Quantum 1 HW 4

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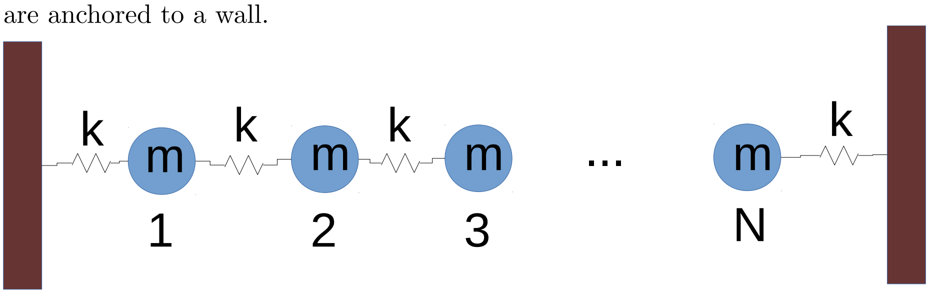
1 Problem 1

We study phonons with a classical system of springs and masses. We have N masses of mass m coupled with springs of spring constant k. Masses 1 and N are anchored to a wall.



We compute the dispersion relation, which is the mode-dependence of the frequency $\omega_{\hat{m}} = \omega_0 \times 2\sin\frac{\hat{m}}{N+1}\frac{\pi}{2}$.

The expected value of the energy in mode j is:

$$< E_j >= (\bar{n}(j) + \frac{1}{2})\hbar\omega_j, \ \bar{n} = \frac{1}{e^{\beta\hbar\omega_j} - 1} \tag{1.1}$$

The total mean thermal energy can be written as a sum of the individual mode terms.

$$< E >= \sum_j (\bar{n}(j) + \frac{1}{2})\hbar\omega_j \tag{1.2}$$

We can separate the $\bar{n}(j)$ and $\frac{1}{2}$ terms of the sum.

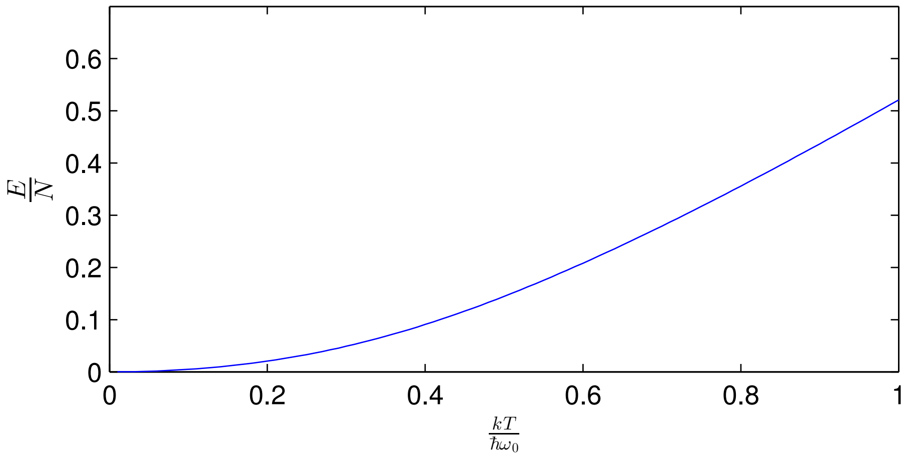
$$< E >= \sum_j \bar{n}(j)\hbar\omega_j + \sum_j \frac{1}{2}\hbar\omega_j \tag{1.3}$$

