Homework 7
Due in class Tuesday, March 1, 2016.

Problem:

Q.1. Starting from the fact that the limiting distribution in the Grand Canonical ensemble is proportional to

$$\exp\left[-\beta\left(V(r)-N\mu\right)+\ln\frac{V^N}{\Lambda^{3N}N!}\right] \quad (1)$$

where $\Lambda=\sqrt{h^2/2\pi mk_B T}$ is the thermal de Broglie wavelength, derive the respective acceptance probabilities for (i) creating and (ii) destroying a particle in a Monte Carlo realization.

Computer Experiment:

Monte Carlo method for the XY spin model. For the following computer experiment, use the LJ code version 0.09 and 'input_v09_pset7.txt' (both available from the Learn website).

- make sure you compile in **two** dimensions (file 'defs.h' uncomment line “#define NDIM 2”)
- build the program by typing: % make 1
- run it by typing: % ./run_me input_v09_pset7.txt

P.1. (i) Run the code using the input T (temperature) from 1 to 10 in step increments of 1 (by editing the input file). (ii) For each temperature, wait until the system equilibrates and calculate the **average order parameter** (column 8 of 'thermo.dat') and its **standard deviation** per temperature. If the order parameter and fluctuations don't seem to settle down, you might want to let it run until its conclusion and average over the whole run, important for high temperatures. (iii) Plot this order parameter vs T including the standard deviation (as error bars) in your data. (iv) Discuss what the order parameter describes in this system and how does the shape of the curve relate to the process that you are simulating. (v) Additionally, explain in simple terms a reason for the observed behavior in the standard deviation.