Homework 1- Lectures 1-3
Early models of Specific Heat in Solids
Due: 1/30/2023

Problem 1

Classical Einstein 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

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

a) Calculate the classical partition function

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

Here $\beta=1/(k_B T)$. Note: in this problem p and x are three dimensional vectors.

b) Using the partition function, calculate the energy expectation value as a function of temperature:

$$\langle E(T) \rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$

c) Calculate the heat capacity:

$$C == \frac{\partial \langle E \rangle}{\partial T}$$

d) Show 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.

Problem 2

Quantum Einstein Solid:
Now consider the same Hamiltonian as in problem 2 quantum mechanically.

a) Express the energy eigenvalues, E_j in terms of k and m.
b) Calculate the quantum partition function

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

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

c) Explain the relationship with Bose statistics
d) Find an expression for the heat capacity.
e) Show that the high temperature limit agrees with the law of Dulong and Petit.
f) Sketch the heat capacity as a function of temperature.

Problem 3

Debye model.

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

b) Guess the element with the highest Debye temperature and the one with the lowest. Explain your reasoning.

c) 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.

Problem 4

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

a) State your assumptions. Leave your answer in terms of an integral that one cannot do analytically.
b) At high T , show the heat capacity goes to a constant and find that constant.
c) At low T , show that $C_v = KT^n$. What is the value of n? Express K in terms of a definite integral.