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

Nov. 5, 2002 **Name: ________________________________**

MIDTERM TEST

Budget your time. Look at all 5 pages. Do the problems you find easiest first.

1. Consider a D-dimensional crystal with N primitive cells, each of volume v, p atoms per cell, Z valence electrons per atom.

a) How many distinct, independent values of **k** are there (assuming periodic boundary conditions)?

b i) How many phonon branches are there?

ii) How many of these branches are optical?

iii) In a high-symmetry direction, how many are longitudinal?

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

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

d) What is the density of electrons n ?

e) What is the ratio of k_F to k_D?

f) What is the ratio of T_F to Θ_D?

2. i) In a simple cubic lattice, what is the distance between a family of (8 5 3) planes?

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

3. For each of these give both the underlying Bravais symmetry *and* the number of atoms in the basis:

CsCl

zincblende (ZnS)

wurzite

graphite

perovskite

4. Which of the following lattices can be decomposed into 2 interpenetrating Bravais sublattices? For those for which you indicate *yes*, indicate the type of the Bravais sublattice. For those for which you say *no*, indicate the smallest number of Bravais sublattices needed to reproduce the [parent] lattice.

fcc

bcc

hcp

honeycomb (2D)

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

a) Which case has the largest angular variation in charge density about an atom (say at a distance 1/4 of the interatomic spacing from the atom)? (Answer M, C, or I to this and the following.)

b) For which are atoms most likely to have 4 nearest neighbors?

c) Which has a nearly uniform electron distribution?

d) Which is the best conductor of electricity and heat?

e) Which is most likely *not* to have optical branches in its phonon dispersion relations?

f) For which is the Madelung constant a relevant concept?

g) For which is the Drude model most appropriate?

h) Which is likely to have the smallest packing fraction?

6. In the Evjen method for the Madelung constant of a linear chain of alternating charges,

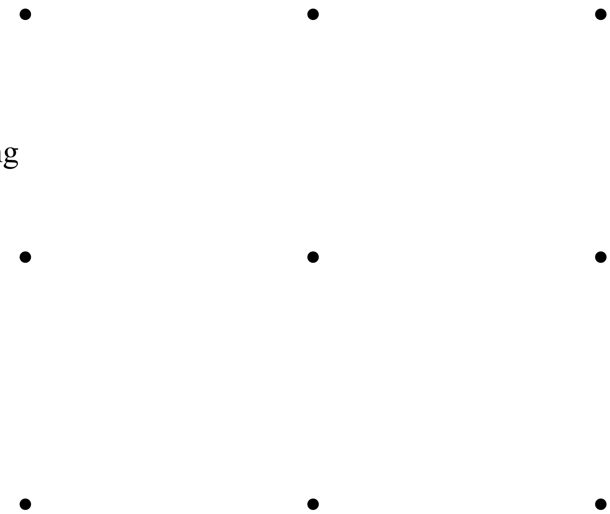
the first term is 1/2 1 2

and the second term is -1 -1/2 0 1/2 1 3/2 2.

(Circle the correct choice for each term.)

7. Consider a 1D chain of atoms of equal mass with an impurity atom of different mass at the origin. Write the ansatz for the displacements u(na,t) associated with a mode localized on the impurity.

8.a) On the square lattice of sites on the right, draw the displacement of the atoms indicated by dots, for a longitudinal phonon with **k** = (π/a) (1, 1).
b) Draw with a solid line an arrow indicating the direction of **k** and with dashed arrows any equivalent directions.
c) What does this indicate about the relation between ω_{LA} and ω_{TA} at this **k**?



d) Indicate the group velocity at this **k**.

9. Consider the phonon dispersion relation on the right.

a) Label each branch as TA, LA, TO, LO as appropriate.

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

c) Why are there more branches along the ΓK direction than along ΓX or ΓL?

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

e) For a comparable crystal but with element(s) having double the mass, what is the primary change you would expect in this graph?

10. In the Debye model in 3D, a) write the energy contribution u(ω) to the internal energy $\int d\omega\, u(\omega)$.
[Do not spend time deriving prefactors that are not on your formula sheet!]

b) Sketch u(ω) vs. ω, and *specify the ω dependence* at small and at large ω [relative to $k_B T/\hbar$].

11. Consider lattice thermal conductivity of a material. We showed that $\kappa = (1/3)\ c\ c_V\ \ell$.

a) Describe the temperature dependence of κ at high T.

b) In 2D, what fraction replaces 1/3?

c) How does the temperature dependence in 2D compare with that in 3D at low T?

12. In neutron scattering, consider the *emission* of a single phonon.

a) Write down the appropriate conservation equations.

b) The sketch at the right is from the text for absorption with the solid approximated by a [1D Bravais] chain. Produce an analogous graph for emission, either by appropriately [re]labeling the axes or by redoing the sketch on the back in a way you find more appealing (with careful labeling of the axes).

c) Why are such sketches not used for electron or photon scattering?

13. Draw lines between items in the lef and the right columns to indicate the best match .

Soft phonon	materials with positive charge carriers
Layered structure	thermal expansion
Stokes and anti-Stokes peaks	cuprate high-temperature superconductor
De Boer parameter	Wiedemann-Franz law for metals
Positive Hall coefficient	Raman scattering
Loschmidt number	importance of zero-point motion van der Waals solid
Grüneisen parameter	ferroelectric instability

Circle any of the [last 4] items in the left column that are dimensionless.

14. For a free electron gas in 3D we showed that the average energy (E/N) in the ground state (i.e. at T=0) is $(3/5)\varepsilon_F$ and the pressure $P = -(\partial E/\partial V)_N$ is (2/3) E/V. For such a gas in 1D,

a) what is the proportionality constant for the average energy (as compared to 3/5) ?

b) what is the proportionality constant for the "pressure" $-(\partial E/\partial L)_N$ (as compared to 2/3) ?

15. What is $\int d^3k \, (df/dT)$, where f is the Fermi distribution function for electrons? (Justify your answer to this quick result, used in homework.)

16. a) Using the density of states $g(\varepsilon)$ and the Fermi distribution function, write expressions for <u>i)</u> the internal energy and <u>ii)</u> the entropy of a Fermi gas (as integrals over ε).

b) What does the Sommerfeld expansion reveal about the T dependence of the electronic specific heat <u>i)</u> in 3D? <u>ii)</u> in 1D?

Do NOT work on this problem before you have completed and checked over the rest of the test!!

BONUS: Consider a 2D Bravais lattice having centered rectangular symmetry. What is the minimum ratio of the longer to the shorter lengths b/a of the sides of the rectangle such that the Wigner Seitz cell has only 4 sides?