Chemistry 40642/60642 Spring 2016
Professor J. Daniel Gezelter Due Friday 3/4/2016

Problem Set 2

You may combine your efforts with other students on the problems but you must acknowledge the contributions of your collaborators.

1. Chandler problem 5.12
2. Chandler problem 5.13
3. Chandler problem 5.21
4. Chandler problem 5.25
5. Monte Carlo simulation of 2-D Ising Model: For this problem you will write a Monte Carlo problem for the two dimensional Ising model on a cubic lattice $L \times L$ (total number of spins is $N = L^2$). Working in small groups ($2-3$ people) is encouraged. You may use parts of the code published in text books (Chandler or Binder and Heermann) or that you find online. If you need copies of an Ising code to get started, I can supply them in a few different languages (python, fortran, Java, JavaScript). The goal of this problem is to gain an understanding of the Ising model's phase behavior and also to enhance your computational skills.

   (a) Show that your random number generator is reliable. That is, does it yield independent, identically distributed random variables, uniformly distributed in the interval $[0, 1]$?

   (b) Write a code for the 2 dimensional Ising model, with $H = 0$. Explain briefly the Monte Carlo method. Explain the main ideas of the code, the clever ideas that save computation time, etc. Discuss briefly the expected effects of boundary conditions. What boundary conditions did you choose?

   (c) Obtain a Monte Carlo "trajectory" of the average spin

$$S(t) = \sum_i \frac{\sigma_i(t)}{N},$$

   where the summation is over all spins in system and t is a particular "step" in the Monte Carlo simulation. For three representative temperatures, plot $S(t)$ as a function of time. Explain the physical behavior of your observations. This exercise will help you estimate the typical number of Monte Carlo cycles (t) for equilibrium to be reached. For periodic boundary conditions, a 20×20 Ising system is sufficient.

   (d) For systems of length $L = 10, 20, 50, 100, 1000$ determine the magnetization $\langle |M_L| \rangle$ and susceptibility χ_L, as a function of temperature (for periodic boundary conditions, work in the range $0.5 < T/T_c < 1.7$). Plot $\langle |M_L| \rangle$ versus T/T_c for different system sizes L on a single plot (and similarly for χ_L). Remarks: (i) obtain χ_L from fluctuation of magnetization, and briefly explain its physical meaning (ii) for convenience use Onsager's T_c.

(e) Use finite size scaling to determine the critical temperature T_c in the limit $L \to \infty$ and the critical exponent β defined by $\langle |M_L| \rangle \sim |T - T_c|^{\beta}$. Compare with Onsager's solution.

(f) Calculate the correlation function

$$\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$$

for various spin separations and temperatures. Explain your observations. For further details see Chandler 6.10.

(g) Summarize briefly Chandler's umbrella sampling technique. Solve 6.16.

(h) Extra Credit: Consider a single spin trajectory $\sigma_1(t)$ as a function of Monte Carlo cycle. This individual spin will flip at random times between state $+1$ and -1 and vice versa. Obtain the distribution (histogram) of cycles (or time) between flipping events. Start with $T > T_c$ and attempt to approach T_c from above. Explain your observations. What happens when $T < T_c$?