

Physics 406, Spring 2012

Midterm I

February 16, 2012

Name Solutions

The five problems are worth 20 points each.

Problem	Score
1	20
2	20
3	20
4	20
5	20
Total	100

1. Your experimental friends present you with a diffraction pattern resulting from a scattering experiment on a three-dimensional solid with one type of atom. This pattern includes (111) and (222) reflection lines. Unfortunately your friends have mixed up their samples since their measurements and cannot recall whether or not this pattern results from the fcc or the bcc sample. Can you help them?

Please note the following bases (of identical atoms) with respect to the cubic lattice axes:

$$\text{Bcc } (000) \left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right)$$

$$\text{Fcc } (000) \left(0 \frac{1}{2} \frac{1}{2}\right) \left(\frac{1}{2} 0 \frac{1}{2}\right) \left(\frac{1}{2} \frac{1}{2} 0\right)$$

Recall that

$$S_G(v_1, v_2, v_3) = \sum_j f_j e^{-2\pi i(v_1 x_j + v_2 y_j + v_3 z_j)}$$

where  $x_j, y_j, z_j$  are fractional atomic coordinates.

bcc:  $S_G = f(1 + e^{-i\pi(v_1 + v_2 + v_3)})$ , or  
 $\uparrow$  identical atoms

$$S_G = \begin{cases} 0 & \sum_i v_i \text{ odd} \\ 2f & \sum_i v_i \text{ even} \end{cases}$$

fcc:  $S_G = f(1 + e^{-i\pi(v_2 + v_3)} + e^{-i\pi(v_1 + v_3)} + e^{-i\pi(v_1 + v_2)})$ , or

$$S_G = \begin{cases} 4f & \text{all } v_i \text{'s odd or even} \\ 0 & \text{otherwise} \end{cases}$$

(111) and (222) lines are OK for fcc, but (111) is forbidden in the bcc lattice (1+1+1=3, odd). So the sample is fcc.

2. Please answer the following conceptual questions:

- a) Why is the energy of a neutron so much smaller than the energy of an electron in radiation beams used to probe crystal structure?

For free particles,

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}.$$

We need  $\lambda = \mathcal{O}(1 \text{ \AA})$  to probe X-tal structure. Since  $m_n \gg m_e$ ,

$E_n \ll E_e$  for the same wavelength.

$$E \sim \frac{1}{m}$$

- b) Aluminum is less dense than uranium. Assuming that these two metals have roughly the same stiffness, what can you say about the expected speeds of sound in these two metals? Please justify your answer.

$$v_s = \sqrt{\frac{Y}{\rho}}$$

Assuming  $Y_{Al} \approx Y_U$ ,

$$\frac{v_s^{Al}}{v_s^U} \approx \sqrt{\frac{\rho_U}{\rho_{Al}}} > 1, \text{ since } \rho_U > \rho_{Al}.$$

Thus the speed of sound is greater in Al.

c) What is the main difference between Einstein and Debye theories of specific heat?

Einstein's theory assumes that each atom oscillates independently w/ freq.  $\omega_E$ . However, neighboring atoms do affect one another, creating sound waves. Thus it is better to consider excitation of sound waves (or collective modes) rather than individual atoms. Debye's theory does just that, assuming that the dispersion relation is linear ( $\omega = v_s q$ ) and that excited waves propagate independently of each other.

3. Please consider a monolayer of Al that is a two-dimensional array of Al atoms in the fcc (100) surface. The cubic lattice constant is 4 Å.

a) Assume that the phonon dispersion in Al is well-described by the Debye approximation (i.e.  $\omega = ck$ ). What is the phonon density of states  $D(\omega)$  for this 2D solid?

$$\text{In 2D, } N(k) = \frac{\pi k^2}{\left(\frac{2\pi}{L}\right)^2}, \text{ where}$$

$\pi k^2$  is the area of the circle with radius  $k$  and BC's result in one state per  $\left(\frac{2\pi}{L}\right)^2$  ( $L^2$  is the area of the square 2D sample).

$$\text{So, } N(k) = \frac{L^2 k^2}{4\pi}$$

$$\omega = ck \Rightarrow N(\omega) = \frac{L^2 \omega^2}{4\pi c^2}$$

$$\text{Now, } D(\omega) = \underset{\substack{\uparrow \\ 1L+1T \text{ mode}}}{2} \frac{dN}{d\omega} = \frac{L^2 \omega}{\pi c^2}$$

b) The speed of sound in Al is  $c = 5 \times 10^3$  m/s. Assuming that this value is also appropriate for our 2D monolayer, what is the Debye temperature for the Al monolayer?

