AMA4004 Statistical mechanics: Ensembles

This assignment contains no hard parts and as such if this report is handed in for the portfolio the maximum mark you can get for it is 8/12.

In order to do this exercise you will need to work through the following materials:

- http://gtribello.github.io/mathNET/GENERALIZED_PARTITION_FUNCTION.html
- http://gtribello.github.io/mathNET/CANONICAL_ENSEMBLE.html
- http://gtribello.github.io/mathNET/ISOTHERMAL_ISOBARIC_ENSEMBLE.html

You must prepare a short report (no more than 3 pages) on one of the following six ensembles. (I will tell you which you are to do)

- The canonical (NVT) ensmeble
- The canonical (NHT) ensemble - H being magnetic field strength
- The Isothermal-Isobaric (NPT) ensemble
- The grand canonical (μVT) ensemble
- The grand canonical (μPT) ensemble
- The microcanonical ensemble

If your report is on any of the first five of the ensembles above you should:

- Write about which thermodynamic variables are constrained in this particular ensemble.
- Derive an expression for the probability of being in a microstate in this ensemble.
- Derive an expression that can be used to calculate the partition function.
- Show that certain ensemble averages can be calculated by taking suitable derivatives of the logarithm of the partition function.
- Explain how you can relate the logarithm of the partition function of this ensemble to a particular thermodynamic potential.
- Derive an expression that relates fluctuations in the value of a extensive quantity with a response function.

If you report is on the microcanonical ensemble you should:

- Explain what the probability of being in a particular state is equal to for the microcanonical ensemble.
- Give an expression for the microcanonical partition function.
- Show how partition functions for all other ensembles can be calculated from the microcanonical partition function.
- Discuss how partition functions that incorporate constraints on microscopic coordinates can thus be calculated.
- Explain the meaning of the term “Potential of mean force”