PHY 555: Solid-state Physics I

Homework #4

Due: 10/17/2022

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*** We showed in class that the heat capacity (i.e., the change in internal energy of the system with change in temperature) and equivalently the entropy of the free electron gas in 3D depended on the density of states at the Fermi level. But there may be many more electrons in the system far below the Fermi level. What is the physical reason that only electrons around the Fermi energy contribute to the heat capacity/entropy?
2. ***10 points*** When we discussed Bravais lattices, we said that there is no base-centered tetragonal, though there is a base-centered orthorhombic. Demonstrate pictorially why this is the case. Also demonstrate pictorially why there is no face-centered tetragonal Bravais lattice.
3. ***5 points*** Consider the centered rectangle Bravais lattice in 2D. Draw the Wigner-Seitz cell.
4. ***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?
5. ***5 points*** Consider the 2D CuO_2 lattice depicted in Fig. 1(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. 1(b). Draw the in-plane primitive unit cell for this case.

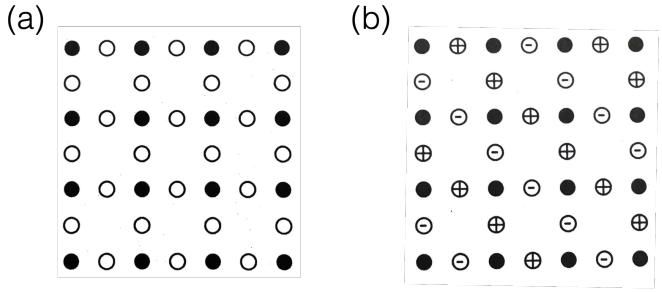

Figure 1: Schematic of 2D CuO_2 planes. (a) All atoms in plane, filled circles are Cu, empty are O. (b) Displaced O atoms, "+" and "−."

Analytical

6. ***30 points*** Suppose we have a function that depends on $\mathbf{k}$ and is periodic in the reciprocal lattice so we can write the discrete Fourier transform

$$F(\mathbf{k}) = F_0 + \sum_{\mathbf{t}_n \neq 0} F_n e^{i\mathbf{k}\cdot\mathbf{t}_n}, \tag{1}$$

where $\mathbf{t}_n$ is a real-space translation vector, F_n are the Fourier coefficients, and we have separated out the $n = 0$ coefficient, which corresponds to the average value of F($\mathbf{k}$).

(**a**) Show that summing Eq. (1) over allowed $\mathbf{k}$ points in the first Brillouin Zone (BZ) gives the average of F($\mathbf{k}$) to be

$$F_0 = \frac{1}{N}\sum_{\mathbf{k}}^{\mathrm{BZ}} F(\mathbf{k}), \tag{2}$$

where N is the total number of $\mathbf{k}$ in the first BZ.

(**b**) Equation (2) is usually very inconvenient to compute exactly, since the number of allowed $\mathbf{k}$ points in the first BZ is very large for a macroscopic crystal. If we want to approximate the sum in Eq. (2) by summing over a smaller subset of $\mathbf{k}$ points, which ones should we choose? To answer this question, we separate the sum over real-space lattice vectors $\mathbf{t}_n$ into "shells" with equal distance to the origin, denoted by (I), (II), (III), etc.:

$$F(\mathbf{k}) = F_0 + \sum_{\mathbf{t}_n^{(I)}} F_n^{(I)} e^{i\mathbf{k}\cdot\mathbf{t}_n^{(I)}} + \sum_{\mathbf{t}_n^{(II)}} F_n^{(II)} e^{i\mathbf{k}\cdot\mathbf{t}_n^{(II)}} + \sum_{\mathbf{t}_n^{(III)}} F_n^{(III)} e^{i\mathbf{k}\cdot\mathbf{t}_n^{(III)}} + \ldots \tag{3}$$

In the spirit of the tight-binding models we have discussed, we assume that F_n decays with shell, i.e., $|F_n^{(I)}| \gg |F_n^{(II)}| \gg |F_n^{(III)}|$. Therefore, for an accurate approximation of the average, we should sum $F(\mathbf{k})$ over $\mathbf{k}$ points such that the sums corresponding to the first few shells vanish.

Consider The case of a cubic lattice. Then the first shell (I) is $\mathbf{t}^{(I)} = (\pm a, 0, 0)$, $(0, \pm a, 0)$, and $(0, 0, \pm a)$. Show that we can make the (I) term in Eq. (3) vanish by summing over *just two* (specifically chosen) $\mathbf{k}$ points.

(**c**) The second shell (II) in the cubic case is: $\mathbf{t}^{(II)} = (\pm a, \pm a, 0)$, $(0, \pm a, \pm a)$, and $(\pm a, 0, \pm a)$. Show that we can make the (I) and (II) terms vanish with the choice of a small number of $\mathbf{k}$ points.

Computational

7. ***40 points*** In the last homework you plotted the density of states for the 3D (simple) cubic tight-binding model, which had a dispersion given by $E_{\mathrm{cubic}}(\mathbf{k}) = E_0 + 2\gamma[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$. In this problem, we will explore the "band structure" of that model, as well as 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. 2(a). Plot the bandstructure, i.e., the band dispersion $E_{\mathrm{cubic}}(\mathbf{k})$ 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: $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma \to \mathrm{R} \to \mathrm{X}$. Note that, as you can see from Fig. 2(a), the different segments of the path may be different lengths. To plot the

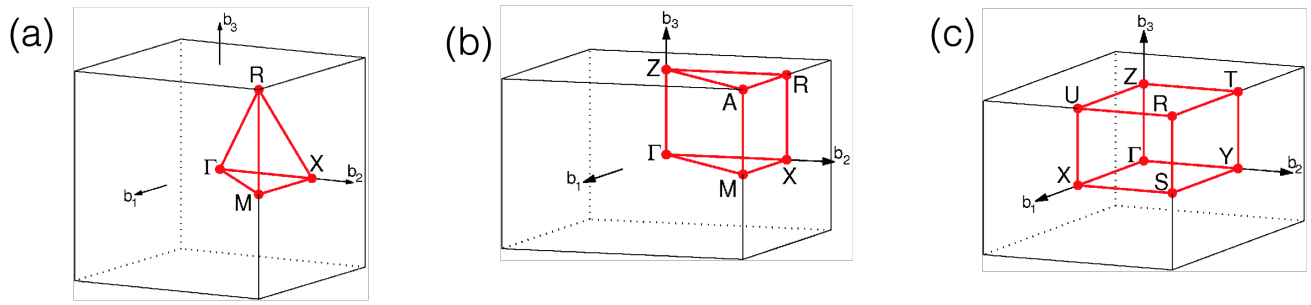

Figure 2: Brillouin zones and high-symmetry **k** points/paths for (a) simple (i.e., primitive) cubic, (b) simple tetragonal, and (c) simple orthorhombic.

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 **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: $\Gamma \to \text{X} \to \text{M} \to \Gamma \to \text{Z} \to \text{R} \to \text{A} \to \text{Z}$. The high-symmetry **k** points in terms of the reciprocal lattice vectors are given in Table 2 and Fig. 2(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 **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 $\Gamma \to \text{X} \to \text{S} \to \text{Y} \to \Gamma \to \text{Z} \to \text{U} \to \text{R} \to \text{T} \to \text{Z}$ (see Table 3 and and Fig. 2(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

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

the three Cartesian directions, given by

$$m_x^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_x^2}\right)^{-1}, \quad m_y^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_y^2}\right)^{-1}, \quad m_z^* = \left(\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_y^2}\right)^{-1}. \tag{4}$$

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?