PHYS545, Test 1, Spring 2014

(1) (5 pts) Use the data in Table 1 (page 116) and/or info below. For room temperature, put the atoms Li, Na, K, Rb, and Cs in order of heat capacity (from lowest to highest). Explain how you made your choice.

(2) (5 pts) (a) This problem is in 2-dimensions. The lattice is a hexagonal lattice with nearest neighber distance a. Draw a crystal where the basis is three atoms A, B, and C where B is $a/4$ to the right of atom A and the C is $a/4$ below atom A. Only show 3 or 4 unit cells.

(3) (5 pts) For the dispersion relation for the 1D lattice of atoms shown in Fig. 7 (page 96), sketch the density of states. Make sure to label any interesting points.

(4) (5 pts) You squeeze a crystal in all three directions so that all three directions of the crystal are smaller by the same factor α. How do the allowed wavevectors of the scattered X-rays change? Explain your answer.

(5) (5 pts) Of the 3 possible ionic crystals, NaCl, KCl, and KBr, which one has largest cohesive binding energy? Give a cogent reason for your choice.

(6) (10 pts) For HCP, the primitive unit cell has vectors $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = (a/2)\hat{x} + (a\sqrt{3}/2)\hat{y}$, and $\vec{a}_3 = (a/\sqrt{3})\hat{y} + (a\sqrt{2/3})\hat{z}$. (a) Give the reciprocal lattice vectors. (b) Give the directions perpendicular to the (1,0,0) and (0,0,1) planes. (c) What is the distance between the (1,0,0) planes? (d) What is the distance between the (0,0,1) planes?

(7) (10 pts) Use the data derived from Fig. 9 (page 115) and/or info below to estimate the speed of sound in solid Ar. For the density of solid Ar, use 1.7 g/cm^3.

(8) (10 pts) Using the positions of the Zn and S in zinc sulfide (pg 17 bottom and table pg 18) obtain an expression for the structure factor (writing f_Z for zinc and f_S for sulfer and there's no special relation between them). Give the four different expressions for the structure factor only in terms of f_Z and f_S for the values (v_1, v_2, v_3) equal to (0,0,1), (1,0,0), (1,1,0), and (1,1,1).

(9) (10 pts) Two atoms of Weirdonium interact with a potential energy that depends on their separation R as $U(R) = A/R^8 - B/R^4$ where A and B are positive constants. When Weirdonium forms a crystal, the $C \equiv \sum_j' p_{ij}^{-8}$ and $D \equiv \sum_j' p_{ij}^{-4}$. (a) Give the units of A, B C and D. (b) Determine the nearest-neighbor distance at equilibrium. (c) Determine the cohesive energy of the crystal.

(10) (10 pts) You have a linear lattice with spacing a. There are 3 atoms in each basis. The atoms are in a line along the lattice with type ABA repeated forever. The lattice is $...(ABA)(ABA)(ABA)....$ Let u_s, v_s, w_s be the displacements of the s-th group of A, B, A respectively. Write down the classical equations of motion for the atoms when only nearest neighbors interact keeping only linear terms in the force. *Do not solve these equations.* Clearly define all of your parameters.

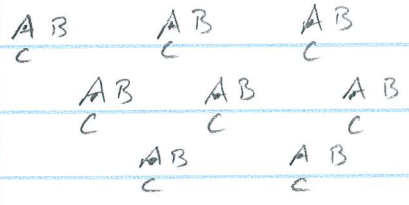
Possibly useful info:

$\cos 30^\circ = \sqrt{3}/2$ and $\cos 60^\circ = 1/2$.

Atomic masses: He(4), Li(7), Na(23), S(32), Cl(35), K(39), Ar(40), Zn(65), Br(80), Rb(85), Cs(133), Wd(333)

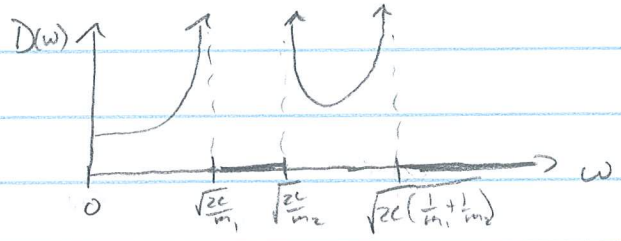
1) The heat capacity is an increasing function of T/Θ. The function is the same for these atoms. As Θ gets smaller T/Θ gets bigger $\Rightarrow$ C_v gets bigger

Li, Na, K, Rb, Cs low to high C_v

2) 

3) The density of states is proportional to $1/d\omega/dk$

$d\omega/dk = 0$ at $\omega = \sqrt{2c/m_1}$ and $\sqrt{2c/m_2}$ and $\sqrt{2c\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}$



$D(\omega) = 0$ for $\sqrt{\frac{2c}{m_1}} < \omega < \sqrt{\frac{2c}{m_2}}$

and $\sqrt{2c\left(\frac{1}{m_1}+\frac{1}{m_2}\right)} < \omega$

4) Since all directions decrease by the factor α, all reciprocal lattice vectors increase by factor $1/\alpha$. Since the X-ray wavevectors are proportional to G, they all increase by a factor of $1/\alpha$.

5) Reason 1) From table pg 14, NaCl has smallest lattice spacing. Thus, will be hardest to pull apart. Reason 2) From Table 7 pg 66, NaCl has the largest lattice energy compared to free ions.

