Physics 361 **Midterm solution** **November 1, 2002**

Due at the end of class. No book or notes.

1. short answer Please briefly justify your answers.

a) (2 points) Many identical spheres are packed in a body centered cubic arrangement and then repacked in a face centered cubic arrangement. In both cases the nearest neighbors are touching. Which packing takes up the lesser volume?

solution: FCC. It is one of the close-packed crystals of maximum density.

b) (3 points) Roughly, how much energy is required to separate an argon atom from its crystal, at very low temperature?

solution: From problems and chapter, the interatomic energy of Argon is about .01 eV. Counting for the 6 neighbors of a surface atom, the required energy is of the order of 0.1 eV.

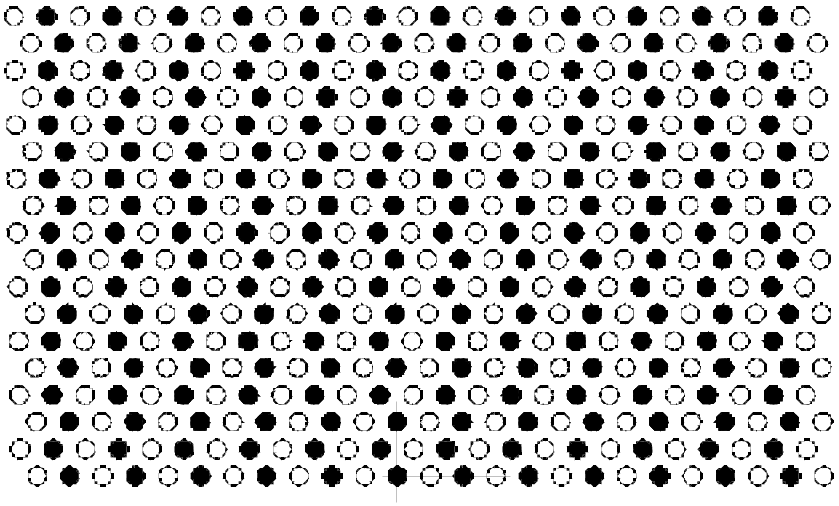
c) (3 points) Which has a larger low-temperature specific heat: diamond or argon?

solution: Low-temperature specific heat depends on the number of vibrational modes with energy less than k_BT. At a given, long wavevector k, diamond vibrates faster, because the bonding is stronger and the atoms are lighter. Both crystals have the same number of modes in the same range of k. Thus a given mode has a higher frequency ω, and there are fewer modes in with energy $\hbar\omega$. Thus Diamond has lower specific heat and Argon has higher.

d) (4 points) A beam of x-rays of energy ϵ diffracts from a powder of many small crystals and onto a screen, forming a pattern of concentric rings. The x-ray energy is then doubled with no change in the geometry. What is the effect on the ring positions?

solution: The set of allowed wavevectors q that cause scattering is unchanged. $|q| = |k|2\sin\theta/2$ where θ is the angle between the incident and the scattered beam. If the x-ray energies double, k doubles and thus $\sin\theta/2$ must decrease by a factor 2. The rings become smaller by this factor.

2. zigzag lattice



The lattice shown is a section of a triangular lattice of black and white atoms. Each atom is separated from its six nearest neighbors by a spacing a.

a) (5 points) Find two primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ such that the displacement vector to any unit cell from a given unit cell has the form $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where n_1 and n_2 are integers. Give the horizontal and vertical co-ordinates of $\mathbf{a}_1$ and $\mathbf{a}_2$.

solution: A horizontal vector from black to the nearest black leads to an equivalent position on the lattice. $\mathbf{a}_1 = 2a\hat{\mathbf{x}}$. A vertical vector from black to the nearest black also leads to an equivalent position, so $\mathbf{a}_2 = \sqrt{3}a\hat{\mathbf{y}}$.

To specify each atom in the lattice, one must specify its unit cell via n_1 and n_2. One must also indicate the position of each atom in a unit cell relative to its origin via a basis vector.

b) (5 points) How many atoms are contained in a primitive cell of this lattice, and what are their basis vectors $\mathbf{b}_1$, $\mathbf{b}_2$, ... relative to the origin shown?

solution: $\mathbf{b}_1 = 0$; $\mathbf{b}_2 = \frac{1}{2}\mathbf{a}_1$; $\mathbf{b}_3 = +\frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$; $\mathbf{b}_4 = -\frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$. Many other choices are possible. It is also OK to give the basis vectors in terms of $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$.

A beam of waves with wavevector $\mathbf{k}_{in}$ can diffract from this lattice in certain directions with wavevectors $\mathbf{k}_{out}$. The scattered wavevectors $\mathbf{q} = \mathbf{k}_{in} - \mathbf{k}_{out}$ that give diffraction lie on a lattice.

c) (4 points) What are two primitive vectors of this lattice? Specify their horizontal and vertical coordinates.

solution: The allowed lattice of $\mathbf{q}$'s satisfy the coherent scattering condition $e^{i\mathbf{q}\cdot\mathbf{R}} = 1$. Thus $\mathbf{q} = n\mathbf{q}_1 + m\mathbf{q}_2$ where $\mathbf{q}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$. Evidently $\mathbf{q}_1 = 2\pi/|a_1|\ \hat{\mathbf{x}} = \pi/a\ \hat{\mathbf{x}}$; $\mathbf{q}_2 = 2\pi/|a_2|\ \hat{\mathbf{y}} = (2\pi/\sqrt{3}a)\hat{\mathbf{y}}$.

d) (4 points) If the black and white atoms scatter identically, what are the allowed wavevectors $\mathbf{q}$ for diffraction?

