PHYS 403: HOMEWORK ASSIGNMENT No. 3: CANONICAL DISTRIBUTION

(Feb 13th, 2020)

HOMEWORK DUE: WEDNESDAY, FEB 26th, 2020

To be handed in during class- Late Homework will not be accepted

QUESTION (1) EINSTEIN PHONONS: This one is to give you a feeling for Einstein phonons (or "vibrons") as they exist in molecules. We will look at the CO_2 molecule, which is linear in shape, and has 4 vibrational modes with frequencies ω_j, with $j = 1, 2, ..4$.

1(a) Write down the canonical partition function for the system of phonons, and then find a result for the specific heat due to these phonons, as a function of temperature T, in terms of the $\{\omega_j\}$.

1(b) Suppose the phonon frequencies are given in temperature units defined as $\theta_j = \hbar\omega_j/k_B$, with the values $\theta_1 = 3360\ K, \theta_2 = 1890\ K$, and $\theta_3 = \theta_4 = 954\ K$. Find the heat capacity of the molecule at a temperature $T = 300\ K$.

1(c) Now, using software of your choice, plot the specific heat of this system as a function of temperature over the temperature range $0 < T < 3000\ K$. Assume that the system remains a low-density gas throughout this temperature range. How accurate do you think this assumption is?

QUESTION (2) ROTATING BODY: Suppose we have an ideal gas of N_o particles in a cylinder of height z_o and radius R_o, rotating with angular velocity Ω_o about its axis. Then it can be shown that the canonical partition function for the gas rotating with the cylinder is given by

$$Z(\Omega_o, \beta) \;=\; Z_o(\beta) Z_{rot}(\Omega_o, \beta) \qquad (0.1)$$

where $Z_o(\beta)$ is the partition function when $\Omega_o = 0$, and the multiplicative factor $Z_{rot}(\Omega_o, \beta)$ is given by an integral over the gas volume of form

$$Z_{rot}(\Omega_o, \beta) \;=\; \left(\frac{1}{V_o} \int dV \exp[-\beta U(r)] \right)^{N_o} \qquad (0.2)$$

in which $U(r) = -\frac{1}{2} m\Omega_o^2 r^2$ is the "centrifugal potential", $V_o = \pi R_o^2 z_o$ is the volume of the gas, and N_o is the number of particles in the gas.

2(a) Show, by direct integration over the the volume of the gas that the free energy is given by

$$F \;=\; F_o \;-\; N_o k_B T\, ln \left(\frac{2k_B T}{m\Omega_o^2 R_o^2} \left(\exp\left[m\Omega_o^2 R_o^2 / 2k_B T \right] - 1 \right) \right) \qquad (0.3)$$

where $F_o(\beta)$ is the free energy when $\Omega_o = 0$.

2(b) Now find the correction $\Delta C_V(T, \Omega_o)$ to the specific heat $C_V(T, \Omega_o = 0)$ as a function of the rotation rate.

END of 3RD HOMEWORK ASSIGNMENT