Exercise 07

NAME:	MATRICULATION NUMBER:
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RESULTS:

7.1		OF 10 P
7.2		OF 8 P
TOTAL		OF 18 P

GENERAL INSTRUCTIONS

- SUBMIT YOUR SOLUTION TO LUCA DONATI (R. 35.17) BEFORE **THURSDAY 16. JUNE AT 8.15 AM**.
- FILL OUT THIS COVER SHEET AND SUBMIT IT ALONG WITH YOUR SOLUTION.
- SHOW HOW YOU ARRIVED AT YOUR ANSWER.

7.1 Einstein model for solids (10 P)

The Einstein solid is a model of a solid based on two assumptions:

- Each atom in the lattice is an independent 3D quantum harmonic oscillator at a fixed position
- All atoms oscillate with the same frequency

Because each atom can vibrate in each spatial direction, a system of N atoms is treated as a system of $3N$ independent harmonic oscillators governed by the Hooke's law:

$$F_i(x) = -k(x - x_0) \tag{1}$$

where $F_i(x)$ is the force acting on the atom i in direction x, k is the constant characteristic of the oscillator and x_0 is the equilibrium position. The frequency of the oscillators is given by

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \tag{2}$$

where m is the mass of the atom and the possible energies are given by

$$E_n = h\nu\left(n + \frac{1}{2}\right) \quad \text{with} \quad n = 0, 1, 2, ... \tag{3}$$

1. Determine the expression for the canonical partition function of a single harmonic oscillator.
2. What is the expression for the canonical partition function of the full system?
3. Write down the expressions for the Helmholtz free energy function $A(N, V, T)$ and the internal energy U.
4. Derive the formula for the heat capacity

   $$C_V = 3Nk\left(\frac{h\nu}{2kT}\right)^2 \frac{1}{\sinh^2\left(\frac{h\nu}{2kT}\right)} \tag{4}$$

   where T is the temperature.
5. The quantity $\frac{h\nu}{k}$ has the dimension of a temperature, it is an intrinsic property of the solid and it is known as Einstein temperature T_E. Plot the quantity C_V as a function of the ratio T/T_E.
6. How can you simplify the equation (4) in the limit of high temperature ($T \gg T_E$) and low temperature ($T \ll T_E$)?

7.2 Two states system (8 P)

Suppose we have a two-state system, specifically, consider a particle such as an electron or proton, which has two spin states, up (+1) and down (-1). Let's apply a magnetic field $\mathbf{B}$, so that the two states can have energy

$$E(\text{up}) = +\boldsymbol{\mu} \cdot \mathbf{B} \ ; \qquad E(\text{down}) = -\boldsymbol{\mu} \cdot \mathbf{B} \tag{5}$$

where $\boldsymbol{\mu}$ is the magnetic momentum and the energy difference between the two states is given by

$$\Delta E = E(\text{up}) - E(\text{down}) = 2\boldsymbol{\mu} \cdot \mathbf{B} \tag{6}$$

1. Write down the partition function Q_1 for a single particle.
2. Assume that $E(\text{down}) = 0$, write down the partition function Q_1^0.
3. What is the partition function Q_N^0 for a system of N particles?
4. Determine the free energy F, the internal energy U, the entropy S and the heat capacity C_V.
5. Plot the internal energy and the heat capacity as a function of the temperature.