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

Oct. 28, 2004 **Name: ___________________________________**

MIDTERM TEST

Budget your time. Look at all 4 pages. Do easiest problems first. Self-prepared "cheat sheet" allowed.

1. Consider a 2D checkerboard lattice of atoms 1 and 2 with form factors f_1 and f_2, with $f_1 = n\, f_2$.
a) If there are reciprocal-lattice points (in 2D space, or rods in 3D space) with intensities having the ratio 25 to 9, what is the value of n?

b) Are there any points in the reciprocal space that have an intensity between these two values?

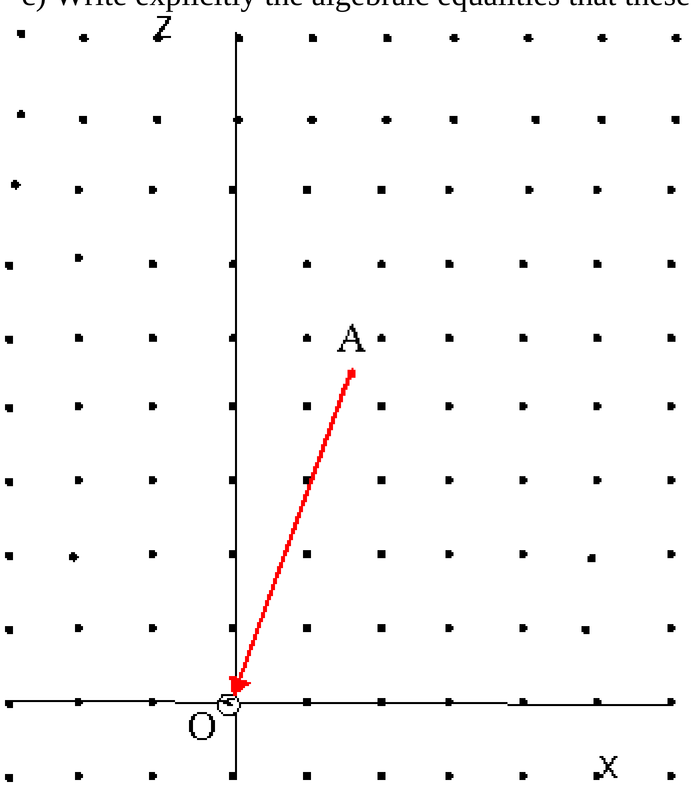
c) Does your answer to part b) change if the lattice is at finite temperature and the atoms vibrate?

2. Consider a plane wave with $\mathbf{k} = (2\pi/a)(-3/2,0,-9/2)$ incident on and elastically scattered by a cubic crystal. You can assume everything happens in the (k_x,k_z) plane, and just drop the middle index.

a) Use the sketch below to find a possible final state $\mathbf{k'}$.

b) What is a possible vector $\mathbf{K}$ that makes this scattering possible?

c) Write explicitly the algebraic equalities that these wavevectors satisfy.



3. i) In a simple cubic lattice, with lattice constant a, what is the interplanar distance d between a family of (9 5 2) planes?

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

4. Recall the Evjen method for the Madelung constant of a NaCl structure. Note the model on the desk.
a) What is the first term, assuming the nearest-neighbor (Na-Cl) spacing is a?

b) What is the contribution to the second term of the series of the atoms involved in the first term? (You are not asked to find the entire second term, which includes contributions from more-distant atoms!)

5. a) For a single-element fcc metal like Cu,
i) how many phonon branches are there?

ii) How many are optical?

iii) How many are transverse?

b) Are there any metals made of a single element that have optical branches? (Explain briefly.)

c) Consider a graphene, i.e. one sheet of graphite, which is a honeycomb array made of a very large number (N) of C atoms. Assume that all the atomic motion occurs within the sheet.
i) How many acoustic branches are there?

ii) How many transverse optical branches are there?

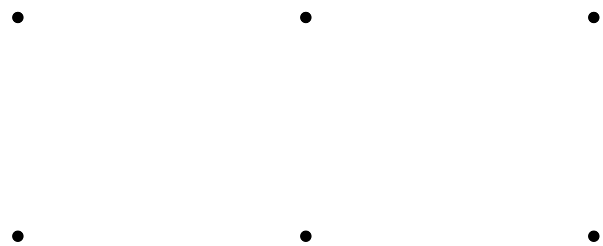
iii) How many distinct values of **k** are there?

c) Now assume that there can also be motion out of (so perpendicular to) the graphene plane.
i) How many acoustic branches are there?

