Homework 4

Due 2/9/2012

1. [20 points] Consider the following wave function that exists in a one dimensional crystal.

$$\psi_k(x,t) = A\exp(ikx - i\omega t)$$

Here, A is a complex constant, and k, ω are (real) wave vector and (positive) angular frequency respectively. Consider this wave function at a fixed time. We consider time $t = 0$ only, without losing any generality (as any phase that results due to a finite, but fixed, time can be included in A), and consider

$$\psi_k(x, t = 0) = A\exp(ikx)$$

Show that the following two statements are true.

[Note: You have an option of doing this problem analytically, or numerically. If you do it numerically, using a computer program, then following this instruction: (1) plotting the real part of ψ_k only, (2) choose a non-trivial phase (i.e. the phase should not be an integer multiple of $\frac{\pi}{2}$) for A, and (3) choose 5 distinct values of G to compare ψ_{k+G} with ψ_k.]

a) $\psi_k(x, t = 0)$ generally differs from $\psi_{k+G}(x, t = 0)$ when x is taken as a continuous variable. Here, G is the reciprocal lattice vector for this crystal.
b) Consider $\psi_k(x, t = 0)$ only at discrete values na, $n =$ integers. That is, we consider x values limited to the lattice points of this crystal. This corresponds to considering (any types of) phonons in this crystal. In this case $\psi_k(x = na, t = 0)$ is exactly equal to $\psi_{k+G}(x = na, t = 0)$ for any reciprocal lattice vector G, and for any complex constant A.

2. [20 points] In class, we set up equations of motion for the monatomic 1D crystal (LN 6, 2nd equation from the bottom of page 4) and for the diatomic 1D crystal (LN 7, the last equation in blue in page 3). Show that for each of these cases, those equations of motion lead to the following continuum elastic wave equation, for long wave length acoustic modes:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

You will recognize this as a wave equation. Here, v is the speed of the sound wave. You must show that you can deduce the correct speed of sound, v, in each case (page 5 of LN 6 and the last equation of page 4 of LN 7) from *this consideration of the equation of motion alone*.

3. [20 points] Kittel 4.5 (see below), but with some changes. Start this problem assuming that the spring constants are C_1 and C_2 ($C_1 \neq C_2$).
   a. Obtain an exact form of ω_k (analogous to that given above in problem 2) valid for any k and for any C_1 and C_2.
   b. Do as Kittel 4.5 says; i.e. plug in $C_1 = C$ and $C_2 = 10C$ and then find ω_k for $k = 0$ and $k = \pi/a$. Sketch the dispersion curves.
   c. Consider $C_1 = C - \delta C$ and $C_2 = C + \delta C$, with $|\delta C| \ll C$. For each of the non-zero phonon energies at $k = 0$ and $k = \pi/a$, use the Tayler expansion of ω_k in terms of δC to evaluate the leading order correction to ω_k from its "unperturbed" value for $\delta C = 0$. At which point is the correction more significant, $k = 0$ or $k = \pi/a$?

4. [10 points] Kittel 4.6 (see below)

5. [Extra credit; 20 points] Kittel 4.4 (see below). Eq. (16a) that this problem refers to is given by $\omega^2 = \frac{2}{M}\sum_{p>0} C_p(1-\cos(pka))$ where p is the neighbor index on one side (1 for the nearest neighbor, 2 for the next nearest, and so on). Please show your derivation of this equation first. Note that this problem is essentially a problem of a 1D crystal: the text refers to "interplanar forces" in a 3D crystal, which might as well be thought of as "interatomic forces" in a 1D crystal for the purpose of this problem.

6. [30 points] Please submit one paragraph description about your final project. Your description must include the title, the summary of what you like to present in a few sentences, the relevance of your project to the solid state physics, and (one to three?) key references. Please come and consult with me, if necessary. This problem is due Feb. 12, and you must submit a digital file (word, pdf, or any common document format) to me by email, or type your paragraph on the course web site (e.g. in a subpage just for yourself in Den).

Kittel problems from chapter 4

4. ***Kohn anomaly.*** We suppose that the interplanar force constant C_p between planes s and $s+p$ is of the form

$$C_p = A\frac{\sin pk_0a}{pa} ,$$

where A and k_0 are constants and p runs over all integers. Such a form is expected in metals. Use this and Eq. (16a) to find an expression for ω^2 and also for $\partial\omega^2/\partial K$. Prove that $\partial\omega^2/\partial K$ is infinite when $K = k_0$. Thus a plot of ω^2 versus K or of ω versus K has a vertical tangent at k_0: there is a kink at k_0 in the phonon dispersion relation $\omega(K)$.

5. ***Diatomic chain.*** Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(K)$ at $K = 0$ and $K = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2.

6. ***Atomic vibrations in a metal.*** Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R. (a) Show that the frequency of a single ion set into oscillation is $\omega = (e^2/MR^3)^{1/2}$. (b) Estimate the value of this frequency for sodium, roughly. (c) From (a), (b), and some common sense, estimate the order of magnitude of the velocity of sound in the metal.