Department of Physics, University of Maryland, College Park

Dec. 17, 2004 **Physics 731: FINAL EXAM** ***Name:*** _____

Easy and hard problems are intermixed; don't get bogged down. You are allowed a personally-prepared sheet of formulas, front side from midterm, back side new.

1. Consider a D-dimensional crystal with volume V, N_c primitive cells, N_a identical atoms, and N_e valence electrons.

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

b) i) What is the volume (in reciprocal space) of the 6^{th} Brillouin zone?

ii) With which other Brillouin zones does it share a bounding plane?

c) What is the number of transverse optical modes?

d) What is the density of electrons?

e) If the material is an insulator or semiconductor, circle the one ratio of these that must be even.

N_e / N_c N_a / N_c N_e / N_a N_c / N_a N_a / N_e N_c / N_e

f) Minimum number of filled or partially filled bands if all electron spins are alligned in the same direction.

2. a) The boundary of the Brillouin zone of an fcc crystal is composed of hexagons and squares. How many hexagons are there? How many squares? Present an argument for how to get these two numbers.

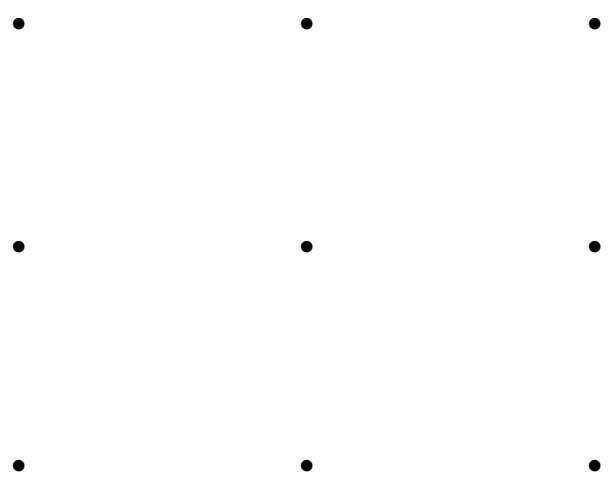
b) On the boundary of the Brillouin zone of graphite, how many hexagons are there? How many rectangles?

c) Why are the boundaries of Brillouin zones composed of planar pieces rather than curved (bowed) ones?

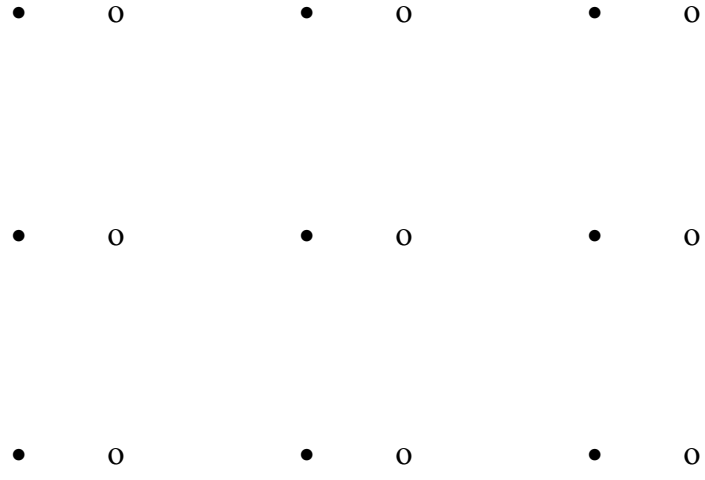
3. For each experimental probe in the left column, mark the letter from the right column that best describes its use. Also mark with E those that rely fundamentally on electric fields and B those that rely fundamentally on magnetic fields.

STM	F. Electronic structure
Photoemission	G. Surface atomic structure
Neutron scattering	H. Surface atomic and electronic structure
X-ray diffraction	J. Fermi surface structure
EXAFS	K. Bulk crystal structure
LEED	L. Surface crystal structure
FIM	M. Lattice vibrations
de Haas van Alphen	N. Near-neighbor atomic spacings

4a.i) On the square lattice of sites on the right, draw the displacement of the atoms indicated by dots, for a longitudinal phonon with $\mathbf{k} = (\pi/a)\ (1/2, 1/2)$.
ii) Why do I not need to specify that the phonon is acoustic?



b.On the 2-site basis square lattice on the right, draw the displacement of the two kinds of atoms for a transverse optical phonon with $\mathbf{k} = (\pi/a)\ (1, 0)$.



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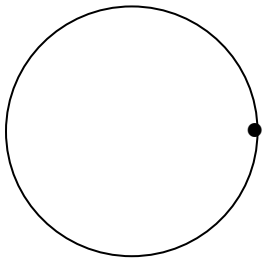
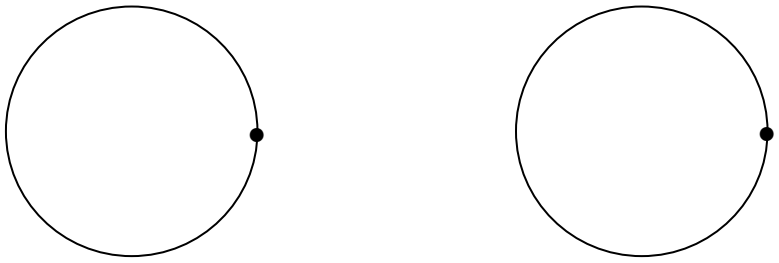
5. The circle below represents the cross-section of a Fermi surface in a plane perpendicular to a constant magnetic field **B**, which points out of this sheet of paper. The dot represents the position of an electron at some instant.



