Phys 155, Winter 2007, Homework 3, due 5pm, Feb 12

(Each problem is 4 points. For problems from the textbook, please note that solutions are included in the textbook. However, use those solutions simply as guide, if necessary. If you do, your answers should show enough details that reflect your own understanding.)

1. *Electrons at surface*
   Problem 3.1 of H&H

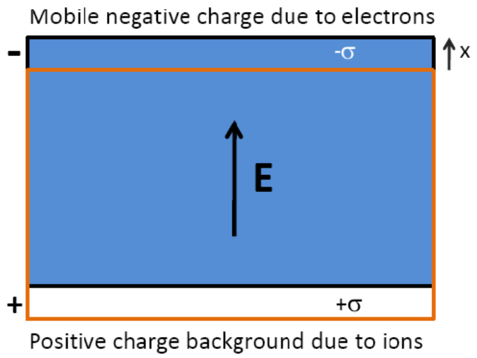
2. *Heat capacity at constant pressure*
   You may recall that the heat capacity measured in laboratory is usually the heat capacity at constant pressure but *not* the heat capacity at constant volume. You may also recall that $C = \frac{\partial E}{\partial T}$ is actually the latter, which is why at some point a subscript V in C_V was sneaked in the lecture note. As you know that in gas (recall ideal gas theory) C_V and C_P are so different from each other, you may wonder how C_V and C_P compare with each other in solids. This problem will clarify this point.
   (a) Consider non-interacting particles. Their statistics need not be specified until (c,d). Assume that the energy ϵ_q (here, q is used as a symbol for all quantum numbers specifying the energy level) of the particle depends on volume as a power law $\epsilon_q \propto V^{-\gamma}$ (e.g. $\gamma = \frac{2}{3}$ for free electron in 3D). Generally, the total energy can be expressed as $E = E_B(V) + E_D(T, V)$, where E_B is the *temperature-independent* but volume dependent energy of the "background," e.g. the potential energy of the static lattice (E_{pot} on slide 16 of Lecture 4), and E_D is the "dynamic" part due to ϵ_q's of our quantum particles. Show that $P = P_B(V) + \gamma E_D/V$, where $P_B = -\partial E_B/\partial V$.
   (b) [Note that in this problem, β means the thermal expansion coefficient, not inverse temperature] Using this result and the equations (7,8) of the note, "00 - Cp and Cv.pdf," show that $\frac{C_P}{C_V} = 1 + \delta$, where $\delta = T\gamma\beta = \frac{T\gamma^2 C_V}{VB}$. Estimate the magnitude of δ for $T = 100\ K$, $\gamma \sim 1$ (typical), and $\beta \sim 3 \times 10^{-4}/K$ (about the maximum from 0 to room temperature).
   (c) Show that for the free electron model $\delta \approx \frac{\pi^2}{3}\left(\frac{T}{T_F}\right)^2$ in the low temperature limit. [It is ok just to show the T^2 behavior]
   (d) Show that, in the low temperature limit of the Debye model, δ vanishes as T^4.

3. *AC conductivity, light propagation, and plasmon, a collective mode of electrons*
   (a) Assuming that $v_d = \tilde{v}_d(\omega)\exp(-i\omega t)$ and $E = \tilde{E}(\omega)\exp(-i\omega t)$, (we will neglect the spatial variation of the wave, assuming a long wavelength $\lambda \gg l$, l is mean free path) show by solving this equation $m\left[\frac{dv_d}{dt} + \frac{v_d}{\tau}\right] = -eE$ (note the correctness of sign here as opposed to the neglected sign in lecture) that the AC conductivity can be written as $\sigma(\omega) = \sigma_D/(1 - i\omega\tau)$, where σ_D is the DC Drude conductivity that we discussed in class.

(b) Recall that the complex dielectric constant $\epsilon(\omega)$ is given by (in the cgs unit) $\epsilon(\omega) = 1 + \frac{4\pi i\sigma}{\omega}$. In the limit $\omega\tau \gg 1$, show that $\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$, where ω_p is the plasma frequency given by $\omega_p^2 = \frac{4\pi n e^2}{m}$ (n is the electron number density). Plot the dispersion relation of light in vacuum and in medium with this dielectric constant. Sketch the reflectivity (for normal incident light) $R(\omega) = \frac{(m-1)^2+\kappa^2}{(m+1)^2+\kappa^2}$, where $m + i\kappa \equiv sqrt(\epsilon(\omega))$, as a function of ω near ω_p, by evaluating $R(\omega)$ for $\omega < \omega_p, \omega = 1.1\omega_p, \omega = 1.2\omega_p, \omega = \infty$. Indicate the plasma edge of the reflectivity.

