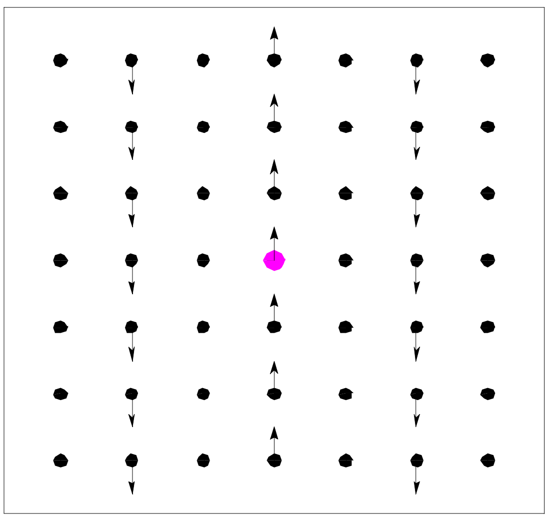
PHYSICS 731 Department of Physics, University of Maryland, College Park

Nov. 1, 2005 Name: ________________________________

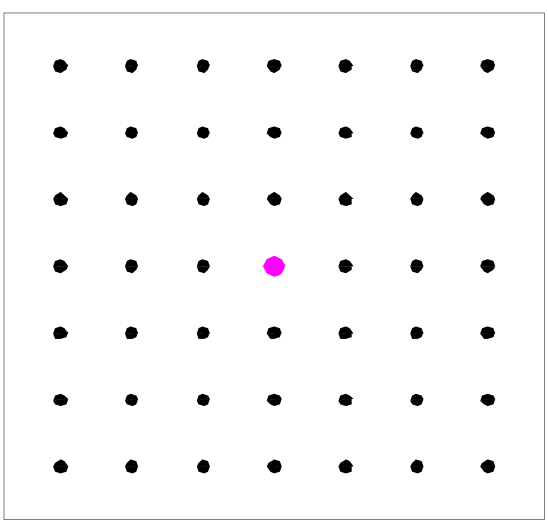
MIDTERM TEST

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

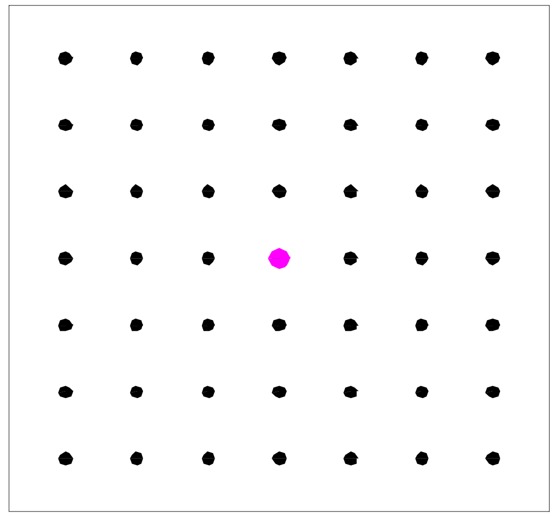
1.a) What is the 2D **k** associated with the depicted displacement pattern? (Assume a = 1 for simplicity.) Is the wave longitudinal or transverse? Acoustic or optical?



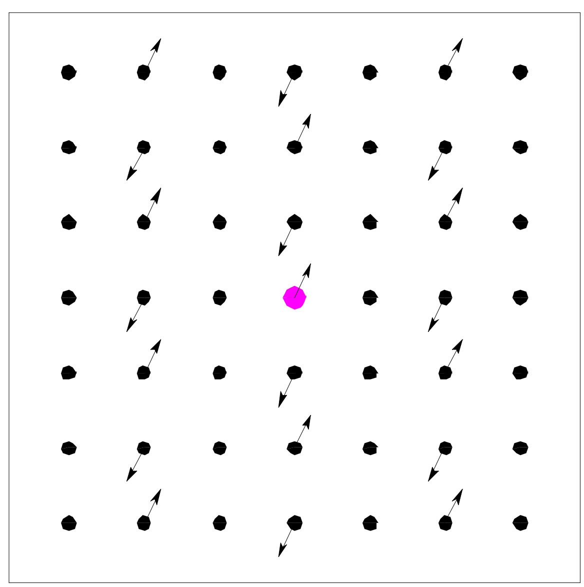
b) Redraw below the arrows [from part a)] for the other polarization. (L if part a is T, or T if part a is L)

