FYS 4130 Statistical Mechanics

Homework 4 Feb 10, 2009

1) Diatomic Gas

Consider a gas of noninteracting diatomic molecules. The rotational energy of the molecules can be modelled as a rigid quantum rotator with energy levels $E_{rot}(l)$ with degeneracy $g(l)$ given by:

$$E_{rot}(l) = l(l+1)\frac{\hbar^2}{2I} \qquad g(l) = 2l+1 \qquad l = 0, 1, 2, ...$$

Where I is the moment of inertia. The Hamiltonian for the system is then:

$$H = \frac{P^2}{2m} + E_{rot}$$

a) Find the canonical partition function of a gas of N non-interacting diatomic molecules. Write this as a product of the partition function for an ideal monatomic gas, Z_I, and a contribution from the rotational energy, $Z = Z_I Z_R$. Leave the partition function in the form of a sum.

b) This sum can be evaluated at the limits of high and low temperature. For the high temperature limit use the partition function to find the energy the specific heat of this gas. This should agree with the equipartition theorem for energy.

c) For the low temperature limit, calculate the sum in the partition function for the lowest temperatures where the rotational motion of the molecules makes a contribution. This will be where only the lowest rotational levels are significant, for $l = 0, 1$. Calculate the energy and specific heat of the gas.

Solution:

a) $Z = \frac{1}{N!}\frac{V^N}{\Lambda^{3N}}(\sum_{l=0}^{\infty}(2l+1)e^{-\beta l(l+1)\hbar^2/2I})^N$

b) $U = 3/2NkT$

c) Keep only $l = 0, 1, 2$ in the sum for the partition function.
$C_v = 3/2Nk + \frac{6N\theta^2}{e^{2\beta\theta}+3}\frac{1}{kT^2}$

2. System of oscillators

Consider a system of N 3 dimensional oscillators, for example the vibrating atoms in a crystal lattice, with the Hamiltonian:

$$H = \sum_{i=1}^{3N} (\frac{P_i^2}{2m} + \frac{1}{2} m\omega^2 q_i^2) \tag{1}$$

a) Calculate the phase space volume.
(The phase space volume has the dimension $n = 6N$)

b) Calculate the entropy and the energy of the system.

Solution:

The phase space volume is

$$\Omega = \frac{1}{(2\pi\hbar)^{3N}} \frac{\pi^{3N}}{(3N)!} \left(\frac{2mE}{m\omega}\right)^{3N} \tag{2}$$

$$S = 3Nk(1 + log\frac{E}{3N\hbar\omega}) \tag{3}$$