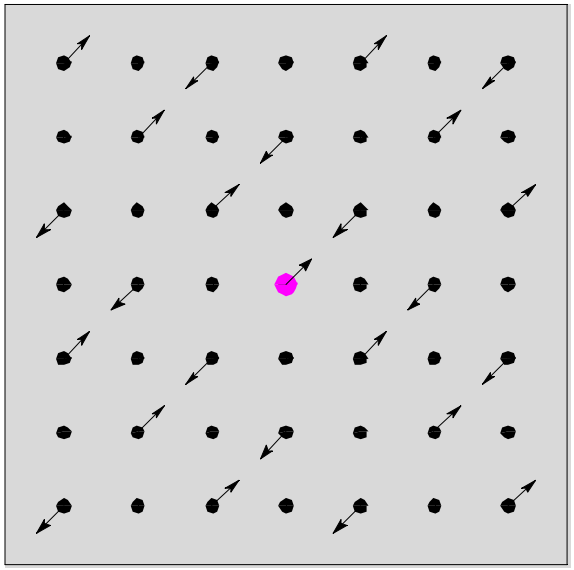
PHYSICS 731 **Department of Physics, University of Maryland, College Park**

Oct. 24, 2006 **Name: _____**

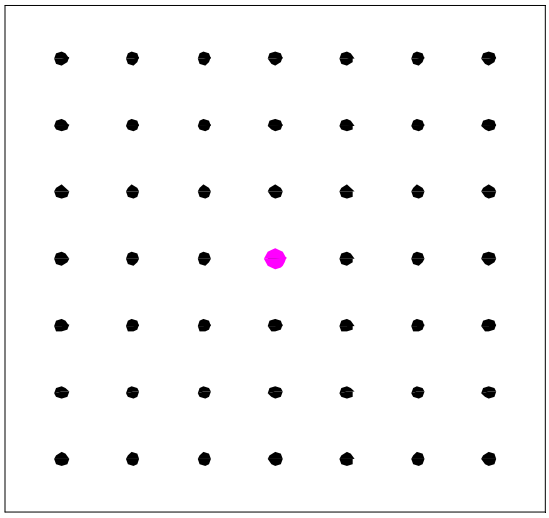
MIDTERM TEST

Budget your time. Look at all 5 pages. Do easiest problems first. Self-prepared "crib sheet" allowed.

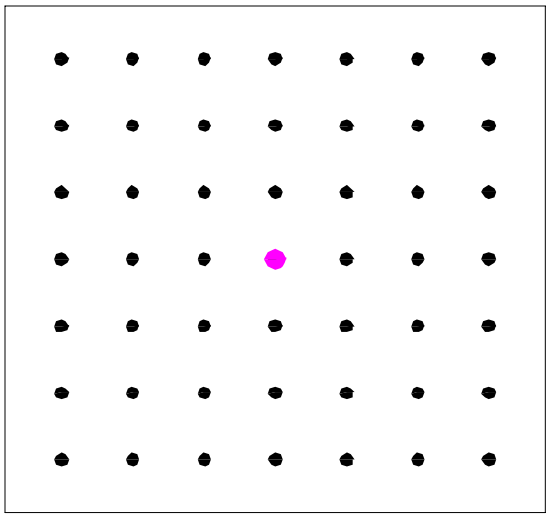
1.a) What is the 2D **k** associated with the depicted displacement pattern? (Assume $a = 1$ for simplicity.) Is the wave longitudinal or transverse? Acoustic or optical?



