QUANTUM MECHANICS I

PHYS 516

Problem Set # 4

Distributed: Feb. 6, 2015

Due: February 16, 2015

Phonons: In one dimension, 100 particles of equal mass m are connected to their nearest neighbors by identical springs with spring constant k. The first and last particles are anchored to brick walls ("brick wall boundary conditions").

a. Draw a sketch.

b. Compute the dispersion relation.

c. This linear chain is in thermal equilibrium with a bath at temperature T. Write down a formal expression for the mean thermal energy.

d. The energy can be written as a sum of two terms. One is temperature-dependent, the other is not. Write down these two terms.

e. Numerically compute the temperature-dependent sum for several values of the ratio $kT/\hbar\omega_0$.

2. Zero Point Energy and Forces: Compute the energy of the temperature-independent term you computed in Problem 1**d.** Assume: $T \rightarrow 0, m = k = \hbar = 1$ and the nearest-neighbor equilibrium spacing is l. Here is a useful piece of information:

$$\sum_{j=1}^{N} \sin \frac{j\pi/2}{N+1} = \frac{1}{2}\frac{\cos\theta + \sin\theta - 1}{1-\cos\theta} \qquad \theta = \frac{\pi/2}{N+1}$$

a. How much energy does it take to keep the atom at position 50 fixed?

b. How much energy does it take to keep the atom at position 25 fixed? At position 24 fixed?

c. What is the force on your finger if you keep the atoms at position 25 fixed? Which direction?

3. Debye Theory of Lattice Vibratins: In three dimensions the mean thermal energy of a phonon mode of energy $\hbar\omega$ is $(\langle n \rangle + \frac{1}{2})\hbar\omega$. Debye guessed that the number of modes within a range $d\omega$ of angular frequence ω behaves like $\mathcal{N} 4\pi\omega^2 d\omega$, where $\mathcal{N}$ is some normalization constant ('fudge factor').

a. If there are N atoms, how many normal modes are there?

b. Assume the most energetic mode has energy $\hbar\omega_D$ (D for Debye). Compute the fudge factor $\mathcal{N}$.

c. Neglect the zero point energy (you studied this [Casimir Effect]) in Problem # 2 above). Show that the mean energy is

$$\langle E \rangle = \int_0^{\omega_D} \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \mathcal{N} 4\pi\omega^2 d\omega$$

d. Define the 'Debye temperature' by $kT_D = \hbar\omega_D$. Introduce a new variable $x = \beta\hbar\omega = \hbar\omega/kT$ and write the integral above in terms of this dimensionless quantity. You should find something like

$$\int_0^{kT_D/kT} \frac{x^3\ dx}{e^x - 1}$$

e. In the high-temperature limit $kT \gg kT_D = \hbar\omega_D$ show $\langle E \rangle \to 3NkT$. What is the specific heat in this limit?

f. In the low temperature limit $kT \ll \hbar\omega_D = kT_D$ show that the mean energy behaves lime $cst. \times T^4$. What is the constant?

g. In this limit how does the specific heat depend on the temperature?