PHYS 425 Midterm Exam 1 F25

Name : Solutions

Make sure your midterm packet contains 6 pages (including this cover page) and 3 questions. The total number of possible points is 50. Write your answers in the space provided and please show all your work. If you need more space, please use the back of the page of the corresponding problem.

- **Partial credit will be given.**
- **You are allowed a standard size notecard with handwritten notes**. Staple it to the exam or put it inside the exam packet.
- **Answers with little to no explanation will not receive partial credit.** Answers that require math should show algebraic steps and if no math is required a written explanation should support your answer.
- **Non-programmable calculators are allowed.**
- **Use the space provided to write your answers.** If you need more space, you can use the backside of the exam sheet. Please make sure to indicate in the space provided if you do.
- **Please make sure I can read your work** and write legibly, in a reasonably neat and coherent way, in the space provided. If I can't read your solution, I will assume it's wrong.
- **Unless otherwise noted, simplify all your work**. This means that you need to need to combine like terms, reduce fractions, etc. If an integral is too complicated to be solved during the midterm, I will ask you to only set it up.
- **Numerical answers should have units!** Unless otherwise noted, units should match the units given in the problem.

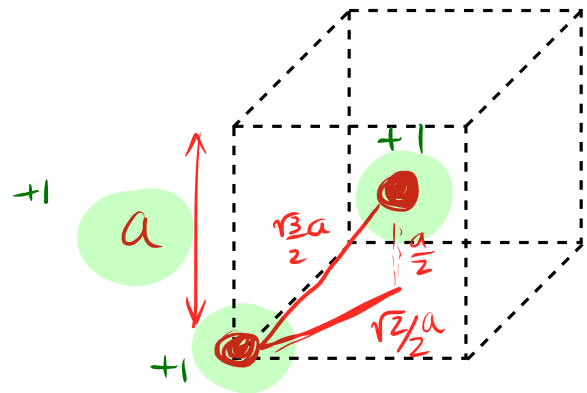
The point distribution is given in the table to the right.

Question	Points	Score
1	20	
2	10	
3	20	
Total:	50	

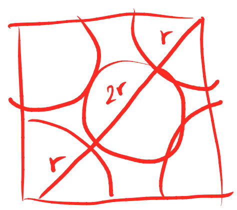
1. (20 points) (*Fe Unit Cell Geometry*)

   A certain thermodynamically stable configuration of iron (ferrite) has a BCC crystal geometry with lattice spacing of 0.286 nm.

   (a) In the simple cubic guidelines below, **draw** the basis for this iron unit cell. **Label** any relevant distances. (*3 points*)



   (b) **Calculate** the atomic packing efficiency for ferrite. (*7 points*)



+2

$4r = \sqrt{3}a$

$\Rightarrow a = \frac{4}{\sqrt{3}} r$

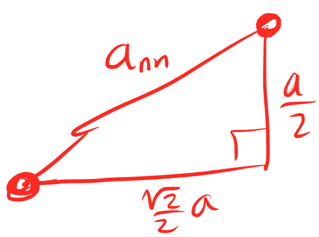
$APF = \frac{N_{atoms} V_{atom}}{V_{cell}}$ +1

+1 $= \frac{2 \left(\frac{4}{3}\pi r^3\right)}{\left(\frac{4}{\sqrt{3}}\right)^3 r^3}$ +1 $= \frac{\sqrt{3}\pi}{8} = .68$

+1

$\boxed{\text{APF} = 68\%}$ +1

   (c) **Find** the nearest neighbor spacing two iron atoms in the ferrite configuration. (*3 points*)



$a_{nn} = \sqrt{\frac{a^2}{4} + \frac{2}{4}a^2}$

$= \frac{\sqrt{3}}{2}a$ +2

+1

$\boxed{a_{\text{nn}} = 0.248 \text{ nm}}$

   (d) A powder diffraction spectrum for ferrite with incident $\lambda = 0.155$ nm X-Rays shows an intensity peak located at $2\theta = 45°$. From the reciprocal lattice vectors below, **circle** the one that corresponds to this peak. Show your work. (*7 points*)

+2

(a) $\vec{G} = \vec{b}_1 + \vec{b}_2$

(b) $\vec{G} = 2\vec{b}_3$

(c) $\vec{G} = \vec{b}_1 + 2\vec{b}_2 + \vec{b}_2$

(d) $\vec{G} = 2\vec{b}_2 + 2\vec{b}_3$

For x-ray diff, $2d\sin\theta = \lambda$ +1

& we know

+2 $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$ & $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

So

$\sqrt{h^2+k^2+l^2} = \frac{2a\sin\theta}{\lambda} = \frac{2(.287\text{nm})\sin(22.5°)}{.155\text{nm}}$