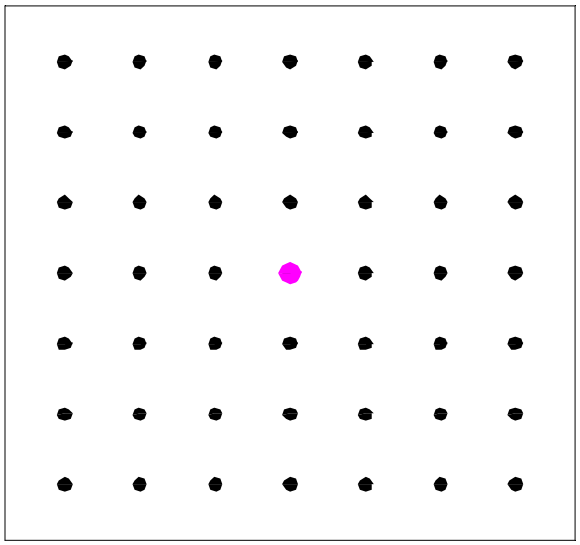
b) Redraw below the arrows [from part a)] for the other polarization. (L if part a is T, or T if part a is L)



c) Redraw below the arrows [from part a)] at a time 1/4 period later.



d) To the 2D **k** associated with the displacement pattern in part a) we add $\mathbf{K} = (4\pi/a)\ (1\ 0)$. Draw the resulting displacement pattern (or describe it).



2. Which of the following are zero, finite, infinite or undefined? Justify your answer enough to indicate that you are not guessing!

- Lattice thermal conductivity when the interatom potential is purely harmonic

- Lattice thermal conductivity for general interatom potential

- Group velocity of a phonon branch at a zone boundary

- Total momentum of [atoms in] a crystal with one phonon of mode **k**,s (**k** not 0)

- Crystal momentum of a crystal with one phonon of mode **k**,s (**k** not 0)

- Displacement **u** of a phonon mode half way between 2 neighboring atoms.

- $\int_0^\infty g(\omega)\, d\omega$

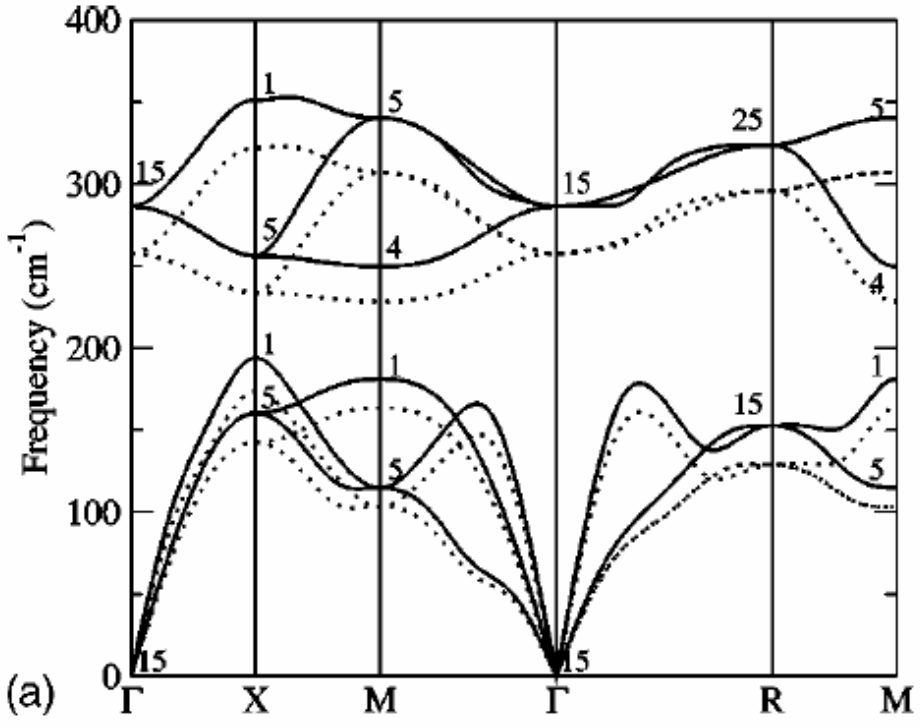
- Ratio of Umklapp to Normal processes in the **jellium** model at finite temperature

- Group velocity at a Van Hove singularity

3. Consider {100}, {111}, and {110} planes of NaCl: which are neutral, which have a net charge? Justify your answer enough to indicate that you are not guessing!

4. a) In a simple cubic lattice, what is the distance between a family of (7 5 2) planes?

b) What is the area of a unit cell of the 2D lattice of these planes?



