PHYS4450 Solid State Physics **Problem Set 3** **Due: 8 March 2013 (Friday)**

All problem sets should be handed in not later than 5pm on the due date. Drop your assignment in the Box in Rm.213.

Please work out the steps of the calculations in detail.

3.0 *Reading Assignment:* On the topic of lattice vibrations, Kittel's Chapter 4 gives a good overview. We treated the topic more formally and emphasized some *general principles*, e.g., **q**'s in 1st BZ, Bloch's theorem, periodic boundary condition and number of allowed **q**'s in B.Z., etc. Christman's Chapter 6 is also good. Chapter 22 of *Solid State Physics* by Ashcroft and Mermin treats the topic at the level I preferred. To get a taste of how vast this topic is, you may want to look at (just browse) the two classics by: Born and Huang, *Dynamical theory of crystal lattices* (1954), and J. Ziman, *Electrons and Phonons* (1960). [The "Huang" in Born and Huang later became the leading figure in solid state physics in China (K. Huang) and educated generations of physicists, especially those in semiconductors, either directly or through his textbooks (written in Chinese and still in print).]

3.1 **(See SQ7) Knowing how many branches to expect.** Consider the compound LaMnO_3. There is one formula per unit cell in the crystalline form. How many branches of phonon dispersion relations are there? How many acoustic branches? How many optical branches?

3.2 **Displaying 2D phonon dispersion relations.** Consider a two-dimensional crystal taking on the square lattice with one atom per basis. The edge of a primitive unit cell is a. The sample is taken to be of size $A = L^2$, where $L = \mathcal{N}a$ with $\mathcal{N} \gg 1$. It will be interesting to set up a lattice vibrational problem and solve for the normal mode frequencies. This is not-too-easy, and we will NOT do it here.

(a) Sketch the reciprocal lattice and construct the first Brillouin zone.

(b) What are the allowed **q**-values? If N (note: this symbol N is different from $\mathcal{N}$) is the total number of unit cells in the crystal, how many allowed wave vectors **q** are there in the first Brillouin zone?

(c) Each allowed **q** occupies a certain area in the reciprocal space. Find the area.

(d) In a unit area of reciprocal space, how many allowed **q**'s are there? Hence, in d^2q (an areal element in the 2D reciprocal space) of reciprocal space, how many allowed **q**'s are there?

(e) Assume that the atoms move only within the plane of the lattice, how many degrees of freedom are there? How many branches do you expect in the dispersion relation $\omega(\mathbf{q})$? [Note $\mathbf{q} = (q_x, q_y)$ are vectors from the center of the Brillouin zone to the allowed values of q_x and q_y.]

(f) **(See SQ9)** Let's say someone has done the normal modes calculation and found the following form for a branch of the dispersion relations:

$$\omega(\mathbf{q}) = \omega(q_x, q_y) = B\sqrt{\sin^2\frac{q_x a}{2} + \sin^2\frac{q_y a}{2}},$$

where B is a constant related to the spring constants and the mass of the atoms. [Note: I am not saying that the form is really correct!]

(i) Sketch the phonon dispersion relation for the wave vector **q** that goes from $\Gamma \to X$ in the first Brillouin zone (here Γ is the BZ center and X is a point at the BZ edge in the $\hat{x}$ or $\hat{y}$-direction (see figure in class notes).

(ii) Sketch the phonon dispersion relation for **q** that goes from $\Gamma \to M$ in the first Brillouin zone along the diagonal in the 1st BZ, i.e., $\mathbf{q} = (x, x)$ for $0 < x < \pi/a$. [Note: You should draw the x-axis of your plot in the proper scale, as compared to (i).] The M-point is at the BZ corner.

(iii) Sketch the phonon dispersion relation for **q** that goes from $X \to M$ in the first Brillouin zone, i.e., for $\mathbf{q} = (\pi/a, x)$ for $0 < x < \pi/a$.