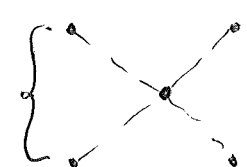
Debye freq.:  $\int_0^{\omega_D} d\omega D(\omega) = 2N$ , or

$$\underbrace{N(\omega_D)}_{\text{from a)}} = N$$

Then  $\frac{L^2 \omega_D^2}{4\pi c^2} = N$ , or

$$\omega_D = \left[ 4\pi c^2 \underbrace{\left( \frac{N}{L^2} \right)}_{\text{2D atomic density}} \right]^{1/2}$$

fcc lattice, (100) surface:

$4\text{\AA}$    $\frac{N}{L^2} = \frac{2 \text{ atoms per cell}}{16\text{\AA}^2}$

So,  $\omega_D = 6.3 \times 10^{13} \text{ s}^{-1}$ ,

and  $\theta_D = \frac{\hbar \omega_D}{k_B} = \underline{\underline{4.7 \times 10^2 \text{ K}}}$ .

4. a) Consider a 3D bcc lattice with the lattice constant  $a$ . Derive corresponding basis vectors for the reciprocal lattice. What is the type of the reciprocal lattice defined by these vectors?

The primitive cell of a bcc lattice is defined by:

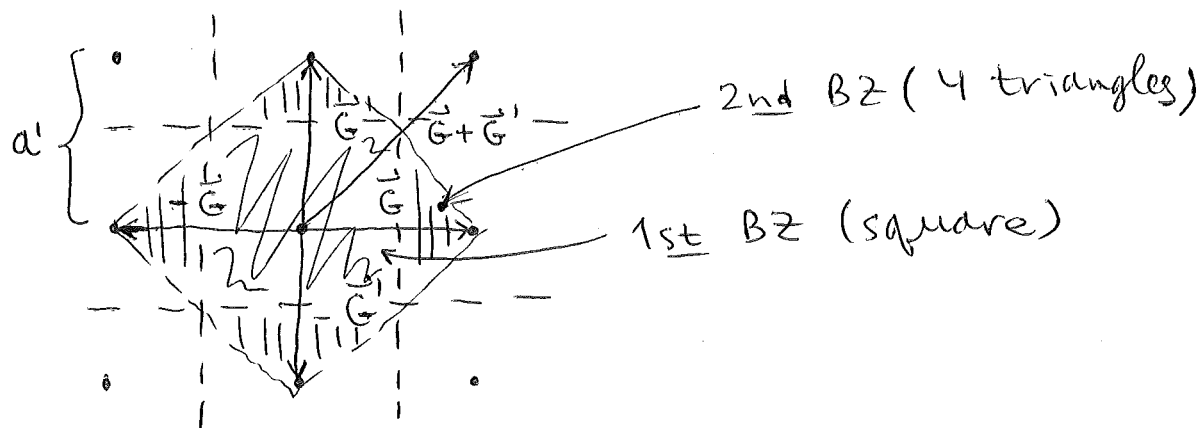
$$\begin{cases} \vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z} - \hat{x}), \\ \vec{a}_2 = \frac{a}{2} (\hat{z} + \hat{x} - \hat{y}), \\ \vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z}) \end{cases}, \quad a - \text{lattice constant}$$

Note that  $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{2}$

Then  $\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{V} = 2\pi \left(\frac{2}{a^3}\right) \left(\frac{a}{2}\right)^2 2 [\hat{z} \times \hat{x} + \hat{x} \times \hat{y}] = \frac{2\pi}{a} (\hat{y} + \hat{z})$ .