$= 1.417$ +1

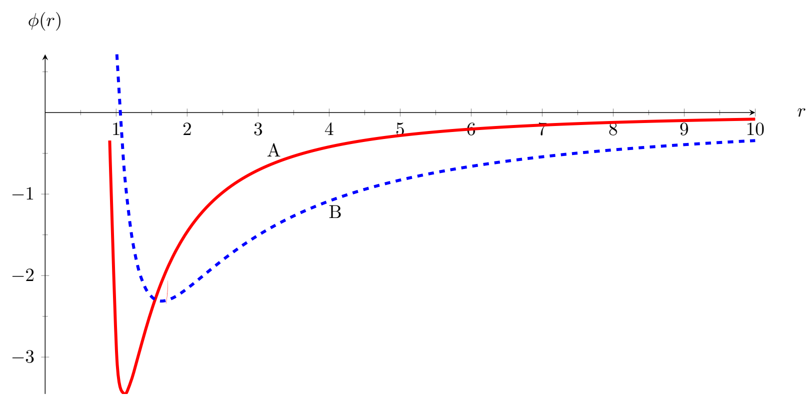
$\approx \sqrt{2}$

(a) has $(hkl) = (1\ 1\ 0)$ +1

So $\sqrt{h^2+k^2+l^2} = \sqrt{2}$

2. (10 points) (Interatomic Potentials)

   Consider the interatomic potentials for two different materials shown below, material A (solid line) and material B (dashed line). You may assume that both materials have similar masses.



For each of the following, **circle** the material with the largest property listed below and briefly **explain** your choice.

(a) equilibrium interatomic spacing (*3 points*)

(Material A / Material B) +1

+1

Interatomic spacing is given by the minimum location of ϕ which is clearly further right for B.

+1

(b) Young's modulus (*3 points*)

+1

(Material A / Material B)

Young's modulus is related to $\phi''(r)$ or the

+1 curvature of ϕ. A has a larger curvature near the minimum.

+1

(c) coefficient of thermal expansion (*4 points*)

+1

(Material A / Material B)

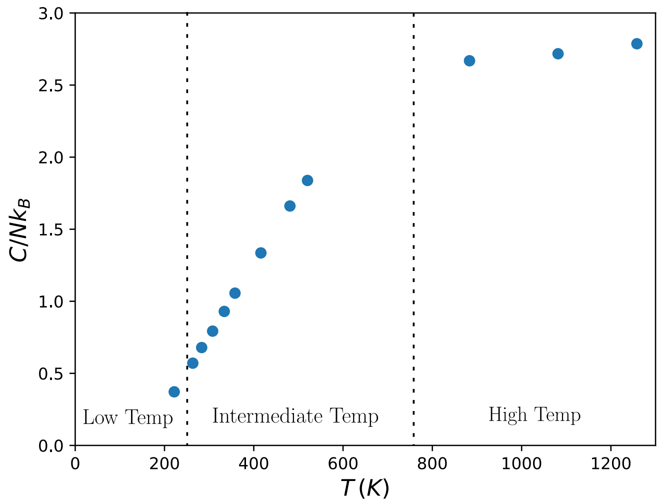
α is related to $\phi'''(r)$ which is expressed through the anharmonicity or asymmetry of ϕ.

+1

B is more asymmetric

+1

3. (20 points) (Models of Heat Capacity)



The plot above shows the experimental heat capacity of diamond as a function of temperature. The temperature range is divided into three regimes: low, intermediate and high temperature.

(a) **Circle** the regime(s) in which each of the following heat capacity models would accurately fit the data above:

(i) Dulong-Petit Model (*1 point*)

(*Low T* / *Intermediate T* / *High T*) +1

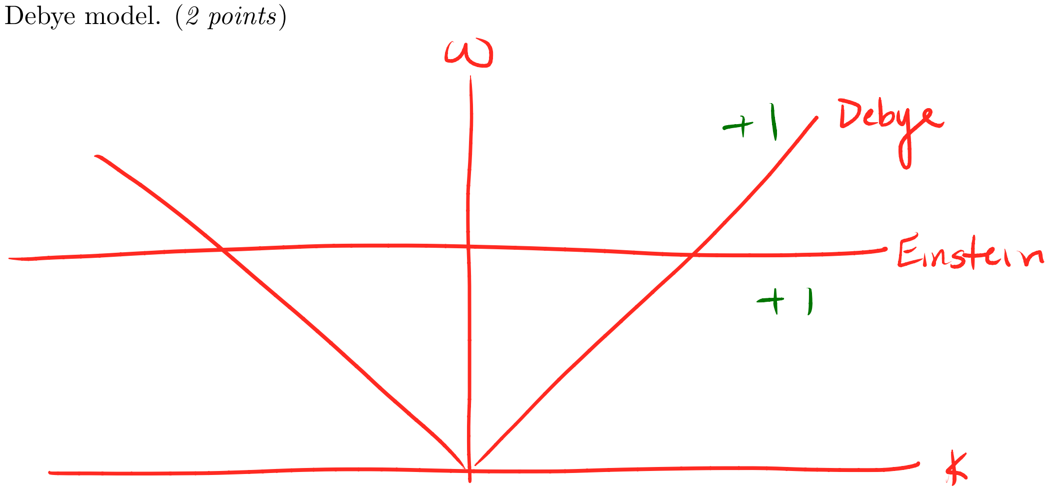
(ii) Einstein Model (*1 point*)