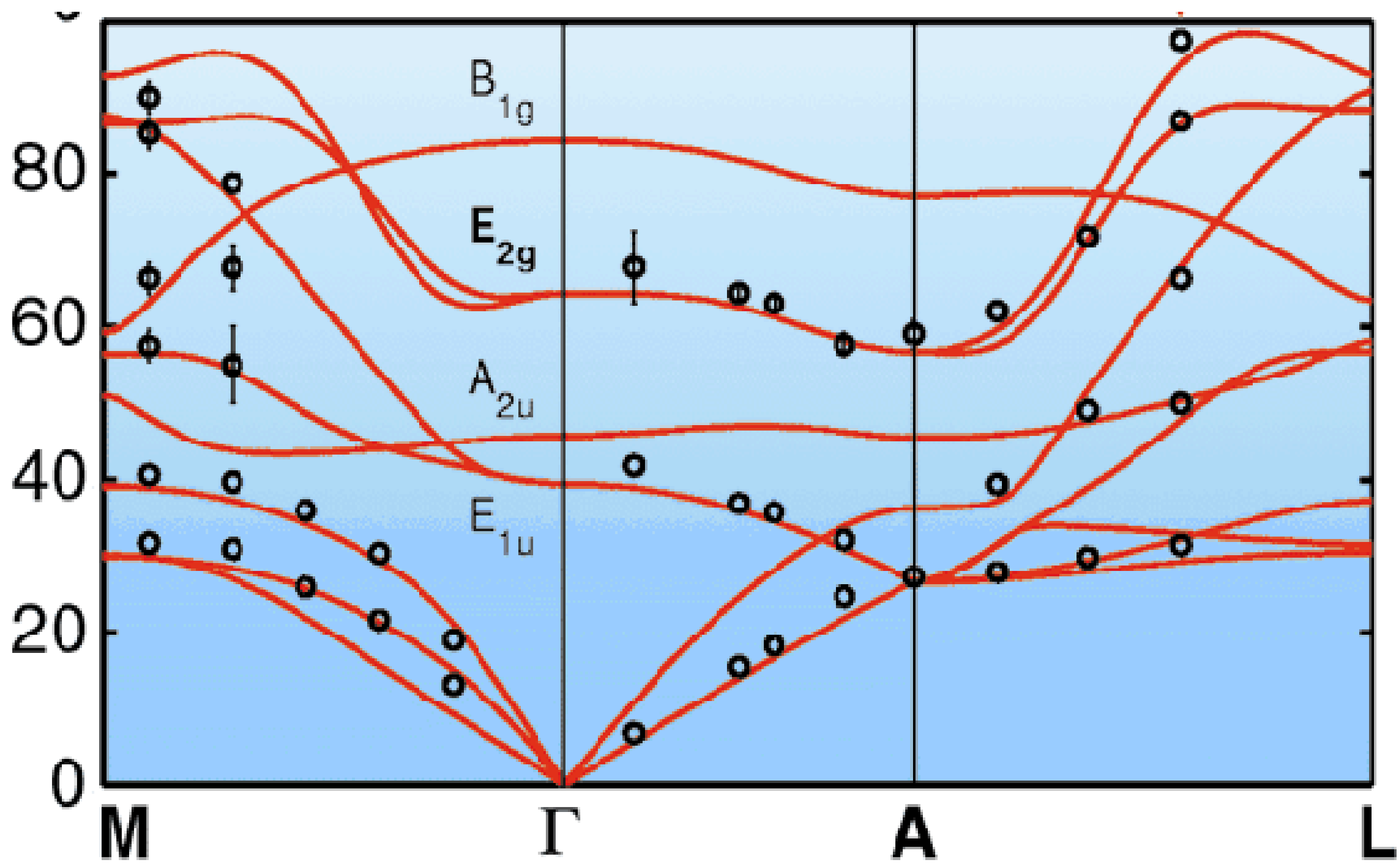


c) Redraw below the arrows [from part a)] at a time 1/4 period later.



d) What is the 2D **k** associated with the displacement pattern depicted below? Is it L-like or T-like?