5. This calculated phonon structure for NiAl appeared in Phys. Rev. B **68**, 214104 (2003). Ignore the numbers 1, 5 15, etc. Focus on either the solid or the dashed lines (not both) until the last items.

a) How many atoms are in the basis?

b) The paper refers to this as a B2 cubic structure. If both atoms were the same, it would reduce to a bcc lattice. What name have we used for this kind of lattice?

c) Which directions/segments (e.g., perhaps ΓX) have 4-fold or 3-fold symmetry?

d) Label each branch: L or T, O or A.

e) Mark on the vertical axis, with arrow[s], the frequencies at which there are Van Hove singularities, if any, that are NOT at special (lettered) points.

f) Up to about what temperature is the Debye approximation good? (Express your answer as a frequency from the vertical axis times fundamental constants.)

g) The paper compares this material to [bcc] W. What is the most striking difference in the phonon dispersion curves for W compared to NiAl?

h) The difference between the solid and the dashed curves is that one represents the crystal at ambient pressure and the other at very high pressure. Which set of curves is for high pressure? Briefly justify your choice, to show that you are not guessing.

i) The figure contains a plot of the Grüneisen parameter of each mode. The likely range of these is i) ⅛ – ½ ii) 1 – 3 iii) 10 – 100 iv) $10^{23} – 10^{25}$ (circle one interval)

j) For which branches and near which lettered positions do you expect the Grüneisen parameter to be largest? (On what basis are you deciding?)

k) i) Of the 4 chemical types of bonding, which two do you expect to contribute most to the total energy of NiAl?

ii) What sorts of measurements could you make to decide which of these two is the more important?

6. The following expression appeared in homework:

$$\exp\left\{-v\int\frac{d\mathbf{k}}{(2\pi)^d}\sum_s\frac{\hbar}{2M\omega_s(\mathbf{k})}(\mathbf{q}\cdot\epsilon_s(\mathbf{k}))^2\coth\frac{1}{2}\beta\hbar\omega_s(\mathbf{k})\right\}$$

a) In the **Debye** model, what is the approximation for $\omega_s(\mathbf{k})$?

b) Neglecting the factor $(\mathbf{q}\cdot\epsilon_s(\mathbf{k}))^2$, rewrite the integral in the **Debye** approximation.

c) For dimension d=2 find the integrand in the limit of very small **k** [again neglecting $(\mathbf{q}\cdot\epsilon_s(\mathbf{k}))^2$] and show thereby that the integral diverges at **k** = 0.

d) What is the physical significance of this result?

7. Consider a d-dimensional crystal with N primitive cells, each of volume v, p atoms per cell, Z valence electrons per atom, and Z_a protons per atom.

a) What is the volume (in reciprocal space) of the first Brillouin zone?

b) i) What is the value of the structure factor $\boldsymbol{S}(\mathbf{K})$ at $\mathbf{K} = 0$ (assuming the form factor is 1)?

ii) If $p = 1$, what is the ratio $\boldsymbol{S}(2\mathbf{K})/\boldsymbol{S}(\mathbf{K})$?

c) What is the density of electrons n ?

d) i) What is the ratio of ϵ_F to $\hbar\omega_D$? How does it compare to T_F/Θ_D?

ii) How, roughly, does $\epsilon_F / \hbar\omega_D$ depend on atomic mass M? (Through which parameter?)

Compare, then, $\epsilon_F / \hbar\omega_D$: **iii)** for the 2 alkalis Li (Z_a=3) and Na (Z_a=11) and **iv)** for Na and Al (Z_a=13).

8. a) In zincblende, i) what lattice is formed by the Zn atoms?

ii) To what structure would it reduce if the Zn and S atoms were the same?

iii) Which of the 4 types of bonding predominates in this crystal?

b) i) What type of Bravais lattice is a perovskite such as $BaTiO_3$?

ii) What type of Bravais lattice would be formed by the Ba and Ti atoms (if identical)?

iii) What type of Bravais lattice would be formed by the Ba and O atoms (if identical)?