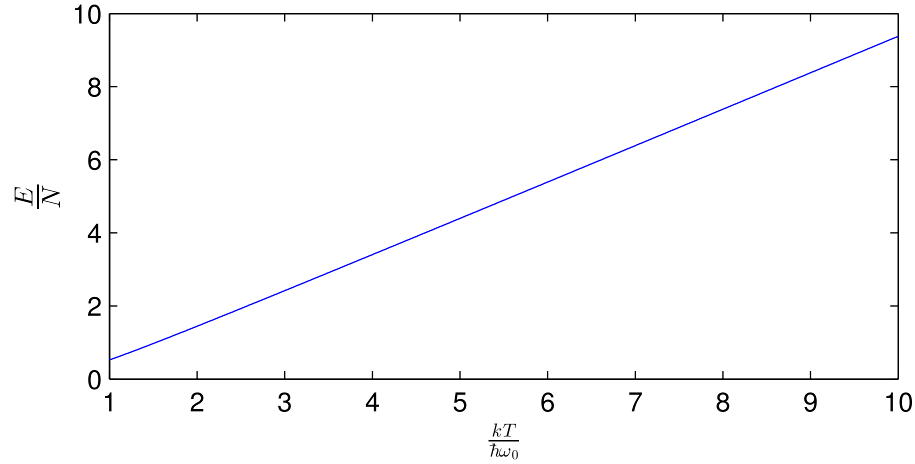
The left term depends on the temperature ($\beta = \frac{1}{kT}$), the right term is temperature independent.

We expand the left sum:

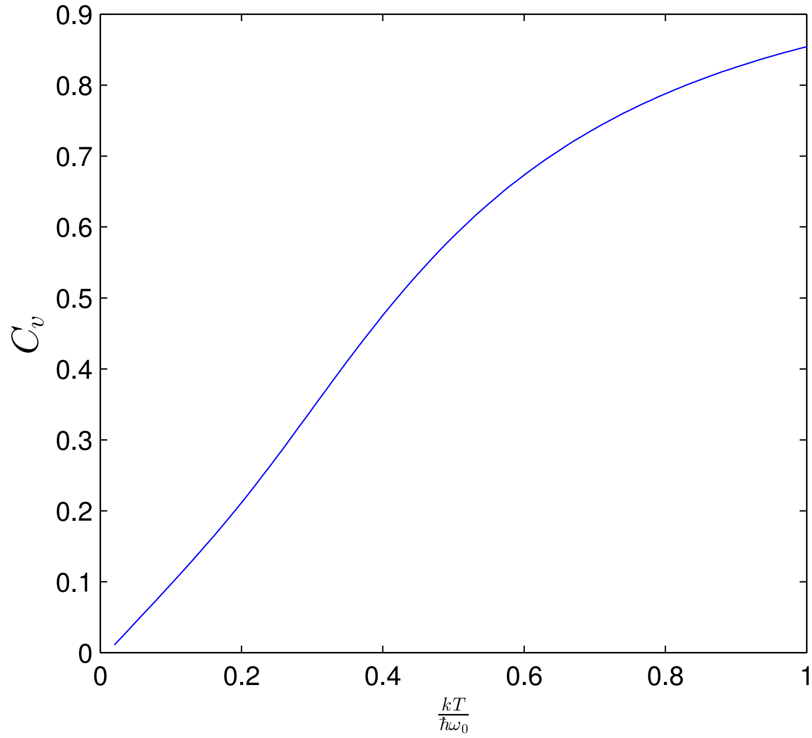
$$\sum_j \bar{n}(j)\hbar\omega_j = \sum_j \frac{\hbar\omega_j}{e^{\frac{\hbar\omega_j}{kT}} - 1} \tag{1.4}$$

We set $\hbar\omega_0 = 1$ and plot the energy versus temperature. We separately graph $kT < \hbar\omega_0$ and $kT > \hbar\omega_0$ to highlight the different behavior.





We can clearly see a linear energy vs. temperature dependence for $kT > \hbar\omega_0$. In the high temperature limit all of the phonon modes are excited, so adding more energy directly increases the temperature.
The low-temperature regime is more interesting. To further investigate the behavior we numerically compute the specific heat as a function of temperature by taking the derivative of the energy vs. temperature function.