2. This phonon dispersion relationcharacterizes a relatively new superconductor.

a) How many atoms are there per unit cell?

b) Which point (M, Γ, A, or L) is the center of the first Brillouin zone?

c) Label each band at Γ as A or O, and T or L.

d) Why are there fewer branches along ΓA than along ΓM or AL?

e) Label spots on the branches THAT ARE NOT AT ONE OF THE LETTERED HIGH-SYMMETRY POINTS at which there are Van Hove singularities in the DOS.

f) Which one of the branches is best approximated with the Einstein approximation?

g) Which one of the branches is best approximated with the Debye approximation?

h) Are the numbers on the vertical axis in units of Hz? Explain very briefly.

3. Circle those of the following 6 which vanish for a purely harmonic lattice:

Deviation of specific heat from Dulong-Petit law
Grüneisen constant
Umklapp processes
inverse of lattice thermal conductivity ($1/\kappa$)
thermal expansion of lattices
sound velocity

4. Consider a 1D chain of atoms (all the same element) at positions na and $(n + ¼)a$, for all integer n.

a) Circle the one of the following that correctly gives the reciprocal lattice vectors K_m: (all integers m)

$2\pi m/a$ $\quad$ $m\pi/a$ $\quad$ $m\pi/2a$ $\quad$ $m\pi/4a$

b) Which of the K_m are extinguished by the structure factor?

c) What is the ratio of the two intensities of the surviving spots (neglecting Debye-Waller)?

d) How (qualitatively) will the Debye-Waller factor change your answer to part c?

5. Consider crystals held together predominantly by metallic (M), covalent (C), and ionic (I) bonding.

a) Which is most likely to apply to a semiconductor

b) Which is likely to have the highest electrical conductivity?

c) For which is the Evjen method a useful concept?

d) For which can the cohesive energy be estimated using the uncertainty principle?

e) For which does the electron density become smallest between 2 atoms?

f) For which is the electron density most nearly uniform?

6. For each of the following non-Bravais crystals, indicate 1) the number of atoms in the [smallest possible] basis, 2) the underlying Bravais lattice associated with that basis, 3) for crystals containing different elements, the kind of crystal that would result if all the atoms were the same element:

a) Zincblende

b) Wurzite

c) NaCl

d) CsCl

e) Perovskite (skip part 3!)

7. In the following, consider stacking sequence and in-plane symmetry.

a) What is the difference between hcp and fcc crystal structure?

b) What is the difference between hcp and (3D) hexagonal crystal structure?

c) What is the difference between hcp and graphite crystal structure?

8. a) For a simple cubic lattice (with lattice constant *a*), what is the distance between {531} planes?

b) What is the area of a primitive cell in such planes?

9. Consider a nanotube having interior radius *R*. Suppose we pack atoms into it that can be approximated as spheres with the same radius *R*. What is the packing fraction?

10. Suppose the dispersion of an *optical* branch in 1D can be written $\omega(k) = \omega_0 - A(a)\cos(k\,a)$. Compute the Grüneisen parameter γ_k.

11. a) Show that $\int_0^\infty g(\omega)\hbar\omega\left(\frac{1}{e^{\hbar\omega/k_BT}-1}\right)d\omega$ has units of energy. What energy does it represent?

b) Show that its high temperature limit has the expected classical form (cf. 12.e, below).

c) In the low temperature limit why is it okay to replace the term in parentheses by $e^{-\hbar\omega/k_B T}$ in the Einstein model but not in general?

12. a) For free electrons (Sommerfeld model), the density of states (DOS) $g(\varepsilon)$ is proportional to ε^{α}; find (don't just write down) the value of α in 1D and 3D.

b) Write the value of $\int_0^{\varepsilon_F} g(\varepsilon)d\varepsilon$ (assuming 3D, n atoms per volume, a Bravais lattice, and valence Z).

c) Write the value of $\int_0^{\infty} g(\varepsilon)f(\varepsilon)d\varepsilon$.

d) Write the value of $\int_0^{\infty} g(\varepsilon)d\varepsilon$.

e) Write the value of $\int_0^{\infty} g(\omega)d\omega$ for phonons in this lattice (cf. 11.b).

f) What [unusual characteristic] do [the functional forms of] the DOS of the Einstein model and the DOS of the Drude model have in common?