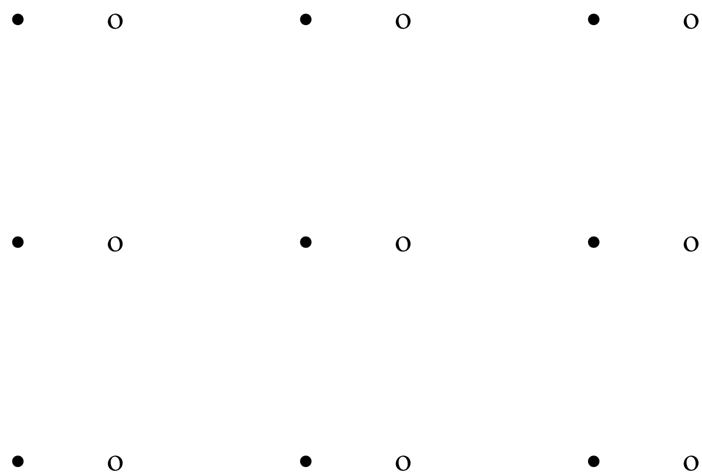
ii) How many transverse optical branches are there?

iii) Describe the reciprocal lattice.

6a. On the square lattice of sites on the right, draw the displacement of the atoms indicated by dots, for an acoustic transverse phonon with **k** = (π/a) (-1/2, 1/2).



b.On the 2-site basis square lattice on the right, draw the displacement of the two kinds of atoms for a longitudinal optical phonon with **k** = (π/a) (0, 1).



7. Consider a 1D chain of atoms of equal mass, spacing *a*, and just nearest-neighbor coupling $K(a) = \phi''(a)$, with the interatomic potential $\phi(x)$ given by the Lennard-Jones potential with constants ε and σ or *A* and *B*.

a) Find the Grüneisen parameter γ_k, showing that it is independent of k.

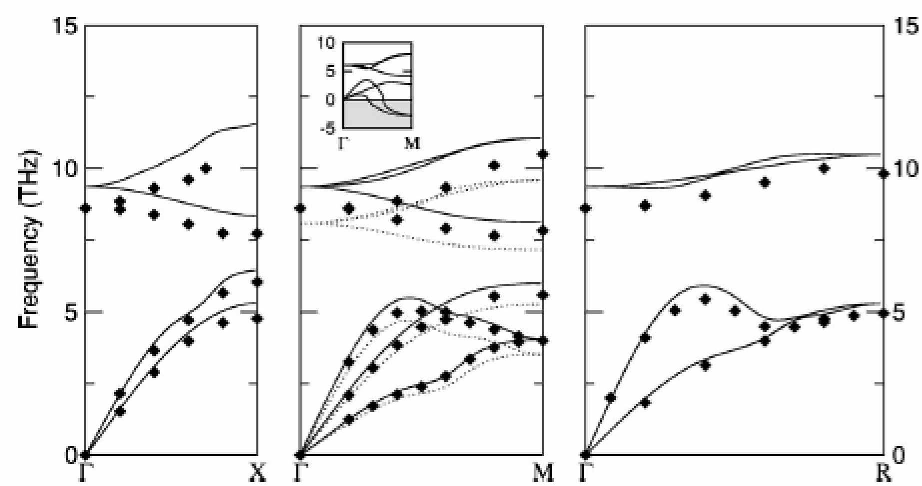
b) What is γ in terms of the van der Waals constants A and B or ε and σ? (No need to do messy arithmetic.)

c) Unrelated to the above, what is the speed of sound, again in terms of the van der Waals constants?

8. a) For a Bravais crystal with *Z* electrons per atom, what is the ratio of k_F to k_D?

b) What is the ratio of T_F to Θ_D in terms of k_F and k_D? What further information do you need to proceed? How might you find it?

9. The phonon dispersion curves depicted below are from a Phys. Rev. B article published a few months ago. The solid lines were computed, the black diamonds are from experiment.



a) Label each branch as TA, LA, or O. (Ignore the dotted curves.)

b) What is the most likely number of atoms in the basis?

c) Would you guess that the crystal has more than one element in it? (Why?)

d) Would you expect that the crystal is fairly isotropic or is it strongly planar? (Why?)

e) Why are there more branches in the middle panel (i.e. along ΓM) than in the left panel (along ΓX)?

f) Mark on the vertical (Frequency) axis the values at which there are Van Hove singularities in the DOS.

g) Draw a sketch to the right of the 3 panels of the density of states, with frequency on the vertical axis and DOS on the horizontal, using the vertical scale of the panels to the left.

10. Consider crystals held together predominantly by metallic (M), covalent (C), and ionic (I) bonding.
a) Name a property that is largest for crystals with M and smallest for those with C bonding.

b) Name a property that is largest for crystals with M and smallest for those with I bonding.

c) For which can you estimate the cohesive energy without quantum mechanics?