(c) At room temperature, Na metal is a bcc crystal with a = 4.29 Å. Its electron density is determined by one free electron contributed per Na. Express the plasma frequency ω_p in eV. Given the room temperature data in page 89 of H&H, $\tau \sim 2.6 \times 10^{-14}$ s, show that the assumption of (b), $\omega\tau \gg 1$, is indeed satisfied. What are the wave lengths of light with this plasma frequency, in vacuum and in Na metal?

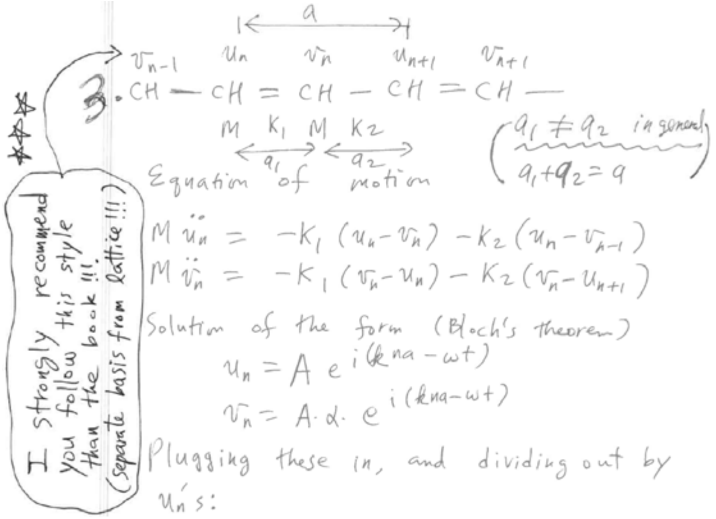
(d) Consider a macroscopic piece of metal, such as Na. For long wavelength phenomena, we can model it as consisting of uniform positive charge density consisting of metal ions and uniform negative charge density consisting of electrons. The two charge densities cancel each other, ensuring that the whole crystal is neutral. Let's assume that the two charge densities are un-deformable rectangular block, and also let's assume that the positive charge block is fixed in space, while the negative charge block is movable. Consider a small displacement x of the negative charge density in one direction, as shown in the figure with a great exaggeration of the amount x just to make the point clear. The result is a development of two surface charge layers, $+\sigma$ and $-\sigma$, (don't confuse these symbols with the conductivity symbol above, despite the unfortunate same notation used here and in the literature). Applying Gauss law $\mathbf{\nabla} \cdot \mathbf{E} = 4\pi\rho$, ($\rho$ is the volume charge density) set up the equation of motion for the negative charge block as a whole, and show that its frequency of oscillation is exactly the plasma frequency given in (b).



4. *Bloch's theorem and phonon*

Show that the "wave functions" that were used in solving the classical coupled oscillator problem do indeed satisfy Bloch's theorem. Identify and write explicitly the function $u_{\mathbf{k}}(\mathbf{x})$ for mon-atomic wave function, (2.8) of H&H, and di-atomic wave function, (2.17) of H&H (by which

I mean <u>two</u> expressions including the displacement for mass M as well as the displacement for mass m). (Note added: in fact, in place of (2.17) I would much prefer the following style, using u and v with the same integer index n.)



3. CH — CH = CH — CH = CH —

$\left(\begin{array}{l} \underbrace{a_1 \neq a_2 \text{ in general}} \\ a_1 + a_2 = a \end{array}\right)$

Equation of motion

$$M \ddot{u}_n = -K_1 (u_n - v_n) - K_2 (u_n - v_{n-1})$$
$$M \ddot{v}_n = -K_1 (v_n - u_n) - K_2 (v_n - u_{n+1})$$

Solution of the form (Bloch's theorem)

$$u_n = A e^{i(kna - \omega t)}$$
$$v_n = A \cdot \alpha \cdot e^{i(kna - \omega t)}$$

Plugging these in, and dividing out by u_n's:

I strongly recommend you follow this style than the book !!! (Separate basis from lattice !!!)

5. *Divalent metal in 2 dimensions in nearly free electron approximation*

This problem is related to Figure 4.5 (a) of H&H. Also, Figure 13.1 and its discussions may be helpful.

