PHYS*4150: Midterm Exam

Date: Monday March 4, 2019 7-9pm

This exam consists of four problems. Please answer all of them. If any of your answers are marked on this page, please hand it in along with your answer booklet at the end of the exam.

Problem 1 (20 pts): Multiple choice and short answer

Please answer all questions in this section. Provide 1 or 2 sentences (at most) to explain your answer. Points are evenly distributed.

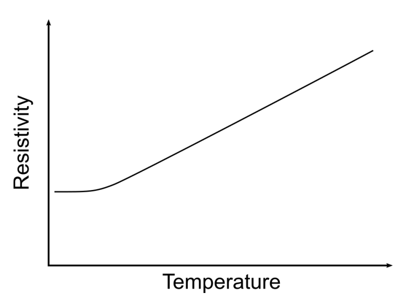
1. The typical density of conduction electrons in a metal is approximately:

   a) $10^{-18}\,\mathrm{m}^{-3}$ *b*) $10^{-8}\,\mathrm{m}^{-3}$ *c*) $10^{8}\,\mathrm{m}^{-3}$ *d*) $10^{18}\,\mathrm{m}^{-3}$ *e*) $10^{28}\,\mathrm{m}^{-3}$

2. In the context of the free electron model, which of the following ***most accurately*** describes the Fermi energy (ε_F) and chemical potential (μ)?

	ε_F	μ
a)	Energy of the highest occupied electron state at $T = 0$	Energy required to add an electron to the system
b)	Energy of the highest occupied electron state	Energy required to add an electron to the system in the ground state
c)	Energy required to add an electron to the system in the ground state	Energy of the highest occupied electron state at $T = 0$
d)	Energy required to add an electron to the system	Energy of the highest occupied electron state

3. For the graph of resistivity vs. temperature shown below for a typical metal, which region would the Drude model most accurately describe?



4. Under what condition does a metal become transparent to electromagnetic radiation?

5. State the main difference between the Drude and Sommerfeld models of metals.

6. In the free electron model, would you expect a metal with a relatively large Fermi energy (ε_F) to be harder or softer than a metal with a relatively small Fermi energy.

7. List the three cubic Bravais lattices in order of ***decreasing*** primitive unit cell volume. Assume all have a cubic cell side length of a.

8. State the mathematical relationship between the real and reciprocal lattice.

9. Assuming a simple cubic lattice, rank the following Miller planes by the density of atoms in the plane: (111), (121), (100), (411).

10. Which one of the following statements regarding x-ray diffraction is false?

    a) the relative intensity of diffracted peaks depends on the composition of the lattice

    b) x-rays predominantly scatter off of electronic planes

    c) the diffraction pattern is a direct measurement of the real-space lattice

    d) higher energy incident x-rays result in a larger Ewald sphere and more visible diffracted peaks

Problem 2 (20 pts): 1D free electron gas

The Schrödinger equation for a 1-dimensional free electron gas is written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x) = \varepsilon\Psi(x), \tag{1}$$

with general solutions of the form

$$\Psi(x) = \sqrt{\frac{1}{L}}e^{\mathrm{i}\mathbf{k}\cdot x}, \tag{2}$$

where L is the length of the metal and $\mathbf{k} = k_x\hat{x}$.

a) Use periodic boundary conditions to show that solutions are quantized by the relation:

$$k_x = 2\pi\frac{n}{L}, \quad n = 0, \pm 1, \pm 2... \tag{3}$$

Sketch the 1-dimensional k-space and state the k-space volume per allowed value of $\mathbf{k}$.

b) Show that the electron density is equal to $n = 2k_F/\pi$, where k_F is the magnitude of the Fermi wavevector.

c) Show that the 1-D density of states, $D(\varepsilon)$, for this free electron gas is

$$D(\varepsilon) = \frac{\sqrt{2m}}{\pi\hbar}\frac{1}{\sqrt{\varepsilon}}. \tag{4}$$

Sketch $D(\varepsilon)$.

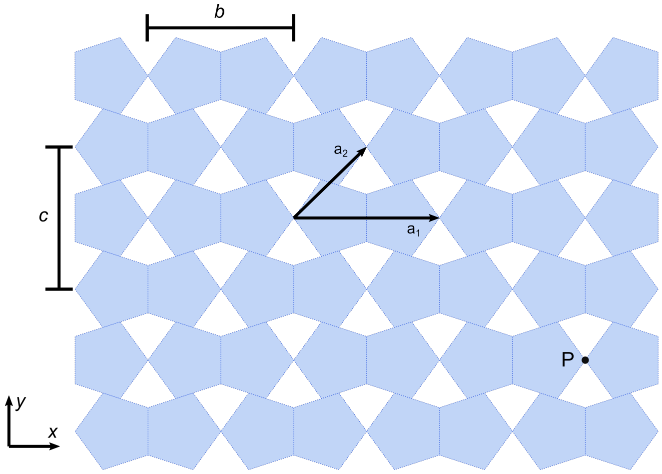
d) Show that the ground-state energy density ($u = U/L$ at $T = 0$) of the system is equal to

$$u = \frac{1}{3}n\varepsilon_F. \tag{5}$$

e) The 1-D density of states is ***not*** finite at $\varepsilon = 0$. Give a simple explanation as to why the ground-state energy is finite, despite this fact.