   - (iv) Use your artistic mind and put the segments of the dispersion relations in (i), (ii) and (iii) into ONE figure, i.e., draw the dispersion relation with the horizontal axis for $\mathbf{q}$ running from $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$. (Note that the different segments on the horizontal axis are of different "lengths". This is the "pro" way of expressing dispersion relations.) **(See SQ 9)**
   - (v) What is the highest frequency? What is the corresponding $\mathbf{q}$ for the highest frequency?
- (g) The dispersion relation $\omega(\mathbf{q}) = \omega(q_x, q_y)$ can actually be plotted as a 3D plot, with q_x, q_y being the x and y-axes, and the frequency $\omega(q_x, q_y)$ being the z-axis. Using a numerical package, e.g., Mathematica or Matlab or Mathcad, try it out. **(See SQ 9)**
- (h) Looking at your results in part (g). If we need a computer to diagonalize a dynamical matrix to get at the dispersion relation, there will be a matrix problem for each value of $\mathbf{q}$. Do you think it is really necessary to perform the dispersion relation calculation for every $\mathbf{q}$ *all over* the 1st BZ? Can we simply work on a smaller portion of the BZ and obtain the rest by symmetry? Why? Comment on how small a zone one can use for this problem by inspecting your results.

3.3 **(See SQ10) Debye model for a 2D solid.** In Problems 3.2, you worked on the phonon dispersion relation of a 2D (square lattice of lattice constant a) solid of the following form

$$\omega_s(\mathbf{q}) = \omega_s(q_x, q_y) = B_s \sqrt{\sin^2 \frac{q_x a}{2} + \sin^2 \frac{q_y a}{2}}.$$

Let's say there are THREE acoustic branches (for in-plane and out-of-plane vibrations). They are labelled by a branch label s, with possibly different B_s $(s = 1, 2, 3)$ characterizing the behavior of each branch. Usually, two of them are identical. For this problem, let's say all the B_s are different.

- (a) Invoke the Debye approximation to study the heat capacity of this 2D system. You may either refer to class notes Ch.VII or simply follow the steps below.
   - (i) Find the $q \rightarrow 0$ behavior of the branches. This picks up the linear part of the dispersion relation.
   - (ii) The Debye APPROXIMATION implies that we would keep the linear form of the branches and extend it to higher q. Using the idea that $\frac{A}{(2\pi)^2} 2\pi q dq = D(\omega) d\omega$, where $D(\omega) d\omega$ is the number of normal mode frequencies within the interval ω to $\omega + d\omega$. Find the contribution to the phonon density of states $D_s(\omega)$ for each of the branches. Then ADD up the contributions from the branches to find $D(\omega)$.
   - (iii) However, we know that there are only a finite number of normal modes (thus normal mode frequencies) in a branch (recall: number of allowed $\mathbf{q}$'s in 1st BZ), and thus a finite number of modes in the three branches. Using this number, fix the Debye frequency ω_D so that the correct number of modes is accounted for. Find also the corresponding Debye temperature θ_D.
   - (iv) Extract the temperature dependence of C_V at low temperatures for the 2D solid. (Contrast the answer with 3D behavior due to phonons.)
- (b) Now, summarize the **phonon contribution** to the low temperature heat capacity in different spatial dimensions (1D, 2D, 3D).
- (c) (Optional but rather interesting (no bonus points):) What if the dimension d is taken to be continuous, i.e., d is no longer restricted to 1,2,3, but say $d = 1.5 or 1.7$? [Remark: There is a class of objects called fractals. They can be characterized by a fractional dimension. For those interested in reading a paper on the phonon DOS in fractals (with fractional dimension), see the famous paper by E. Domany *et al.*, Phys. Rev. B **28**, 3110 (1983).]

3.4 **Magnon contribution to heat capacity.** In class, we mentioned that the low-energy excitation of a ferromagnetic ground state takes on the form of spin waves (c.f. elastic waves in the case of lattice vibrations). The quanta of excitation is called magnon (c.f. phonon). There is a key difference though – the dispersion relation has the form of $\omega = Cq^2$.

(a) Consider a 3D system. How does the magnon contribution to the low-temperature heat capacity? [Arguing the T-dependence will be sufficient. You need to use what you learned in statistical mechanics. Getting the density of modes $D(\omega)$ will be a proper starting point.]

(b) Consider a 2D system. How does the magnon contribution to the low-temperature heat capacity? [Arguing the T-dependence will be sufficient. Contrast the result with 2D phonon contribution.]

It will be educational to construct a hand-waving argument for these magnon results (see SQ10).

3.5 **Beyond nearest neighbor interaction – and Kittel's problem 4.4.** In the examples discussed in lectures, we assumed nearest-neighbor interaction for simplicity. (An appendix gives a general treatment of setting up the dynamical matrix.) However, experiments indicate that (since interactions are electrical (Coulombic) in nature) there are interactions beyond nearest neighbors. There are many interesting effects when one goes beyond nearest-neighbor interactions. In particular, an **infinite-range interaction** leads to some special effects!

