Department of Physics, University of Maryland, College Park

Dec. 16, 2002 **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.

I. 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) What is the volume (in reciprocal space) of the n^{th} Brillouin zone?

c) What is the ratio of the number of occupied **k** modes for electrons (at T=0) to the number of transverse acoustic modes?

d) What is the density of electrons?

e) If the material is an insulator or semiconductor, circle which of these must be even. (Justify your choice!)

$Z \qquad p \qquad D \qquad pZ \qquad pZD$

2. In general electron or phonon dispersion relations can be written as $\varepsilon(\mathbf{k})$ [or $\hbar\omega(\mathbf{k})$] = **const** + **coef** $k^{\mathbf{x}}$ for small $k = |\mathbf{k}|$. In each case specify the values (or the signs in cases where you have no information about the value) of the three parameters **const**, **coef**, and **x**.

a) acoustic phonon

b) optical phonon

c) plasmon

d) magnon

e) electron in electron gas (jellium) in Hartree-Fock (use $F(k/k_F)$)

f) electronic band in tight-binding approximation

g) electron in 3rd band in 1-D nearly-free-electron approximation

3. 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 2D,

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

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

4. Suppose a 1-D band can be described by the tight-binding dispersion relation $\varepsilon(k) = \varepsilon_0 - 2\gamma \cos(ka)$, $\gamma > 0$.

a) For what values of ε are there Van Hove singularities?

b) If the effective mass m^* at the bottom of this band is *three* times the bare electron mass m_e, express γ in terms of m_e and other fundamental constants.

5. Circle all of the following which change sign when the subscript e becomes h (for holes):

k_e $\quad \dot{k}_e$ $\quad \varepsilon_e$ $\quad v_e$ $\quad \dot{v}_e$ $\quad m_e$ $\quad q_e$

6. a) i) In k-space, for free electrons, what is the *ratio* of the radii of the cylinders representing the second and the first (n=0) Landau levels? ii) What can be said about the corresponding the orbitals in real space?

b) Find the strength of the magnetic field H such that the ratio of the occupation of the first Landau level to that of the second level is 4/3. [As usual, neglect electron spin.]

c) At this value of H, what is the highest Landau level that is occupied [near the equator or belly of the free-electron sphere, if the axis is in the direction of H]?

d) Draw a sketch of the density of states.

7. Consider the 5 lettered orbitals in the figure:

a) Which is/are open?

b) Which is/are hole-like?

c) i) Which cannot be seen in a deHaas vanAlphen experiment?

ii) Give the reason why not for each choice.

iii) For those that *can* be seen, indicate for which there will be beats associated with their oscillations.

d) To perform the deHaas vanAlphen or related experiments, the H field should be in some "intermediate" range of strength. What becomes problematic if the H field becomes i) too strong and ii) too weak?

8. In homework you found the effective mass for the electron gas in the Hartree-Fock approximation at **k** = 0.

a) Sketch how you did this.

b) In Hartree-Fock, what is the electron speed |**v**(**k**)|? [You may express your answer using F(x).] Draw a graph of it (vs. *k*) and include a dotted line of |**v**(**k**)| for the usual (i.e. Hartree) free-electron velocity.

c) What (qualitatively) happens to the effective mass as *k* increases (compared to the value at **k** = 0?

9. For Al, we argued in homework that the pseudopotential could be written $U(\mathbf{q}) = -U_0/(q^2 + \kappa^2)$.

a) In the <100> direction, write the sizes of the first two band gaps in the nearly-free electron approximation. It is easiest to express your answer in terms of k_X.

b) i) What is the source/origin of κ? ii) For Na, do you expect κ to be larger or smaller (or the same) than for Al? By what about what ratio? (Explain your reasoning.)

10. Explain why the Drude model is a better approximation for a (free-electron like) metals than for an electron gas described by Maxwell-Boltzmann statistics (as in a semiconductor). To what in the metal do the values of electron speed c, mass m, and relaxation time τ correspond?

11. a) What assumptions are made in writing the Boltzmann equation?

b) Which, if any, are not used for the relaxation-time approximation?

c) Which, if any, additional assumptions are used for the relaxation-time approximation?

12. a) How can one tell from the specific heat if the Fermi energy lies in an energy gap?

b) Why is a gap necessary for a surface state?

c) Since both insulators and semiconductors have their Fermi energy in an electron-energy gap at T=0, what is the difference between them?

13. a) For what values of b_n does $\psi(x) = \Sigma_n b_n\phi(x - na)$ satisfy the Bloch criterion of Bloch's theorem?

b) If $H = H_0 - e\mathbf{E}\cdot\mathbf{r}$, H_0 a periodic electron potential, find $[T_\mathbf{R}, H]$, i.e. the commutator of H with the translation operator $T_\mathbf{R}$.

14. For each item below, pick the best match (capital letter) from the list of 5 at the right.

a) Is neglected in Hartree-Fock

b) Exactly cancel for jellium (2 letters)

c) Would be most affected if muons replaced electrons

d) Would be reduced by the greatest percentage if the electron gas were fully polarized (spins all aligned).

e) Is often well approximated by a term proportional to (electron density)$^{2/3}$

f) Is often well approximated by a term proportional to (electron density)$^{1/3}$

A. Kinetic energy

B. Electron-electron interaction

C. Electrostatic energy of attraction to positive background

D. Exchange interaction

E. Correlation

15. a) In photoemission, do you expect the bulk density of states to be best reproduced in the emitted spectrum if the final electron energy is about 10 eV, 70 eV, or 400 eV? Explain briefly.

b) In photoemission, do you expect the *surface* density of states to be best reproduced in the emitted spectrum if the final electron energy is about 10 eV, 70 eV, or 400 eV? Explain briefly.

Do these only after completing the rest of the exam and checking it over.

Give an example of an application of simple harmonic oscillators that we did not then discuss in terms of a Bose-Einstein distribution.

Suppose a positron is created in a solid and emerges to the vacuum. How is it affected by the various contributions to the work function? Should its mean free path be similar to that of an electron as given in the universal curve? (Why?)