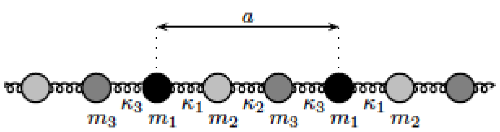
FÍSICA DA MATÉRIA CONDENSADA

Problemas – 3ª Série*

1 **Second Neighbor Diatomic Chain*** Consider the diatomic chain from Exercise 10.1. In addition to the spring constant κ between neighboring masses, suppose that there is also a next nearest-neighbor coupling with spring constant κ' connecting equivalent masses in adjacent unit cells. Determine the dispersion relation for this system. What happens if $\kappa' \gg \kappa$?

2 **Triatomic Chain***
Consider a mass-and-spring model with three different masses and three different springs per unit cell as shown in this diagram.



As usual, assume that the masses move only in one dimension.

(a) At $k = 0$ how many optical modes are there? Calculate the energies of these modes. Hint: You will get a cubic equation. However, you already know one of the roots since it is the energy of the acoustic mode at $k = 0$

(b)* If all the masses are the same and $\kappa_1 = \kappa_2$ determine the frequencies of all three modes at the zone boundary $k = \pi/a$. You will have a cubic equation, but you should be able to guess one root which corresponds to a particularly simple normal mode.

(c)* If all three spring constants are the same, and $m_1 = m_2$ determine the frequencies of all three modes at the zone boundary $k = \pi/a$. Again you should be able to guess one of the roots.

3 **Einstein Solid**
(a) *Classical Einstein (or "Boltzmann") Solid:*
Consider a three dimensional simple harmonic oscillator with mass m and spring constant k (i.e., the mass is attracted to the origin with the same spring constant in all three directions). The Hamiltonian is given in the usual way by

$$H = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2$$

▷ Calculate the classical partition function

$$Z = \int \frac{\mathbf{dp}}{(2\pi\hbar)^3} \int \mathbf{dx}\, e^{-\beta H(\mathbf{p},\mathbf{x})}$$

Note: in this problem $\mathbf{p}$ and $\mathbf{x}$ are three dimensional vectors.

▷ Using the partition function, calculate the heat capacity $3k_B$.

▷ Conclude that if you can consider a solid to consist of N atoms all in harmonic wells, then the heat capacity should be $3Nk_B = 3R$, in agreement with the law of Dulong and Petit.

(b) *Quantum Einstein Solid:*
Now consider the same Hamiltonian quantum mechanically.

▷ Calculate the quantum partition function

$$Z = \sum_j e^{-\beta E_j}$$

where the sum over j is a sum over all eigenstates.

▷ Explain the relationship with Bose statistics.

▷ Find an expression for the heat capacity.

▷ Show that the high temperature limit agrees with the law of Dulong of Petit.

▷ Sketch the heat capacity as a function of temperature.

(See also exercise 2.7 for more on the same topic)

4 Debye Theory I

(a)‡ State the assumptions of the Debye model of heat capacity of a solid.

⊳ Derive the Debye heat capacity as a function of temperature (you will have to leave the final result in terms of an integral that cannot be done analytically).

⊳ From the final result, obtain the high and low temperature limits of the heat capacity analytically.

You may find the following integral to be useful

$$\int_0^\infty dx \frac{x^3}{e^x - 1} = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} = 6 \sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{15}$$

By integrating by parts this can also be written as

$$\int_0^\infty dx \frac{x^4 e^x}{(e^x - 1)^2} = \frac{4\pi^4}{15}.$$

(b) The following table gives the heat capacity C for potassium iodide as a function of temperature.

T(K)	C(J K^{-1}mol^{-1})
0.1	8.5×10^{-7}
1.0	8.6×10^{-4}
5	.12
8	.59
10	1.1
15	2.8
20	6.3

⊳ Discuss, with reference to the Debye theory, and make an estimate of the Debye temperature.

5 Debye Theory II

Use the Debye approximation to determine the heat capacity of a two dimensional solid as a function of temperature.

⊳ State your assumptions.

You will need to leave your answer in terms of an integral that one cannot do analytically.

⊳ At high T, show the heat capacity goes to a constant and find that constant.

⊳ At low T, show that $C_v = KT^n$ Find n. Find K in terms of a definite integral.

If you are brave you can try to evaluate the integral, but you will need to leave your result in terms of the Riemann zeta function.

6 Diatomic Einstein Solid*

Having studied exercise 2.1, consider now a solid made up of diatomic molecules. We can (very crudely) model this as a two particles in three dimensions, connected to each other with a spring, both in the bottom of a harmonic well.

$$H = \frac{\mathbf{p_1}^2}{2m_1} + \frac{\mathbf{p_2}^2}{2m_2} + \frac{k}{2}\mathbf{x_1}^2 + \frac{k}{2}\mathbf{x_2}^2 + \frac{K}{2}(\mathbf{x_1} - \mathbf{x_2})^2$$

Here k is the spring constant holding both particles in the bottom of the well, and K is the spring constant holding the two particles together. Assume that the two particles are distinguishable atoms.

(For this problem you may find it useful to transform to relative and center-of-mass coordinates. If you find this difficult, for simplicity you may assume that $m_1 = m_2$.)

(a) Analogous to exercise 2.1 above, calculate the classical partition function and show that the heat capacity is again $3k_B$ per particle (i.e., $6k_B$ total).

(b) Analogous to exercise 2.1 above, calculate the quantum partition function and find an expression for the heat capacity. Sketch the heat capacity as a function of temperature if $K \gg k$.

(c)** How does the result change if the atoms are indistinguishable?