aligned} M_{ij\mathbf{k}} &= \langle \Phi_{i\mathbf{k}} | H | \Phi_{j\mathbf{k}} \rangle \\ S_{ij\mathbf{k}} &= \langle \Phi_{i\mathbf{k}} | \Phi_{j\mathbf{k}} \rangle \\ \det|M_{ij\mathbf{k}} &- E S_{ij\mathbf{k}}| = 0 \end{aligned}$$

to the semi-empirical expressions:

$$\begin{aligned} M_{ij\mathbf{k}} &= E_i \delta_{ij} + \sum_{\mathbf{t}_I} e^{i\mathbf{k}\cdot\mathbf{t}_I} \int \phi_i^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_j(\mathbf{r}-\mathbf{t}_I) d^3r \\ S_{ij\mathbf{k}} &= \delta_{ij} \\ \det|M_{ij\mathbf{k}} &- E\delta_{ij}| = 0 \end{aligned}$$

where $\Phi_{i\mathbf{k}}$'s are the Bloch sums, ϕ_i's are the atomic-like orbitals, $\mathbf{t}_I$ runs over nearest neighbor lattice sites, and $V_a(\mathbf{r}-\mathbf{t}_I)$ is the atomic-like potential centered on site $\mathbf{t}_I$.

Analytical

2. ***20 points*** Consider the empirical tight-binding treatment of s and p electrons on an FCC lattice. In this case, each lattice site has twelve nearest neighbors $\mathbf{t}_I$: $(a/2)(0, \pm1, \pm1)$, $(a/2)(\pm1, 0, \pm1)$, $(a/2)(0, \pm1, \pm1)$. The relevant interaction integrals are:

$$\int \phi_s^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_s(\mathbf{r}-\mathbf{t}_I) d\mathbf{r} = V_{ss\sigma}$$

$$\int \phi_s^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_{p_x}(\mathbf{r}-\mathbf{t}_I) d\mathbf{r} = l_x V_{sp\sigma}$$

$$\int \phi_{p_x}^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_{p_x}(\mathbf{r}-\mathbf{t}_I) d\mathbf{r} = l_x^2 V_{pp\sigma} + (1-l_x^2) V_{pp\pi}$$

$$\int \phi_{p_x}^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_{p_y}(\mathbf{r}-\mathbf{t}_I) d\mathbf{r} = l_x l_y (V_{pp\sigma} - V_{pp\pi})$$

$$\int \phi_{p_x}^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t}_I) \phi_{p_z}(\mathbf{r}-\mathbf{t}_I) d\mathbf{r} = l_x l_z (V_{pp\sigma} - V_{pp\pi})$$

where ϕ_i's are the atomic-like orbitals; $V_{ss\sigma}$, $V_{sp\sigma}$, $V_{pp\sigma}$, and $V_{pp\pi}$ are the adjustable parameters; and $\mathbf{l}$=(l_x,l_y,l_z) is the unit vector in the direction of $\mathbf{t}_I$.

(**a**) Assume that the s orbitals do not interact with the p orbitals. Show that the dispersion of the s-orbital derived band is given by

$$E(\mathbf{k}) = E_s + 4V_{ss\sigma}\left[\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_z a}{2}\right)\cos\left(\frac{k_x a}{2}\right)\right]$$

where E_s are the onsite energies.

(**b**) For the p orbital manifold, show that the matrix elements are given by:

$$\begin{aligned} M_{p_x p_x \mathbf{k}} &= E_p + 2\cos\left(\frac{k_x a}{2}\right)\left[\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_z a}{2}\right)\right](V_{pp\sigma} + V_{pp\pi}) \\ &\quad + 4\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)V_{pp\pi} \\ M_{p_x p_y \mathbf{k}} &= -2\sin\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y a}{2}\right)(V_{pp\sigma} - V_{pp\pi}) \end{aligned}$$

Computational

3. ***25 points*** Use the results of problem **2** to calculate the dispersion of the s and p bands in an FCC crystal along the path L $\to$ Γ $\to$ X $\to$ K $\to$ Γ (see Fig. 1 and Table 1 for high-symmetry $\mathbf{k}$ points/paths). Use the following parameters (all in Ha): $V_{ss\sigma} = -0.5$, $V_{pp\sigma} = 0.5$, $V_{pp\pi} = -0.05$, $E_s = 9$, $E_p = 0$. Use $a = 10.67$ Bohr for the lattice constant.

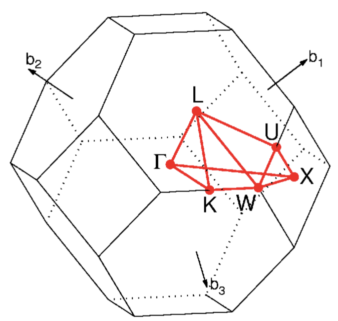

Figure 1: Brillouin zone and high-symmetry points/lines for the face-centered cubic Bravais lattice. (b_1, b_2, and b_3 correspond to the reciprocal lattice vectors of FCC, written below as $\mathbf{g}_1$, $\mathbf{g}_2$, and $\mathbf{g}_3$.)

Table 1: High-symmetry $\mathbf{k}$ points of the face-centered cubic lattice.

	$\times\mathbf{g}_1$	$\times\mathbf{g}_2$	$\times\mathbf{g}_3$
Γ	0	0	0
K	3/8	3/8	3/4
L	1/2	1/2	1/2
U	5/8	1/4	5/8
W	1/2	1/4	3/4
X	1/2	0	1/2