

# Physics 215B: Homework Problem Set 2

Due: January 23, 2008

## 1. Phonon Frequencies and Energies. 30 points.

The  $q=0$  optic phonon modes of diamond (made of  $^{12}\text{C}$ ) lie at  $1330\text{ cm}^{-1}$ . [The unit  $\text{cm}^{-1}$  is called *wavenumbers* (or occasionally *inverse centimeters*) and is used as a unit of energy, see Wikipedia <http://en.wikipedia.org/wiki/Wavenumber>]

- (i) Calculate the frequency  $\omega$  in  $\text{s}^{-1}$ , and the energy  $\hbar\omega$  in  $\text{meV}$ . What is the wavelength?
- (ii) calculate the corresponding length scale  $x_o = \sqrt{\hbar/M\omega}$  in  $\text{\AA}$ , and the momentum scale  $p_o = \sqrt{M\hbar\omega}$  in both  $g - \text{cm/s}$  and atomic units. Interpret the value of  $x_o$ .

## 2. Molecular Vibrations. 10 points.

Consider an equilateral triangle shaped molecule  $Z_3$  made of three identical atoms ( $Z$ ). Determine how many molecular vibrations this molecule has, and sketch the corresponding eigenvectors.

## 3. Debye-Waller Factor. 30 points.

Adopt the assumptions of the Debye model, so that polarization vectors  $\vec{\epsilon}_{k\nu}$  consist of a longitudinal mode polarized parallel to  $\vec{k}$ , and two transverse modes perpendicular to  $\vec{k}$  (all are mutually perpendicular), with density of states given by the Debye expression.

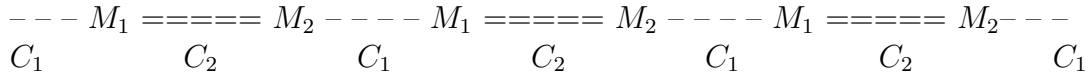
- (i) Show that, in three dimensions, the Debye-Waller factor is given by

$$2W = \langle (\vec{q} \cdot \vec{u})^2 \rangle = \frac{3}{2} \frac{\hbar^2 q^2}{M\hbar c k_D}.$$

- (ii) Show that in one or two dimensions, the Debye-Waller factor diverges.
- (iii) Graphene is a single layer of graphite, that is, a single layer of C atoms bonded  $sp^2$ -like in a honeycomb lattice. Single, essentially unsupported, layers of graphene can be synthesized and studied, although they do not remain flat but are substantially warped. The divergent D-W factor that one calculates for a 2D layer [part (ii) of this problem] seems to say that the r.m.s fluctuation of a C atom in graphene is not finite, i.e. the graphene crystal should not exist. Try to reconcile the theory with reality.

**4. Vibrating Diatomic Chain of Atoms.** 30 points.

Consider a 1D chain of atoms with alternating masses  $M_1$  and  $M_2$ , and also alternating near-neighbor spring constants  $C_1$  and  $C_2$ . Denote the unit cell length by  $a$ , the actual positions of the atoms within the cell does not matter.



- (i) Use Newton's laws to calculate the phonon dispersion relations  $\omega_{k\nu}$ . Verify that you obtain the correct (simpler) result when  $M_1 = M_2$ ,  $C_1 = C_2$ .
- (ii) Next let  $C_1 = C_2$  and  $M_1 \gg M_2$  (think in terms of PdH, where the mass ratio is roughly 100:1). Sketch the dispersion relations in the 1st Brillouin zone, and give the expressions for the energies at  $k = 0$  and  $k = \pi/a$  to lowest order in  $M_2/M_1$ . Give the exact expression for the sound velocity.
- (iii) Briefly interpret both phonon branches, taking into consideration the large mass difference.