Problem set 2: Computational Molecular Physics

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April 28, 2015

(Please send the solution by e-mail to **tahereh.ghane@gmail.com** by **Fri. 1.05 (2pm)** at the latest.)

1 Canonical Ensemble

(10 points)

1- Initiating from the definition of average energy in canonical ensemble ($< E >= \Sigma_i P_i E_i$) and using canonical partition function prove that: $< E >= -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$

2- Starting from the entropy of canonical ensemble ($S = -k_B \Sigma P_r ln P_r$) and using the definition of Helmholtz free energy ($A = -k_B T ln Z$), prove that: $A = E - TS$

2 Ensemble Averages

(20 points)

We have a system with 2 spins with magnetic moments μ_1 and μ_2, respectively, which is in thermal equilibrium with a bath of temperature T. Consider an external magnetic field B which interacts with each spin according to $E(i, \pm) = \pm \mu_i B$ assuming that the spins do not interact with each other. First, prove that partition function calculated as :

$$Z = 4cosh(\beta B \mu_2) cosh(\beta B \mu_1)$$

Then, using the definition of Z calculate:

(a) The average value of total internal energy of the system ($< E >$),

(b) The entropy of the system,

(c) The Helmholtz free energy,

(d) If the contributions to the total magnetization M are $m_i(\pm) = \pm \mu_i$ calculate the average value of the magnetization of the system at T.

(Note1: The spins can only be "up" (+) or "down" (-) relative to magnetic field with $E(i, +) = \mu_i B$ and $E(i, -) = -\mu_i H$, respectively.