Homework 4

Due 2/3/2011

1. [15 points]
   To make an estimate of the typical phonon energy scale, it is sensible to assume that an atom of mass M is vibrating at its site with an effective spring constant. Assume that it is moving along a certain direction only, i.e. consider a strictly one dimensional simple harmonic Hamiltonian (SHH) problem, as appropriate for a normal mode. Let Δx be the uncertainty of the position of the atom due to the zero point motion.
   a. Using the minimum uncertainty relation ($\Delta x \Delta p = \hbar/2$) valid for the ground state of a SHH, the virial theorem ($\langle T \rangle = \langle V \rangle$) valid for any eigen-state of a SHH, $\langle T \rangle = \frac{\Delta p^2}{2M}$, and the zero point energy = $\frac{1}{2}\hbar\omega$, express the phonon energy $\hbar\omega$ in terms of Δx, M and $\hbar$.
   b. Estimate $\hbar\omega$ for a carbon (C) atom and a copper (Cu) atom, respectively, assuming that $\Delta x \approx 0.05$ Å.
   c. In graphene, the actual phonon energy scale is ≈ 100 meV. In a high temperature superconducting ("high-Tc") cuprates, the phonon mode of mainly Cu character has the energy scale ≈ 10 meV. From these values, make an estimate of Δx, in terms of the percentage of bond length, which is 1.42 Å in graphene, and 1.92 Å in a high-Tc cuprate. [So, this part is the reverse of part b.]
   d. This part is continuation of part c. So far, we've been considering the zero point energy only, which means that we were considering the zero temperature limit. At room temperature, consider the Bose-Einstein distribution function $n(\hbar\omega)$ with zero chemical potential (i.e. the Planck distribution function function). By equating $\frac{1}{2}\hbar\omega + n(\hbar\omega)\hbar\omega$ with $\langle T \rangle + \langle V \rangle$, find the percentage increase of Δx relative to its zero temperature value for graphene and the high Tc cuprate, respectively. Use properties listed in a, except the minimum uncertainty relation which does not hold any longer for excited states.

2. [10 points]
   In class, we set up the eigenvalue equation for a di-atomic 1D chain with masses M_1 and M_2. That equation is

$$\begin{pmatrix} 2C - M_1\omega_k^2 & -C\left(1 + e^{-ika}\right) \\ -C\left(1 + e^{ika}\right) & 2C - M_2\omega_k^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

   The eigenvalues are (I am not asking you to derive these)

$$\omega_k = \sqrt{\frac{C}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka}\right)}$$

   a. Show explicitly that when $k = 0$, the two normal modes correspond to $u = v$ (acoustical mode; in phase within the basis) and $M_1 u + M_2 v = 0$ (optical mode; out of phase within the basis).
   b. Show explicitly that when $k = \frac{\pi}{a}$ (or $-\frac{\pi}{a}$) the two normal modes correspond to $u = 0$ or $v = 0$ (local vibrations out of phase between neighboring cells).

3. [15 points] Kittel 4.5, 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

5. [10 points; extra credit; but you should try this!] Kittel 4.4