Consider a 2 dimensional simple square crystal with a divalent atom per unit square. I.e., there are two valence electrons contributed by each atom that occupies a square of dimensions a x a.

(a) In the free electron approximation, what is the Fermi momentum k_F. In particular, show that $k_F > \pi/a$, $1.1\ \pi/a$, and $k_F < \sqrt{2}\ \pi/a$.

(b) Draw the reciprocal lattice, including your origin of choice, nearest neighbor lattice points, and next nearest neighbor lattice points. Draw Brillouin zones (BZ's) that correspond to each lattice point that you included. Then, draw in the Fermi surface in the free electron approximation. Do this in the repeated zone scheme, i.e., draw all Fermi surfaces corresponding to all zones that you included.

(c) Now look at the zone corresponding to the origin of your choice. Sketch all free electron dispersions that are folded into this zone along two vertical lines defined by $k_x = 0.9\ \pi/a$ and $k_x = \pi/a$. Take your x-axis as k_y from $-\pi/a$ to π/a. In the plot, show where is the Fermi energy and also indicate the non-spin degeneracy of each dispersion curve that you plotted. Now, let's turn on potential $V(G=2\pi/a)$, and define $\Delta \equiv |V(2\pi/a)|$. Assume that Δ is a very small number compared to any energy separation between dispersion curves in your plots, but still a finite number. To the leading order in Δ, explain quantitatively what happens to the dispersion curves, and plot new dispersion curves.

(d) Using your results of (c) and the fact that Fermi surface is orthogonal to the BZ face for a weak potential (We covered this in class. A more mathematical proof will be provided in the next homework set. This property tends to be true also for strong potentials, due to high symmetry of the BZ face, but it doesn't have to), determine the geometry of Fermi surface(s) under the weak crystal potential. In the repeated zone scheme, extend the sketch of new dispersions you made in (c) to k_y from $-3\pi/a$ to $3\pi/a$. Explain why the Fermi surface can be thought of a small “cigar” shaped electron pocket and a small “circle” shaped hole pocket. Explain why there should be a definite relationship between the areas of the “cigar” shape and the “circle” shape, and state what is the relationship. (“circle” may be more appropriately called “diamond” or “star”)

Tips

2. (a) For the dynamic part, you can use the following expression for the Helmholtz free energy, $F = E - TS = -k_B T \ln Z$ where $Z = \sum_i \exp(-E_i/k_B T)$, Z is the partition function and E_i is the energy of each configuration (“ensemble”). $E_i = \sum_q \epsilon_q$, where the summation is over each occupied quantum orbital for that given configuration (i.e. for bosons same q can repeat). Pressure P is given by $-\left(\frac{\partial F}{\partial V}\right)_T$. Examine where the volume dependence of F comes from.

   (b) Note that there are two ways to express $\left(\frac{\partial P}{\partial T}\right)_V$. One way is to use the equation of state derived in (a) and the other is to use eq. (7) of the note “Cp and Cv”.

   (c) For this part, E_B can be set to 0. Note that the leading order term for $B = -V\left(\frac{\partial P}{\partial V}\right)_T$ is temperature independent (You need to explain this yourself).

   (d) For this part, E_B should be taken as finite (see slide 16 of Lecture 4). Again, you need to explain that the leading term of $B = -V\left(\frac{\partial P}{\partial V}\right)_T$ is temperature independent. Incidentally, note that γ is the Grüneisen constant of slide 156 of Lecture 4.

3. Plasmon is described well in Kittel (Chap. 14) or Aschcroft and Mermin (Chap. 1). Also, see 13.6 of H&H.
   (b) Recall that in non-magnetic isotropic medium, the dispersion relation is given by $\epsilon\omega^2 = c^2k^2$. Negative ϵ means a damped wave, in which case the wave does not propagate, i.e. the light will be totally reflected at the surface, and is forbidden inside the material.
   (c) Here is a useful conversion formula from λ to energy for light in vacuum. $\hbar\omega(eV) = 12398/\lambda(\text{Å})$.
   (d) This part should be really simple despite many words. If you have a problem applying Gauss law, ask for help. You will notice that this oscillation represents another simple harmonic oscillator, whose quantum is called “plasmon,” which is routinely measured in the core level photoelectron spectroscopy and the electron energy loss spectroscopy. Plasmon is a mixed mode of photons and electrons.

4. The wave function of lattice vibrations is defined only on atomic positions. Still you can give a definition of $u_{\mathbf{k}}(x)$ as though it was a function defined for all values of x, using conditional expressions.