Assume first that the area inside the circle corresponds to filled states (and those outside correspond to empty.) Draw a *dashed* arrow from the dot indicating the direction of the electron velocity. Draw a solid arrow indicating the direction of d**k**/dt. Draw a dotted arrow showing the direction of the acceleration.

Now do the same below for the case when the filled states lie outside the circle. On the left circle, draw the 3 arrows appropriate for hole quantities (those with subscript h); on the right circle, draw the 3 arrows for the $\mathbf{k}_e$ of a missing electron

HOLE



6. Consider an electron gas (Sommerfeld model) in a uniform constant magnetic field H.

a) Find the value of H (in terms of k_F) so that the 5^{th} Landau level lies just outside the Fermi sphere.

b) For this value of H, write an expression for the ratio of the occupation of the 4^{th} level to the lowest level.

7. Suppose that the effective mass tensor is diagonal but that $M_{zz} = 2\ M_{xx} = 2\ M_{yy}$

a) What is the ratio of the cyclotron mass for an H field in the z direction compared to that with H in the x direction?

b) What is the ratio of the cyclotron mass for an H field in the z direction compared to the specific heat effective mass?

c) Assume in the following that the electron effective mass is isotropic, so scalar. Indicate the dependence of each of the following on it:

i) Density of states g(ε) (Sommerfeld model)

ii) Period for an electron going around an orbit in a constant H field.

iii) Size of a band gap in the nearly-free electron model.

iv) Phonon dispersion curves (be careful!)

v) Total kinetic energy (Sommerfeld model)

8. For each item in the left column, find the best match from the right column:

____Elemental (single-element) hcp but not fcc	a) Has 2 different elements
____Graphene but not graphite	b) Has a filled *d*-band
____Copper but not sodium	c) Has close-packed layers
____Diamond but not graphite	d) Has sp^3 hybrid orbitals
____Zincblende but not diamond	e) Must have optical phonons
	f) Has a reciprocal lattice consisting of rods
	g) Has only longitudinal phonons

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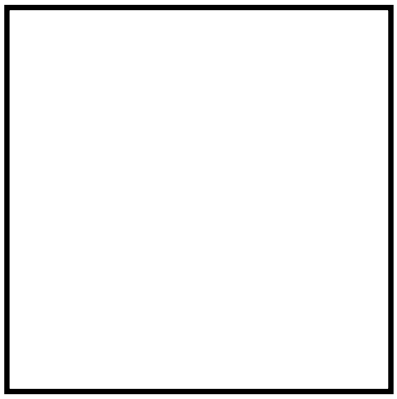
9. Recall that a nearest-neighbor tight-binding model (with no overlap) for a square lattice, lattice constant a, can be written $\varepsilon(\mathbf{k}) = -2\gamma\,(\cos k_x a + \cos k_y a)$.

a) On a plot of the first Brillouin zone, draw the contour corresponding to $\varepsilon(\mathbf{k}) = 0$.



b) Suppose this lattice sheet is wrapped into itself seamlessly along the *y* direction so that the resulting cylinder (pointing along *x*) has the following allowed distinct values of k_y : 0, $\pi/2a$, $-\pi/2a$, π/a. What is the circumference of the tube (i.e. what is the repeat distance in the *y* direction)?

c) Plot $\varepsilon(k_x)$, indicating which (if any) bands are degenerate. On the plot above of the first Brillouin zone, indicate where $\varepsilon(\mathbf{k}) = 0$.

d) Work out the density of states of a 1 D tight-binding model, $\varepsilon(k_x) = -2\gamma \cos k_x a$.

e) Use your result from part d) to sketch the density of states of this wrapped system.

f) Suppose there is an additional electronic state, energy ε_{imp} due to an impurity. What inequalities must ε_{imp} satisfy so as to be localized like a surface state? (What is the physical condition needed?)

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10. a) Show as in homework that $\chi(q)$ of the Lindhard dielectric function in 1D at T=0 has a logarithmic divergence at $q = 2\ k_F$. (Full credit for all the prefactors of $\chi(q)$.)

b) Suppose an electric field acts for time τ so that the whole occupied distribution moves, so that its center of shifts from $k = 0$ to $k = -eE\tau/\hbar$. How does your answer change?

11. For each of the following, indicate whether they are A) positive, B) negative, C) zero, D) undetermined sign and (if not choice C!) are proportional to E) k_F^2, F) k_F, or G) some more complicated expression.

Kinetic energy [Slater] per electron

Exchange energy per electron

Correlation energy per electron

Electron-electron interaction + electron- jellium interaction

Electron-electron interaction + electron- positive-ion background interaction

Workfunction of metal surface

12. a) llustrative DFT calculations are typically presented for $r_s = 2$ and $r_s = 5$. Which corresponds to Na and which to Al? Which would be more likely to describe Cu well?

b) Why is it problematic to try to calculate the gap energy of a semiconductor (so the smallest difference in energy between the highest occupied and lowest unoccupied bands) using Hohenberg-Kohn-Sham theory?

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