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

Nov. 5, 1998 **Name: ___________________________________**

MIDTERM TEST

1. Consider a family of square-lattice planes with $\mathbf{a_1}$ = d (1, 0, 0) and $\mathbf{a_2}$ = d (0, 1, 0).

a) Find $\mathbf{a_3}$ such that this is an fcc crystal.

b) Find $\mathbf{a_3}$ such that this is a bcc crystal.

c) Find $\mathbf{b_3}$ for one case, indicating clearly whether you have picked the fcc or bcc direct lattice.

d) Verify explicitly that this $\mathbf{b_3}$ gives the correct interplanar spacing (in the $\hat{\mathbf{z}}$ direction).

2. Consider the phonon dispersion relations $\omega_1(k) = A \sin(ka/2)$ and $\omega_2(k) = \omega_0 - B \cos(ka)$, where A and B are positive constants with $\omega_0 > A + B$, $A >> B$, for a chain of N pairs of lighter and heavier atoms (in one dimension, with periodic boundary conditions).

a) i) Which branch corresponds to the acoustic modes? Draw as sketch of displacements for $k \to 0$.

ii) What name is given to the other branch? Explain why.

b) Determine the "critical" values ω_c of ω for which there are Van Hove singularities in the phonon density of states.

c) What is the exponent α associated with this singularity (where $g(\omega) \propto |\omega_c - \omega|^\alpha$)?

d) What would be required [though unphysical!] for $g(\omega)$ to go to 0 continuously in 1D?

e) What is $\int g(\omega)\, d\omega$? (Do NOT compute this explicitly; use your knowledge of what this means.) What fraction of this integral is due to the acoustic branch?

f) Based on your answers to the above questions, draw a sketch of $g(\omega)$ vs. ω.

or f') At low temperature T find the power of T with which $\langle \omega^2 \rangle_T$ varies. (Note that this amounts to the Debye approximation at low T.)

3. In STM (scanning tunneling microscopy) experiments, one actually measures electronic density rather than atomic positions. In some materials, one sees phantom atoms: the seeming presence of a non-existent atom between two actual atoms. Is the bonding in this case primarily covalent, ionic, metallic, or van der Waals? Explain briefly.

4. Consider circles of two different radii $r^>$ and $r^<$, arranged in a checkerboard pattern.
a) Solve for the critical ratio $r^>/r^<$. To what face of what ionic crystal structure is this analogous?

b) Suppose the circles are replaced by two different sizes of regular [sides of equal length] octagons (oriented along the symmetry axes). Define $r^>$ and $r^<$ as the distances from the centers to the midpoint of an edge. i) Does the critical ratio increase, decrease, or stay the same? ii) Does the packing fraction at the critical ratio increase, decrease, or stay the same? In both cases, justify your answer.

or b') Can a regular octagon ever be the Wigner Seitz cell of a 2D Bravais lattice? Explain. (What is the largest number of sides a regular polygon can have and still be the Wigner-Seitz cell of a 2D Bravais lattice?)

5. What property of x-rays and thermal neutrons is comparable in size?

6. What two excitations are coupled to form a polariton?

7. Place the letter representing the best match in the blank in front of each of the following statements about lattice properties:

___	Reason why in phonon dispersion $\omega(-k) = \omega(k)$.	a. Finite size of real systems
___	In a scattering process, wavevector is conserved only up to a reciprocal lattice vector [$k' = k + K$]	b. Harmonic approximation of lattice vibrations
___	As $k \to 0$ there is a branch with $\omega \propto k$.	c. Equipartition of energy
___	Thermal conductivity does not diverge as $T \to 0$.	d. Lattice-translation invariance/
___	High-temperature lattice specific heat is independent of T.	e. Inversion symmetry
___	Property of all Bravais lattices but not all lattices with bases.	f. Time-reversal symmetry

8. In homework you used the equation $\overleftrightarrow{\mathbf{D}}(\vec{\mathbf{k}}) = \sum_{\vec{\mathbf{R}}} \sin^2(\tfrac{1}{2}\vec{\mathbf{k}}\cdot\vec{\mathbf{R}})[A\overleftrightarrow{\mathbf{1}} + B\hat{\mathbf{R}}\hat{\mathbf{R}}]$, with $A = 2\phi'(d)/d$ and $B = 2[\phi''(d) - \phi'(d)/d]$. Verify explicitly that for a 1D Bravais chain with only nearest-neighbor interactions, this equation produces the result $\omega(k) = 2\sqrt{K/M}\;|\sin(ka/2)|$.

Show that for a Bravais lattice the dynamic matrix can be written as

$$D(\vec{k}) = -2\sum_{\vec{R}} \overleftrightarrow{D}(\vec{R})\sin^2(\tfrac{1}{2}\vec{k}\cdot\vec{R})$$