(a) Study how we get the equation of motion in a 1D monatomic chain of atoms of mass M with nearest neighbor interaction (see for example class notes). Now let's see how we can get at Kittel's Eq.(16a) in Chapter 4. Following Kittel's notations, let C_p be the "spring constant" that relates the net displacement to the force between two atoms (1D chain) that are pa apart, where p is an (positive and negative) integer and a is the lattice constant. Then we write the force on the n-th atom as

$$F_n = \sum_p -C_p(u_n - u_{n+p}),$$

where u represents the displacement and the sum is over all other atoms. Of course we expect C_p to drop with the separation labeled by p. Then write down the equation of motion for the n-th atom. Now using the standard procedure in looking for the normal modes and show that the following dispersion equation arises:

$$\omega^2 M = -\sum_p C_p(e^{iqpa} - 1).$$

Noting that from translational symmetry, we have $C_p = C_{-p}$, and hence show that Eq.(16a) of Kittel follows, i.e.,

$$\omega^2 = \frac{2}{M}\sum_{p>0} C_p(1 - \cos qpa). \tag{1}$$

(b) Now try the simplest possible case of $C_p = K$ for $p = 1$ and $C_p = 0$ for $p \geq 2$. Show that Eq.(1) reduces to the dispersion relation for 1D monatomic chain with nearest-neighbor interactions only.

(c) Using Eq.(1) and taking the long wavelength limit (i.e., $pqa \ll 1$), derive an expression for the velocity of sound in terms of C_p.

(d) Check whether $\omega^2(q) = \omega^2(-q)$?

(e) **(Kohn anomaly: This is Kittel Problem 4.4**) Suppose that C_p takes on the form

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

where A and Q are constants and p runs over all integers. From the form, Q is something in the reciprocal space. Discuss how C_p drops with p (or with pa which is the separation between two atoms). This is a form applicable to metals. Using C_p in Eq.(1), write down an expression for $\omega^2(q)$.

Now, pay attention to ω_q and the particular value $q = Q$. See if you can plot $\omega(q)$? Show that something strange will happen at $q = Q$, by showing that $d\omega^2/dq$ is infinite when $q = Q$. Technically, $\omega(q)$ has a vertical tangent at $q = Q$ or it is described as having a "kink" at $q = Q$.

Remarks: In the case under consideration, ω^2 versus q or ω versus q has a vertical tangent at $q = Q$. This is called the Kohn's anomaly, after Walter Kohn. It is related to the form of C_p, which says that the interaction, while drops with the separation as $1/pa$, also oscillates with the separation. By oscillating, it implies some characteristic length given by $1/Q$. This particular Q then reflects itself in the phonon dispersion relation. [See W. Kohn, Phys. Rev. Lett. **2**, 393 (1959) for more detail. The author won the 1998 Nobel Chemistry prize for his foundation work on the density functional theory in 1963 (later developed into powerful computational methods for studying molecules and solids).] A second remark is that a similar form of interaction as given by C_p also appears in magnetism under the context of magnetic interaction in metals (indirect exchange). The interaction is called the RKKY interaction, with one of the K's being Kittel. Another remark is about **softening of some phonon modes and structural phase transitions**. When a solid's phonon dispersion relation shows a mode with a finite $\mathbf{q}$ that the corresponding ω becomes very small, it means that a bit of energy is sufficient to excite that mode. The particular mode is described as "soft" mode. The implication is that the system now prefers to show a particular wavevector of $\mathbf{q}$, just like the original solid wants to show a wavevector of $2\pi/a$ due to the periodicity of a in the crystal. This preference signifies another period emerges, thus possibly a change in the structure of the crystal.

3.6 **Melting of Solids.** This is a simple question, but the physics is nice. In SQ8 on quantum harmonic oscillator, the TA has shown that the displacement $\hat{X}$ (or $\hat{u}$ if you like) can be given as $\hat{u} = \sqrt{\frac{\hbar}{2M\omega}}(\hat{a}^\dagger + \hat{a})$. Recall that in stat mech, $\langle A \rangle$ is the statistical average (that could involve both an expectation value and an average based on the Canonical Distribution (see PHYS4260 Class Notes Ch. V).