(*Low T* / *Intermediate T* / *High T*) +1

(iii) Debye Model (*1 point*)

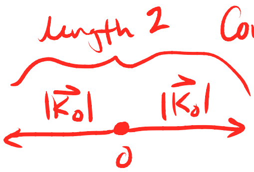
(*Low T* / *Intermediate T* / *High T*) +1

(b) In the space below **sketch** and **label** the assumed *dispersion relation* by (i) the Einstein model and (ii) the Debye model. (*2 points*)



For the following, consider the 1 dimensional Debye solid.

(c) **Find** an expression for the density of states, $g(\omega)$. (*3 points*)



Count states

$$N = \sum_{|k|<|K_0|} 1 = 2\,\frac{L}{2\pi}\int_0^{K_0} dk \quad +1$$

$$= 2\,\frac{L}{2\pi}\int_0^{\omega_0}\frac{d\omega}{v} \quad +1$$

$$\boxed{g(\omega) = \frac{L}{\pi v}} \quad +1$$

(d) **Find** an expression for the Debye frequency, ω_D. (*2 points*)

Introduce cutoff ω_D so that

$$N = \int_0^{\omega_D} g(\omega)\,d\omega = \frac{L\omega_D}{\pi v} \quad +1$$

$$\boxed{\omega_D = \frac{\pi v N}{L}} \quad +1$$

(e) **Show** that the Debye model for a 1 dimensional solid predicts a heat capacity with a linear dependence in temperature for the <u>*low temperature*</u> regime. (*10 points*)

We have $g(\omega)$ so

$$\langle E\rangle = \int_0^{\omega_D} \hbar\omega(\vec{k})\, n_{BE}(\omega(k))\, g(\omega(k))\, d\omega$$

$$= \frac{L\hbar}{\pi v}\int_0^{\omega_D}\frac{\omega}{e^{\beta\hbar\omega}-1}\,d\omega \quad +2$$

let $x = \beta\hbar\omega \rightarrow d\omega = \frac{dx}{\beta\hbar}$ $+1$

So $$\langle E\rangle = \frac{L\hbar}{\pi v}\left(\frac{1}{\beta\hbar}\right)^2\int_0^{\beta\hbar\omega_D}\frac{x}{e^x-1}\,dx \quad +2$$

For the low temp limit, $T\rightarrow 0$ implies $\beta\hbar\omega_D \rightarrow \infty$ so $+2$

$$\int_0^\infty \frac{x}{e^x-1} = \frac{\pi^2}{6}$$

which makes

$$\langle E\rangle = \frac{\pi L k_B^2}{6v\hbar}T^2 \quad +1$$

and thus

$$C = \frac{\partial\langle E\rangle}{\partial T} = \boxed{\frac{\pi L k_B^2}{3v\hbar}T} \quad +2$$

Some useful info, you may tear this page off the exam packet:

$$1\,\mathrm{u} = 1.66 \times 10^{-27}\ \mathrm{kg}$$

$$1\,\mathrm{eV} = 1.602 \times 10^{-19}\ \mathrm{J}$$

$$k_B = 1.38 \times 10^{-23}\ \mathrm{J/K} = 8.62 \times 10^{-5}\ \mathrm{eV/K}$$

$$N_A = 6.022 \times 10^{23}\ \mathrm{mol}$$

$$h = 6.626 \times 10^{-34}\ \mathrm{J\,s} = 4.136 \times 10^{-15}\ \mathrm{eV\,s}$$

$$e = 1.602 \times 10^{-19}\ \mathrm{C}$$

$$R = N_A k_B = 8.38 \times 10^{3}\ \mathrm{J/(kg\,K)}$$

$$\int_0^\infty \frac{x}{e^x - 1}\,dx = \frac{\pi^2}{6}$$

$$\int_0^\infty \frac{x^2}{e^x - 1}\,dx = 2\zeta(3)$$

$$\int_0^\infty \frac{x^3}{e^x - 1}\,dx = \frac{\pi^4}{15}$$

$\zeta(3) = 1.202\ldots$ (leave as $\zeta(3)$ if needed)

$$\int d^3x = \int_0^{2\pi} \int_0^{\pi} \int_0^{R} r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$\int d^2x = \int_0^{2\pi} \int_0^{R} r\, dr\, d\phi$$