PHY 555: Solid-State Physics I
Homework #2
Due: 09/20/2024

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** Explain why crystal momentum $\hbar k$ does not correspond to the true momentum of electrons in a periodic potential, but is still a useful quantity.

2. **5 points** Argue that the "overlapping band" situation shown in Fig. 1 is not possible for an electron in a one-dimensional periodic potential. (**Hint**: What type of differential equation is the Schrödinger equation in 1D? How many solutions does it have for a given energy? What do the band dispersions we have analyzed look like with respect to $\pm k$?) What does this imply about the locations of band extremea for 1D potentials?
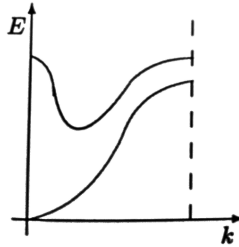

Figure 1: Impossible bands in 1D periodic potential.

3. **5 points** Why do all simple Bravais lattices (i.e., those *without* a basis) have to contain just one type of element? Why can we have a composite lattice (i.e., *with* a basis) that also only contains one type of element?

4. **5 points** Consider the 2D CuO_2 lattice depicted in Fig. 2(a) (filled circles are Cu and empty circles are O) which is a common building block for high temperature superconductors.

   (a) Draw a possible primitive unit cell, as well as the basis vectors. What is the Bravais lattice?

   (b) In some cases, the O atoms may be distorted in and out of plane, as indicated by the "$+$" and "$-$" in Fig. 2(b). Draw the in-plane primitive unit cell for this case.

Analytical

5. **15 points** Show that for wavefunctions in Bloch form, i.e., $\psi_k(x) = u_k(x)e^{ikx}$, the expectation value of the kinetic energy operator can be written as

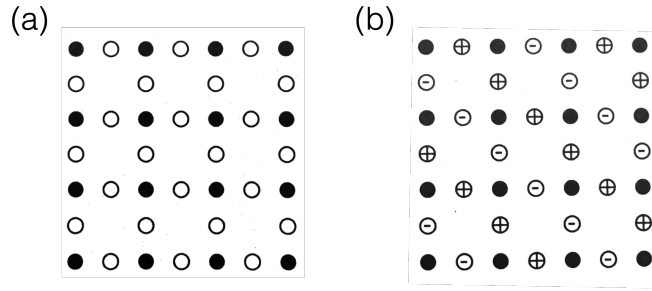$$\langle \psi_k | \frac{p^2}{2m} | \psi_k \rangle = \langle u_k | \frac{(p + \hbar k)^2}{2m} | u_k \rangle \tag{1}$$

over...

Figure 2: Schematic of 2D CuO_2 planes. (a) All atoms in plane, filled circles are Cu, empty are O. (b) Displaced O atoms, "+" and "−."

6. **30 points** We discussed in class that the electronic structure is given by the Bloch wavefunctions evaluated at k's in the first Brillouin zone. At a given k, say k_0, there are an infinite number of solutions to the Schrödinger equation, labeled by n, at increasing energies E_{nk_0}. Because the eigenfunction ψ_{nk_0} form a complete set we can actually use them to represent the wavefunction and energies *at any other k*.

   (**a**) Consider the expansion the crystal wavefunction in terms of Bloch functions of the form:

$$\psi_k(x) = \sum_n c_{nk} \left[e^{i(k-k_0)x} \psi_{nk_0}(x) \right]. \qquad (2)$$

   Show that if we know the wavefunctions (ψ_{nk_0}) and energies (E_{nk_0}) at k_0, we can determine the wavefunction and energies at any other k. **Hint:** It is sufficient to show that the matrix elements of the Hamiltonian with respect to the basis functions in the square brackets in Eq. (2) can be determined if ψ_{nk_0} and E_{nk_0} are known.

   (**b**) Consider a given energy state n and k-point k. Assume that this state is nondegenerate. Treat $\hbar(k - k_0)p/m$ as a perturbing potential and write the energy E_{nk} up to second order in $k - k_0$ using nondegenerate perturbation theory.

   (**c**) Consider the case where k_0 is a band extremum. Show that the energy versus k can be written as a quadratic dispersion around k_0, with an "effective mass" different from the free-electron mass.
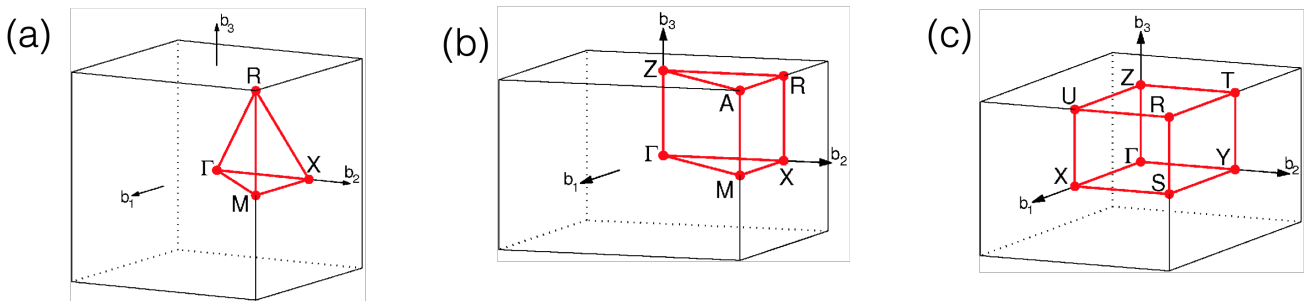
Computational

Figure 3: Brillouin zones and high-symmetry **k** points/paths for (a) simple (i.e., primitive) cubic, (b) simple tetragonal, and (c) simple orthorhombic.