2 Problem 2

The temperature-independent zero-point energy is:

$$< E_{zp} >= \sum_j \frac{1}{2}\hbar\omega_j \tag{2.1}$$

The mode frequencies are $\omega_{\hat{m}} = 2\omega_0 \sin \frac{\hat{m}}{N+1}\frac{\pi}{2}$. We can rewrite this using:

$$\sum_j \sin \frac{j\frac{\pi}{2}}{N+1} = \frac{1}{2}\frac{\cos\theta + \sin\theta - 1}{1-\cos\theta}, \;\; \theta = \frac{\frac{\pi}{2}}{N+1} \tag{2.2}$$

$$< E_{zp} >= \hbar\omega_0 \frac{\cos\theta + \sin\theta - 1}{1-\cos\theta} \tag{2.3}$$

We can now calculate the zero-point energy of both the complete 100-atom system and the sum of individual sub-systems. We take $m = k = \hbar = 1$ to simplify the calculations. We now calculate zero-point energies for different values of N.

The energy to fix the mass at position 50 is:

$$< E_{zp}(100) > - < E_{zp}(50) > - < E_{zp}(49) >= 1.00778 \tag{2.4}$$

The energy to fix the mass at position 25 is:

$$< E_{zp}(100) > - < E_{zp}(24) > - < E_{zp}(75) >= 1.0113 \tag{2.5}$$

The energy to fix the mass at position 24 is:

$$< E_{zp}(100) > - < E_{zp}(23) > - < E_{zp}(76) >= 1.0117 \tag{2.6}$$

It requires additional energy $-3.92e^{-4}$ to hold mass 24 fixed compared to mass 25. With $F = -\nabla V$, the gradient of the energy is the energy difference divided by the separation between masses, so $F_{25} = 3.92e^{-4}/\ell$ and the force is toward the left wall.

3 Problem 3

Debye's theory of lattice vibrations estimates the number of normal modes within $d\omega$ of ω to be $K4\pi\omega^2 d\omega$. In a 3-D lattice of N atoms there will be 3N normal modes. If the highest Debye normal mode is ω_D, then we can calculate the constant K:

$$\int_0^{\omega_D} K4\pi\omega^2 d\omega = 3N \tag{3.1}$$

$$K = \frac{9N}{4\pi\omega_D^3} \tag{3.2}$$

The mean thermal energy of a phonon mode with frequency ω is $(< N > +\frac{1}{2})\hbar\omega$. The phonons will obey Bose-Einstein statistics, so $< N(\omega) >= \frac{1}{e^{\beta\hbar\omega}-1}$. Neglecting the zero-point energy term $\frac{1}{2}\hbar\omega$, we find the mean thermal energy for the Debye model:

$$< E >= \int_0^{\omega_D} \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} K4\pi\omega^2 d\omega \tag{3.3}$$

We now define the Debye temperature, $kT_d = \hbar\omega_D$, and substitute $x = \beta\hbar\omega$.

$$\frac{dx}{d\omega} = \beta\hbar \tag{3.4}$$

$$d\omega = \frac{1}{\beta\hbar} dx \tag{3.5}$$

$$K = \frac{9N}{4\pi\omega_D^3} = \frac{9N\hbar^3}{4\pi k^3 T_D^3} \tag{3.6}$$

$$< E >= \frac{9N(kT)^4}{(kT_D)^3} \int_0^{\frac{kT_D}{kT}} \frac{x^3}{e^x - 1} dx \tag{3.7}$$

In the high temperature limit we use the approximation $e^x - 1 \approx x$ for $x \ll 1$. We then have:

$$< E >= \frac{9N(kT)^4}{(kT_D)^3} \int_0^{\frac{kT_D}{kT}} x^2 dx \tag{3.8}$$

$$< E >= 3N \frac{(kT)^4}{(kT_D)^3} \frac{(kT_D)^3}{(kT)^3} = 3NkT \tag{3.9}$$

In the low temperature limit the upper limit of integration approaches infinity. We can then evaluate the definite integral:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \Gamma(4)[\frac{1}{1^4} + \frac{1}{2^4} + \frac{1}{3^4}...] = 6\frac{\pi^4}{90} \tag{3.10}$$

$$< E >= \frac{3N\pi^4(kT)^4}{5(kT_D)^3} \tag{3.11}$$

We find the specific heat by taking the derivative of the thermal energy with respect to temperature. The specific heat is porportional to T^3 in the low temperature limit.