One way to consider melting of a solid is consider the fluctuations in the displacement. [The idea is like random walks. The walk could go to the left or to the right. If we consider the square of the displacement, it will always be positive. In random walk, $\langle x^2 \rangle \sim t$ shows the diffusive behavior, where t is time or the number of steps in the random walk.] So, we are led to consider the quantity $\langle u^2 \rangle$. Show that for an oscillator (a normal mode)

$$\langle u^2 \rangle = \frac{\hbar}{2M\omega}(2\langle \hat{a}^\dagger \hat{a} \rangle + 1) = \frac{\hbar}{M\omega}(\langle n \rangle + \frac{1}{2}),$$

where $\langle n \rangle$ is just the thermal average excitation of the oscillator.

(a) Show that at a temperature $T > \Theta_D$, where Θ_D is the Debye temperature, one could argue that

$$\langle u^2 \rangle \sim \frac{\hbar^2 T}{M\Theta_D^2}.$$

You are welcome to work out the prefactor.

(b) Here is something called the **Lindemann criterion** of melting. Let a be the lattice constant (at ordinary temperature where the solid is still a solid). Lindemann says that when $\langle u^2 \rangle$ becomes "comparable" to a^2, the solid melts! Experiments showed that "comparable" means $\langle u^2 \rangle / a^2 \sim 0.2$ or so. Using this criterion, obtain an expression for the melting point T_m of a solid.

(c) *Melting at $T = 0$ or not-forming-a-solid even at $T = 0$* An extension of (a) and (b) is to take it to $T = 0$. Show that for $T \to 0$,

$$\langle u^2 \rangle \sim \frac{\hbar}{2M\omega} \sim \frac{\hbar^2}{2M\Theta_D}.$$

For a solid, the frequency ω can be related to the bulk modules B through $\omega = \sqrt{\frac{B}{M}}$, where B can be estimated by equating the change in potential energy for a displacement of $u \sim a$ (which is $\sim Ba^2$) to a typical interaction energy $\mathcal{V}(a)$ between the atoms. As in the Lindemann criteria, the important quantity is the ratio

$$\Lambda \equiv \frac{\langle u^2 \rangle}{a^2},$$

which is called the *de Boer parameter*. Show that at $T = 0$,

$$\Lambda \sim \frac{\hbar}{a} \frac{1}{\sqrt{M\mathcal{V}}}.$$

Now, if $\Lambda \geq 0.2 - 0.3$ at $T = 0$, then the atoms cannot form a solid even down to $T = 0$. Understand? Now, look at the expression. State the conditions on the mass and the interaction $\mathcal{V}$ that a material would remain a liquid down to $T = 0$. Connect your observation to the fact that helium remains a liquid at normal pressure – something that you learned before about zero-point motion prevents helium from solidification. This is sometimes called *quantum melting.* It is perhaps another form of *quantum phase transitions.* The latter is a fashionable research area. Here, the transition is not driven by temperature. It is $T = 0$ physics. By varying the mass M of the atoms or the interaction (if one can do that experimentally), one can control the quantum fluctuations (zero point motion) and drive a system from a solid phase to a liquid phase. You see – this is rather old physics. But physicists often like coining a fancy term and revive a research field.

Remark: **Wigner crystal?** Once upon a time, there was an interesting idea. Let's say there are N electrons ($N \gg 1$). Take the equivalence of N positive charges, turn them into a uniform charge distribution that forms the background. The system of this background positive charges and the N electrons is then a neutral system. The question is: Can the N electrons form a regular array of electrons in such a positively charged background? Such a structure is called a **Wigner crystal**. Will it be stable against quantum melting? Can this exist in 3D? 2D? 1D? Fascinating questions! (This is similar to the plum-pudding model of J.J. Thomson for an atom in the early 20th century.) I think in recent years, Wigner crystals have been realized experimentally in 1D and 2D systems. As to 3D, I have not followed the progress.

Important: You must attach a signed copy of the following declaration to your homework. You may also download the form in the website listed below.

I declare that the assignment here submitted is original except for source material explicitly acknowledged, and that the same or related material has not been previously submitted for another course. I also acknowledge that I am aware of University policy and regulations on honesty in academic work, and of the disciplinary guidelines and procedures applicable to breaches of such policy and regulations, as contained in the website http//www.cuhk.edu.hk/policy/academichonesty.

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