solution: If the atoms all scatter identically, we have a triangular lattice whose primitive vectors are *eg.* $\mathbf{a}'_1 = a\hat{\mathbf{x}}$ and $\mathbf{a}'_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}\sqrt{3}\hat{\mathbf{y}}$. Thus $\mathbf{q} = n\mathbf{q}'_1 + m\mathbf{q}'_2$, with $\mathbf{q}'_i \cdot \mathbf{a}'_j = 2\pi\delta_{ij}$. $\mathbf{q}'_2$ is evidently vertical. Applying the dot product condition with $\mathbf{a}'_2$, we get $\mathbf{q}'_2 = (4\pi/\sqrt{3}a)\ \hat{\mathbf{y}}$. $\mathbf{q}'_1 \equiv q_x\hat{\mathbf{x}} + q_y\hat{\mathbf{y}}$. Applying the dot product with $\mathbf{a}'_1$, $2\pi = q_x a$, so $q_x = 2\pi/a$. Applying the dot product with $\mathbf{a}'_2$, we infer $q_x\frac{1}{2}a + q_y\sqrt{3}a/2 = 0$, so $q_y = -q_x/\sqrt{3} = -(2\pi/\sqrt{3}a)$.

If all the atoms are connected by identical springs with spring constant A, vibrational waves can propagate in the lattice. There is no vibration perpendicular to the plane of the crystal. Long-wavelength compressional vibrations propagate at a speed $c_\parallel = (3/4)a\sqrt{A/M}$, where M is the average mass per atom. This speed is the same in all propagation directions. Transverse waves propagate at a speed $c_\perp = c_\parallel/\sqrt{3}$, also the same for all propagation directions.

e) (15 points) Find the specific heat c_v as a function of temperature T for very low T in terms of the given quantities, $\hbar$ and the Boltzmann constant k_B . That is, find the temperature derivitive of the energy per unit area.

solution: We express the total energy E at temperature T using the thermal average phonon number $\langle n\rangle$ in each mode. Every mode can be labeled by its wavevector $\mathbf{k}$ and its polarization s. The energy $E_{\mathbf{k}s}$ in a given mode is given by $\hbar\omega_{\mathbf{k}s}(\frac{1}{2} + \langle n\rangle_{\mathbf{k}s})$. At low temperatures, the modes that contribute have $\omega_{\mathbf{k}s} = c_s|k|$. For a mode with energy $\hbar\omega$, $\langle n\rangle = (e^{\beta\hbar\omega} - 1)^{-1}$. Thus the total energy is given by

$$E = E_0 + \sum_{s=1}^{2}\sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}s}\,\langle n\rangle_{\mathbf{k}s} = E_0 + \frac{(\text{area})}{(2\pi)^2}\sum_s \int 2\pi k\ dk\ \hbar c_s|k|(e^{\beta\hbar c_s|k|} - 1)^{-1}.$$

Defining $x = \beta\hbar c_s|k|$,

$$E = E_0 + \sum_s \frac{(\text{area})}{(2\pi)}\beta^{-1}(\beta\hbar c_s)^{-2}\int dx\ x^2(e^x - 1)^{-1}$$

$$= E_0 + (\text{area})(2\pi)^{-1}\beta^{-3}[(\hbar c_\parallel)^{-2} + (\hbar c_\perp)^{-2}]\int dx\ x^2(e^x - 1)^{-1}$$

Denoting the [...] as $(\hbar c)^{-2}$ and the numerical integral as I, This yields

$$E = E_0 + (\text{area})(2\pi)^{-1}\beta^{-3}(\hbar c)^{-2}I$$

Now using $c_v = (d/dT)(E/(\text{area}))$ and noting that $\beta^{-1} = k_B T$,

$$c_v = (2\pi)^{-1}3k_B(k_B T)^2(\hbar c)^{-2}I$$

Using the given formula for $c_\perp$ and $c_\parallel$, and the tabulated value for I, this gives

$$c_v = (8.15...)\ k_B^3 T^2 M/(Aa^2)$$

f) (6 points) Find the specific heat for high temperatures.

solution: At high temperature, each mode has k_BT of energy, and each atom has two modes. Thus $E = Nk_BT$; $c_v = nk_B$, where n is the density of atoms. n is 4 atoms per rectangle of area a_1a_2 or $(2/\sqrt{3}a^2)$. Thus $c_v = 4k_BT/(\sqrt{3}a^2)$.

Suppose the mass ratio of white to black atoms is changed from 1 to nearly 0 with fixed average mass M.

g) (5 points) How does the specific heat change in the various temperature regimes? Where does the main change occur?

solution: *low temperature*: Since the mean mass per unit area is fixed, the speeds of sound are fixed, and there is no change in the low-temperature specific heat. *high temperature*: At very high temperatures, each atom again has $2k_BT$ of energy as before, so there is no difference in the specific heat here, either. Now, however, there are optic modes involving motion of the light masses that have arbitrarily high frequencies ω_o. Thus one can have temperatures much larger than all the acoustic $\hbar\omega$'s but much lower than the optic $\hbar\omega$'s. These optic modes contribute negligibly to the specific heat at such temperatures, and the acoustic modes give k_BT of energy per atom. Thus the c_v rises from the T^2 form of e) at low temperatures, to a plateau of k_B per atom, and then to another plateau of $2k_B$ per atom when the temperature exceeds $\hbar\omega_o$

n	$\int_0^\infty dx \frac{x^n}{e^x-1}$	$\int_0^\infty dx \frac{x^n}{e^x+1}$
1	1.64	0.82
2	2.40	1.80
3	6.49	5.68