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7. **40 points** . In this problem, we will explore the "band structure" of the 3D (simple) cubic tight-binding model, which has a dispersion given by $E_{\text{cubic}}(\mathbf{k}) = E_0 + 2\gamma[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$. We will also look at it's generalization to tetragonal and orthorhombic. (Below, tables of high-symmetry $\mathbf{k}$-points and Brillouin zones are adapted from https://arxiv.org/pdf/1004.2974.pdf.)

(a) Consider the simple cubic Brillouin Zone depicted in Fig. 3(a). Plot the bandstructure, i.e., the band dispersion $E_{\text{cubic}}(\mathbf{k})$ along the high-symmetry paths through the Brillouin Zone. Use $E_0 = 0$, $\gamma = -0.5$ Ha and $a = 1$ Bohr. See Table 1 for the high-symmetry $\mathbf{k}$ points in terms of the reciprocal lattice vectors. Use the path: $\Gamma \to X \to M \to \Gamma \to R \to X$. Note that, as you can see from Fig. 3(a), the different segments of the path may be different lengths. To plot the band structure correctly this should be taken into account, i.e., the range of the x axis between high-symmetry points should be proportional to the distance between them in reciprocal space.

Hint: For some inspiration of how the bandstructure should be plotted, see e.g., Fig. 7 in the Sec. V.4 of the textbook or Appendix B of https://arxiv.org/pdf/1004.2974.pdf. Of course in those cases they have multiple bands where you will have only one (since you have one orbital per site).

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

	$\times \mathbf{g}_1$	$\times \mathbf{g}_2$	$\times \mathbf{g}_3$
Γ	0	0	0
M	1/2	1/2	0
R	1/2	1/2	1/2
X	0	1/2	0

(b) We can generalize the tight-binding model to treat a tetragonal crystal ($a = b \neq c$, $\alpha = \beta = \gamma = 90°$): $E_{\text{tet}}(\mathbf{k}) = E_0 + 2\gamma[\cos(k_x a) + \cos(k_y a)] + 2\gamma_z \cos(k_z c)$. Plot the dispersion along the path: $\Gamma \to X \to M \to \Gamma \to Z \to R \to A \to Z$. The high-symmetry $\mathbf{k}$ points in terms of the reciprocal lattice vectors are given in Table 2 and Fig. 3(b). Note that the same label may correspond to a different point in the cubic and tetragonal cases (by convention). For the parameters, use $E_0 = 0$, $\gamma = -0.5$ Ha, $\gamma_z = -0.2$ Ha, $a = 1$ Bohr, and $c = 1.5$ Bohr.

Table 2: High-symmetry $\mathbf{k}$ points of the simple tetragonal lattice

	$\times \mathbf{g}_1$	$\times \mathbf{g}_2$	$\times \mathbf{g}_3$
Γ	0	0	0
M	1/2	1/2	0
A	1/2	1/2	1/2
R	0	1/2	1/2
X	0	1/2	0
Z	0	0	1/2

(c) We can further generalize to the case of an orthorhombic crystal ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$): $E_{\text{orth}}(\mathbf{k}) = E_0 + 2\gamma_x \cos(k_x a) + 2\gamma_y \cos(k_y b) + 2\gamma_z \cos(k_z c)$. Plot the dispersion along the path $\Gamma \to X \to S \to Y \to \Gamma \to Z \to U \to R \to T \to Z$ (see Table 3 and and Fig. 3(c)). For the parameters, use $E_0 = 0$, $\gamma_x = -0.5$ Ha, $\gamma_y = -0.2$ Ha, $\gamma_z = -0.1$ Ha, $a = 1$ Bohr, $b = 1.5$ Bohr, and $c = 2.0$ Bohr.

(d) For the cubic, tetragonal, and orthorhombic cases (parts **(a)**, **(b)**, **(c)**), plot the effective mass in the three Cartesian directions, given by

$$m_x^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_x^2}\right)^{-1}, \quad m_y^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_y^2}\right)^{-1}, \quad m_z^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_y^2}\right)^{-1}. \tag{3}$$

over...

Table 3: High-symmetry **k** points of the simple orthorhombic lattice

	$\times \mathbf{g}_1$	$\times \mathbf{g}_2$	$\times \mathbf{g}_3$
Γ	0	0	0
R	1/2	1/2	1/2
S	1/2	1/2	0
T	0	1/2	1/2
U	1/2	0	1/2
X	1/2	0	0
Y	0	1/2	0
Z	0	0	1/2

along the same paths through the BZ as in parts **(a)**, **(b)**, **(c)**. Analytic expressions for the effective mass can be obtained from the expressions for $E(\mathbf{k})$ given above. Note that the effective mass will diverge at some **k** points, so you should zoom in around m^* to observe the effective mass around the band extrema. When does m^* diverge? What happens to the effective masses at the extrema when the symmetry is lowered from cubic to tetragonal to orthorhombic?