Likewise,  $\vec{b}_2 = \frac{2\pi}{a} (\hat{z} + \hat{x})$ ,  $\vec{b}_3 = \frac{2\pi}{a} (\hat{x} + \hat{y})$ .  
This is an fcc RL with  $a' = \frac{4\pi}{a}$ .

b) Draw a square 2D reciprocal lattice with the lattice constant  $a'$ , and show the 1<sup>st</sup> and 2<sup>nd</sup> Brillouin zones on the drawing. Provide a step-by-step explanation of how the zones have been drawn.



- Choose a RL point
  - From this point, draw 4 shortest RL vectors:  $\pm \vec{G}, \pm \vec{G}'$
  - Draw 4 lines bisecting these vectors.
- The square area enclosed by these lines is the 1<sup>st</sup> BZ.
- Draw 4 next-shortest vectors:  $\pm \vec{G} \pm \vec{G}'$  and bisect them with lines. 4 triangles enclosed by these lines & not included into 1<sup>st</sup> BZ make the 2<sup>nd</sup> BZ.

5. a) Derive an expression for the average energy of a QM simple harmonic oscillator (SHO) which is at thermal equilibrium with temperature  $T$ .

The average energy

$$\bar{E} = \frac{\sum_{n=0}^{\infty} n \hbar \omega e^{-\frac{n \hbar \omega}{k_B T}}}{\sum_{n=0}^{\infty} e^{-\frac{n \hbar \omega}{k_B T}}} =$$

$$= - \frac{\partial}{\partial (1/k_B T)} \log \left[ \sum_{n=0}^{\infty} e^{-\frac{n \hbar \omega}{k_B T}} \right] =$$

$$= - \frac{\partial}{\partial (1/k_B T)} \log \left[ \frac{1}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \right] = - \frac{1 - e^{-\frac{\hbar \omega}{k_B T}}}{(1 - e^{-\frac{\hbar \omega}{k_B T}})^2} (-e^{-\frac{\hbar \omega}{k_B T}}) \times$$

$$\times \hbar \omega = \frac{e^{-\hbar \omega / k_B T}}{1 - e^{-\hbar \omega / k_B T}} \hbar \omega =$$

$$= \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1}$$

- b) Use this equation to derive the expression for the specific heat  $C_v$  (per mole of substance) according to Einstein's theory.

Acc. to Einstein's theory,

$U = 3N \frac{\hbar \omega_E}{e^{\hbar \omega_E / k_B T} - 1}$ , since all  $3N$  oscillators vibrate at the same freq.  $\omega_E$ .

Then  $C_v = \left( \frac{\partial U}{\partial T} \right)_v = -3N (\hbar \omega_E) \frac{1}{(e^{\hbar \omega_E / k_B T} - 1)^2} e^{\frac{\hbar \omega_E}{k_B T}} \times$

$$\times \left( -\frac{\hbar \omega_E}{k_B T^2} \right) = 3N k_B \underbrace{\left( \frac{\hbar \omega_E}{k_B T} \right)^2}_{R} \frac{e^{\hbar \omega_E / k_B T}}{(e^{\hbar \omega_E / k_B T} - 1)^2}$$

$\frac{\theta_E}{T}$ , where  $\hbar \omega_E \equiv k_B \theta_E$



c) Examine the high- and low-temperature limits of this expression. Compare the high-T limit to the results of the classical theory. What is the T-dependence of the low-T limit? How does it compare with experimental data?

$T \gg \theta_E$  (high-T limit):

$$C_v = 3R \left( \frac{\theta_E}{T} \right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T} - 1)^2} \approx$$

$$\approx 3R \left( \frac{\theta_E}{T} \right)^2 \frac{1}{\left( \frac{\theta_E}{T} \right)^2} = 3R, \text{ the classical result.}$$

$T \ll \theta_E$  (low-T limit):

$$C_v \approx 3R \left( \frac{\theta_E}{T} \right)^2 e^{-\theta_E/T} \sim e^{-\theta_E/T}.$$

The T-dependence is exponential, whereas experiments show that

$$C_v \sim T^3 \text{ as } T \rightarrow 0.$$

The exponential decrease is much faster than warranted by experiment.