Exam, Physics 155

Tuesday, March 02, 2010

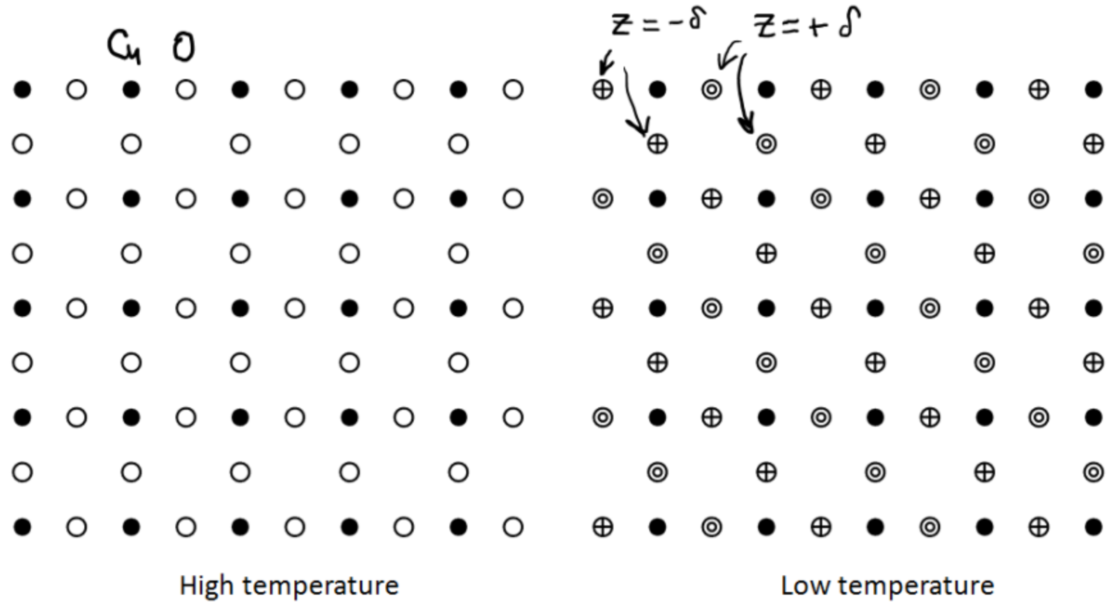
You can ask me if you need to use a calculator but do not have one.

1. [40 points; 30 points for acef, 10 points for bd] Consider a one dimensional crystal with the lattice constant a. Assume that the basis consists of only one atom, and that there is one valence electron per unit cell. This would be a model of a one dimensional H crystal.
   a. Use either the nearly free electron theory with a small potential $U_{G=2\pi/a}$ or the tight binding theory with a small hopping amplitude $t = -\langle s|H|s \pm 1\rangle$ to <u>derive and sketch</u> the energy dispersion of the lowest energy band. You should clearly mark the position and value of the wave vector corresponding to the boundary of the first Brillouin zone. You should clearly note how $U_{G=2\pi/a}$ or $t = -\langle s|H|s \pm 1\rangle$ affects the energy dispersion. For the tight binding band, you can assume, as non-zero matrix elements in addition to t, $\langle s|s'\rangle = \delta_{ss'}$ and $\langle s|H|s\rangle = \varepsilon_0 - \alpha$.
   b. What would be the electrical conduction property? Namely, would the material be a metal or a insulator? Explain. [You should give your answer without considering the electron-electron interaction first, should you wish to include the electron-electron interaction in this discussion.]
   c. Assume a harmonic potential between nearest neighbors to <u>derive and sketch</u> the phonon dispersion relation. Assume ion mass M and spring constant C.
   d. Assume $T \ll T_F, \theta_D$. In the temperature dependence of the heat capacity, would it be possible to separate out the electron contribution and the phonon contribution? Explain briefly. You do not need to derive the temperature dependence [especially for the electron part].
   e. Suppose that below a certain low temperature, the material goes into a phase with a "dimerization" in the sense that the uniform lattice constant a becomes alternating a_1 and a_2, with one longer than the other. The new lattice constant is $a_1 + a_2 = 2a$. Let us call this low temperature phase a "dimer phase." Would the material be a metal or an insulator in the dimer phase? Explain your answer using the qualitative behaviors of the electron energy band, including a sketch of the band dispersion as in (a).
   f. In the dimer phase, corresponding to the alternating lattice constants, a_1 and a_2, the spring constant also alternates as C_1 and C_2. <u>Derive and sketch</u> the phonon dispersion relation in the new phase. Label the acoustical branch and the optical branch.

Choose and do only one of 2 and 3. [10 points]

2. An fcc metal goes through a phase transition into a bcc metal. In either structure, the primitive unit cell consists of only one metal atom. Let us assume that the volume change between the two phases is so small that we can ignore it. What is the fractional change in the nearest neighbor distance?

3. The $\mathrm{CuO_2}$ plane of the high temperature superconductor $\mathrm{La_2CuO_4}$ has the following crystal structure at high temperature and at low temperature. In the low temperature phase, some oxygen atoms displace up slightly relative to the $\mathrm{CuO_2}$ plane, and some oxygen atoms displace down slightly, as noted in the figure. In each case, identify the primitive Bravais lattice and the primitive basis.



Choose and do only two problems from 4-7. [20 points * 2]

4. In X-ray diffraction off of a one dimensional crystal, how does the maximum intensity and the width of the line profile (intensity vs. k) scale as a function of the number of atoms in the crystal? Explain it by examining the sum $\sum_s e^{-iksa}$.

5. Consider a piece of metal (e.g. a Na crystal) at $T = 0$. You apply pressure to reduce its volume by one percent. How much does the Fermi energy change (include the sign)? How much does the total electronic energy change? Answer both questions in terms of the percentage change.

6. Consider a two dimensional square lattice with one atom per unit cell.

Suppose there are two valence electrons per unit cell. Clearly explain why the area of the Fermi surface within the free electron model is equal to the area of the first Brillouin zone. Discuss the Fermi surface (FS) formation (their rough shape and the connectivity) within the *nearly* free electron model. Identify electron pocket FSs and hole pocket FSs. Explain how you identified them (i.e. what is the definition of an electron pocket or a hole pocket and how did you apply the definition)?

7. The lattice specific heat of a certain form of carbon shows a temperature dependence T^2 instead of the usual T^3 dependence in the low temperature limit. What can you infer about the structure of this form of carbon? The [short or long] derivation of the temperature dependence is required here [different from part (d) of the first problem].

Choose and do only three problems from 8 through 12. [5 points * 3]

8. What are the physical effects that can be explained only by going beyond the harmonic approximation in the theory of phonons? List two such effects and explain qualitatively why those necessitate going beyond the harmonic approximation.

9. What is the definition of a metal? What is the definition of an insulator? The answer may not be unique, but you should give a clear answer from what we covered in class, in terms of the band structure.

10. What is the definition of an acoustical phonon? What about an optical phonon? Which one corresponds to the uniform translation of all atoms in the unit cell when viewed locally (i.e. length scale much less than the wave length)? [The "uniform translation" should not be part of any definition.]

11. What is an Umklapp scattering and why is it important? Take an example to explain it. For instance, you can explain it using a scattering process in which there are two phonons in the initial state and one phonon in the final state.

12. What is the most interesting and intriguing science fact that you learned in this class? State it and explain it.