Problem 3 (20 pts): Crystal lattices

Consider the pattern of pentagons below:



One set of primitive cell vectors are labelled $\mathbf{a_1}$ and $\mathbf{a_2}$. The constants b and c give the relative scales of the $x-$ and $y-$directions, respectively.

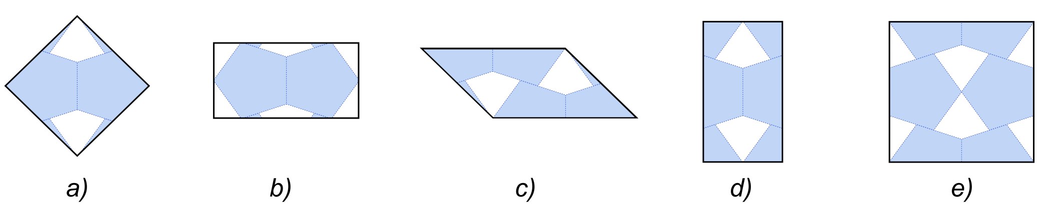
a) Write point P interms of the primitive vectors $\mathbf{a_1}$ and $\mathbf{a_2}$.

b) Write $\mathbf{a_1}$ and $\mathbf{a_2}$ in terms of the constants b and c and the unit vectors $\hat{x}$ and $\hat{y}$.

c) Express the volume of the unit cell in terms of b and c.

d) How many pentagons are in the primitive unit cell? Briefly justify your answer.

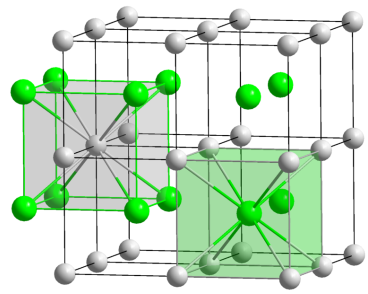
e) Which of the following are unit cells of the lattice? Briefly justify why or why not. For each unit cell state whether it is a primitive cell or not.



f) For ***one*** of the unit cells you identified above, sketch the corresponding Wigner-Seitz cell.

Problem 4 (20 pts): Diffraction and the reciprocal lattice

The crystal structure of cesium chloride (CsCl) is shown below. The larger, green spheres indicate cesium ions and the smaller, grey spheres indicate chloride ions.



CsCl is described by a simple cubic lattice with a 2-pt basis of Cs^+ at (0,0,0) and Cl^- at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The coordinates are written in terms of $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$ where $\mathbf{a_i}$ are the normal primitive cell vectors for a simple cubic cell of side length a.

a) What is the coordination number of the ions?

b) The cubic unit cell has a side length of 4.119 Å. What is the CsCl bond length?

c) Calculate the structure factor for CsCl:

$$S_{\mathbf{K}} = \sum_j f_j e^{\mathbf{i}\mathbf{K}\cdot\mathbf{d_j}} \tag{6}$$

where $\mathbf{d_j}$ are the basis points of the unit cell. Assume atomic form factors of f_{Cs^+}, f_{Cl^-} for the cesium and chloride ions. The reciprocal lattice vectors can be written as $\mathbf{K} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ where $\mathbf{b_i}$ are the primitive lattice vectors of the reciprocal lattice. Consider the cases of $h, k, l \rightarrow$ odd/even to show that the relative intensity of diffracted spots is:

$$|S_{\mathbf{K}}|^2 = \begin{cases} |f_{Cs^+} + f_{Cl^-}|^2, & h+k+l = \text{even} \\ |f_{Cs^+} - f_{Cl^-}|^2, & h+k+l = \text{odd} \end{cases} \tag{7}$$

d) Sketch the reciprocal lattice cubic unit cell. Clearly indicate the scattering intensity of the reciprocal lattice points.

e) What is the volume of the 1st Brillouin Zone?

f) Sketch separately the Miller planes of (110) and (111) in the cubic unit cell. Sketch the view of the lattice on these planes and clearly indicate the Cs^+ and Cl^- ions.