6) a) For the $\vec{b}_i$, will need $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a^3 \begin{vmatrix} 1 & 0 & 0 \\ 1/2 & \sqrt{3}/2 & 0 \\ 0 & 1/\sqrt{3} & \sqrt{2/3} \end{vmatrix} = a^3/\sqrt{2}$

$$\vec{b}_1 = \frac{2\pi\sqrt{2}}{a^3}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi\sqrt{2}}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1/2 & \sqrt{3}/2 & 0 \\ 0 & 1/\sqrt{3} & \sqrt{2/3} \end{vmatrix} = \frac{2\pi\sqrt{2}}{a}\left[\frac{1}{\sqrt{2}}\hat{x} - \frac{1}{\sqrt{6}}\hat{y} + \frac{1}{\sqrt{12}}\hat{z}\right]$$

$$\vec{b}_2 = \frac{2\pi\sqrt{2}}{a^3}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi\sqrt{2}}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1/\sqrt{3} & \sqrt{2/3} \\ 1 & 0 & 0 \end{vmatrix} = \frac{2\pi\sqrt{2}}{a}\left(\sqrt{\frac{2}{3}}\hat{y} - \frac{1}{\sqrt{3}}\hat{z}\right)$$

$$\vec{b}_3 = \frac{2\pi\sqrt{2}}{a^3}(\vec{a}_1 \times \vec{a}_2) = \frac{2\pi\sqrt{2}}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 0 \\ 1/2 & \sqrt{3}/2 & 0 \end{vmatrix} = \frac{2\pi\sqrt{2}}{a}\left(\frac{\sqrt{3}}{2}\hat{z}\right)$$

b) The direction $\perp$ to the (1,0,0) plane is $\hat{b}_1 = \dfrac{\left[\frac{1}{\sqrt{2}}\hat{x} - \frac{1}{\sqrt{6}}\hat{y} + \frac{1}{\sqrt{12}}\hat{z}\right]}{\sqrt{\frac{1}{2}+\frac{1}{6}+\frac{1}{12}} = 3/4}$

" " " " (0,0,1) plane is $\hat{b}_3 = \hat{z}$

c) $d = \dfrac{2\pi}{|\vec{b}_1|} = \dfrac{2\pi}{\frac{2\pi\sqrt{2}}{a}\sqrt{\frac{1}{2}+\frac{1}{6}+\frac{1}{12}}} = \dfrac{a}{\sqrt{2}\sqrt{3/4}} = \sqrt{\frac{2}{3}}\,a$

d) $d = \dfrac{2\pi}{|\vec{b}_3|} = \dfrac{2\pi}{(2\pi\sqrt{2}/a)\sqrt{3}/2} = \sqrt{\frac{2}{3}}\,a$

7) $\Theta = 92K = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{1/3} = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 \text{density}}{\text{mass of 1}}\right)^{1/3}$

$$v = \frac{92K \;\; 1.38\times10^{-23}\,J/K}{1.0546\times10^{-34}\,Js}\left(\frac{40\times1.66\times10^{-27}\,kg}{6\pi^2\;\;1700\,kg/m^3}\right)^{1/3}$$

$$= 1050\ m/s$$

8) $f = \sum_j f_j e^{-i\vec{G}\cdot\vec{r}_j} = f_{zn}\left(1 + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} + e^{-i\pi(v_1+v_2)}\right)$
$+ f_s e^{-i\frac{\pi}{2}(v_1+v_2+v_3)}\left(1 + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} + e^{-i\pi(v_1+v_2)}\right)$

$(0,0,1)$ $\quad f = f_{zn}(1 + -1 + -1 + 1) + f_s e^{-i\pi/2}(1 + -1 + -1 + 1) = 0$

$(1,0,0)$ $\quad f = f_{zn}(1 + 1 + -1 + -1) + f_s e^{-i\pi/2}(1 + 1 + -1 + -1) = 0$

$(1,1,0)$ $\quad f = f_{zn}(1 + -1 + -1 + 1) + f_s e^{-i\pi}(1 + -1 + -1 + 1) = 0$

$(1,1,1)$ $\quad f = f_{zn}(1 + 1 + 1 + 1) + f_s e^{-3i\pi/2}(1 + 1 + 1 + 1) =$
$= 4(f_{zn} + i f_s)$

9) a) A units Energy × length^8, B units Energy × length^4, C & D units none

b) $U_{TOT} = \frac{1}{2}N\left(\frac{AC}{R^8} - \frac{BD}{R^4}\right) \Rightarrow \frac{\partial U}{\partial R} = 0 = -\frac{8AC}{R^9} + \frac{4BD}{R^5}$

$R_0 = (2AC/BD)^{1/4}$

c) $U_{TOT}(R_0) = \frac{N}{2}\left(\frac{AC}{(2AC/BD)^2} - \frac{BD}{\left(\frac{2AC}{BD}\right)}\right) = N\left(-\frac{B^3D^2}{8AC}\right)$

10) The force on u_s is from w_{s-1} and v_s

" " " v_s " " u_s " w_s

" " " w_s " " v_s " u_{s+1}

$$M_A \frac{d^2 u_s}{dt^2} = C_{AA}(w_{s-1} - u_s) + C_{AB}(v_s - u_s)$$

$$M_B \frac{d^2 v_s}{dt^2} = C_{AB}(u_s - v_s) + C_{AB}(w_s - v_s)$$

$$M_A \frac{d^2 w_s}{dt^2} = C_{AB}(v_s - w_s) + C_{AA}(u_{s+1} - w_s)$$

$M_{A,B}$ is the mass of atoms A + B

C_{AA} is the spring constant between 2 A atoms

C_{AB} " " " " " an A and a B atom