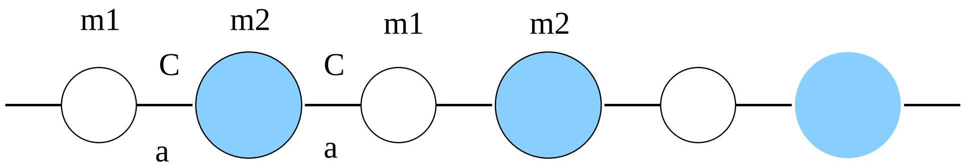
NAME: SOLUTIONS

33-448 Solid State Physics Midterm #2 Wednesday, March 16, 2016

Consider the diatomic chain illustrated in the figure, with alternating masses $m_1 < m_2$ connected by springs of equilibrium length $a$ and spring constant $C$. Most of the following questions should be answered using approximations whose nature you should explain in words or formulas as appropriate. Each question can be answered independently of the others.




In case you wish to know it, here is the dispersion relation for a *monatomic* chain:

$$\omega(K) = 2\sqrt{\frac{C}{m}} \sin \frac{Ka}{2}.$$

DO NOT SOLVE THE EXACT EQUATIONS OF MOTION OR OBTAIN THE EXACT DISPERSION RELATION FOR THE DIATOMIC CHAIN!!

1. What is the speed of sound at low frequency?

   **Answer:** In the limit of low frequency the wavelength greatly exceeds the interatomic spacing, and only the average mass enters. Hence we may apply the dispersion relation of the monatomic chain with $m = (m_1 + m_2)/2$. At small $K$, $\omega \approx \sqrt{C/m}Ka$ and the sound speed $v = \omega/K = \sqrt{C/m}a$.

2. Determine the contribution of the acoustic phonons to the heat capacity at low temperature. Your answer should include correct powers of sound speed $v$ and temperature $T$, but you need not worry about any other details.

> **Answer:** Phonon modes up to $\omega^\star \sim k_B T/\hbar$ can be excited. The number of such modes is proportional to $K^\star = \omega^\star/v$. Since each mode will be excited to approximately $k_B T$ of energy, the total energy $U \sim T^2/v$, and the heat capacity $C_v \sim T/v$.

3. Let $m_1 \ll m_2$ and determine the contribution of the optical phonons to the heat capacity at low temperature (hint: treat these in the Einstein model. I am primarily interested in the dependence on the Einstein frequency $\omega_E$ and the temperature $T$).

> **Answer:** In this limit, masses $m_2$ remain stationary so each mass $m_1$ oscillates independently at the "Einstein" frequency $\omega_E = \sqrt{2C/m_1}$, where the factor of 2 comes because of the two springs connected to it. The occupation probability for this mode vanishes as $\exp(-\hbar\omega_E/k_B T)$ (notice we don't need the exact Bose-Einstein formula in this limit), so the energy $U \approx \hbar\omega_E \exp(-\hbar\omega_E/k_B T)$ and the heat capacity $C_V \sim (\hbar\omega_E/k_B T)^2 \exp(-\hbar\omega_E/K_B T)$.

4. Describe the motions of the atoms for zone boundary phonon modes and determine their *exact* frequencies for all $m_1 < m_2$.

> **Answer:** At the zone boundary, one class of atoms oscillate while the other remains staitionary, for each mode. Hence the frequencies are $\omega_{1,2} = \sqrt{2C/m_{1,2}}$.

5. Describe two interesting things that happen to the dispersion relation at the diatomic chain zone boundary in the limit $m_2 \rightarrow m_1$, and briefly explain why they occur.

> **Answer:**

a. Because the chain becomes monatomic, the acoustic and optical branches merge into a single frequency.

b. Because the lattice constant drops by a factor of 2 when $m_1 = m_2$, the original diatomic zone boundary is eliminated in favor of a new boundary twice as far from the origin of reciprocal space. Hence dispersion relation at the diatomic zone boundary has a nonvanishing slope (sound speed).