Chemistry 40642/60642 — Spring 2016
Professor J. Daniel Gezelter — Due Fri. 1/29/2016

# Problem Set 1

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

1. For the nearest-neighbor Ising model,

$$\mathcal{H} = -H \sum_{n} \sigma_n - \frac{J}{2} \sum_{n,n'}^{N.N.} \sigma_n \sigma_{n'}$$

   with external magnetic field ($H \neq 0$), determine the zero-temperature states as a function of $J$ and $H$. Present the results on a H-J zero-temperature diagram marking clearly which states are favored in the various regions of the diagram.

2. For the one-dimensional Ising model, plot the average energy (actually $E/NJ$), the magnetic susceptibility, and the specific heat all against $kT/J$ between values of 0 and 5. Discuss the specific heat maximum at around $kT/J = 1$.

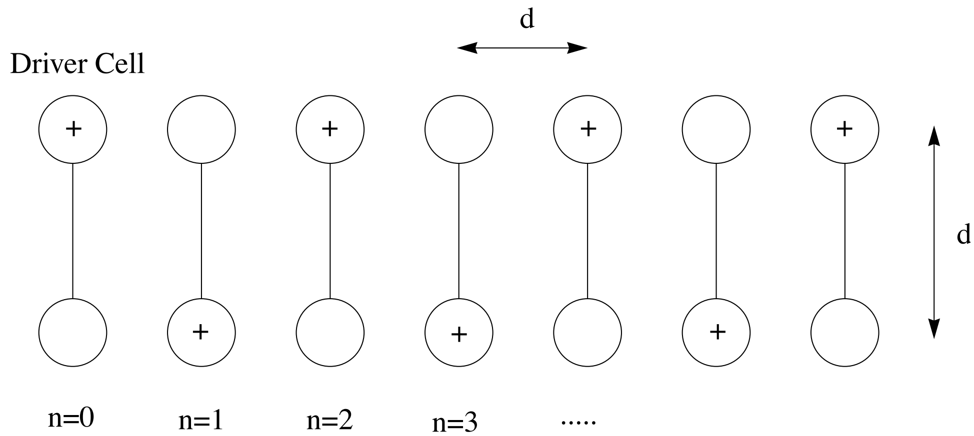
3. For the one-dimensional Ising model, calculate the correlation function ($\langle \sigma_0 \sigma_n \rangle$) between any two sites as a function of the distance between them. Do the calculation for $H = 0$ and then attempt it for $H \neq 0$.

4. In the mean-field theory for the Ising model, we can make the approximation

$$\sum_{n'} J_{nn'} \sigma_{n'} = kT tanh^{-1} \sigma_n$$

   Numerically solve this equation for the nearest-neighbor Ising model. Plot the spin density (i.e. the magnetization) as a function of temperature. Use a physical argument to account for the limiting behavior of the curve as the temperature becomes large.

5. Quantum Cellular Automata: A very hot topic in some departments at Notre Dame is a new logic device built out of coupled molecular parts that can take on logic-like states. In our model of a QCA device, we will use the following picture:




Each cell has one excess electron that can move relatively easily between a pair of metal atoms. There is a single "driver" cell on the left side of the chip that we can force into the "+" state, i.e. the electron is on the upper metal atom. Since we now are experts at the Ising model, we will denote the state of the $i^{\text{th}}$ cell as $S_i$. This variable tells us where the electron is in that cell. In the above diagram, we have $S_1 = -1$ and $S_2 = +1$.

a) Use basic electrostatics to show that the energy between the $m$ and $n$ cells may be written

$$\begin{aligned} E_{mn} &= \frac{q^2}{8\pi\epsilon_0 d}\left(\frac{1}{\sqrt{(m-n)^2}} + \frac{1}{\sqrt{(m-n)^2+1}}\right) \\ &\quad + \frac{q^2}{8\pi\epsilon_0 d}\left(\frac{1}{\sqrt{(m-n)^2}} - \frac{1}{\sqrt{(m-n)^2+1}}\right) S_m S_n \end{aligned}$$

b) Write out the full Hamiltonian for a chain of $N$ cells in a line to the right of the driver cell. Identify constants that could be replaced by a site-dependent field $H_n$ and coupling $J_{n,n'}$.

c) Solve for the partition function in the nearest neighbor approximation.

d) Derive $\langle S_N \rangle$, which is the average magnetization of the $N^{\text{th}}$ spin. Note that this is *not* the same as the average magnetization of the lattice.

e) Plot the $\langle S_N \rangle$ as a function of temperature when $N = 10$, $N = 100$, and $N = 1000$. You may assume $d = 7.5$Å to perform this calculation.

f) If $d = 20$Å, what temperature range would we be able to run our device at and still have a well-defined logic state in cell 1000?