Chemistry 60642 Spring 2016
Professor J. Daniel Gezelter Due Weds. 5/4/2016

Final Exam

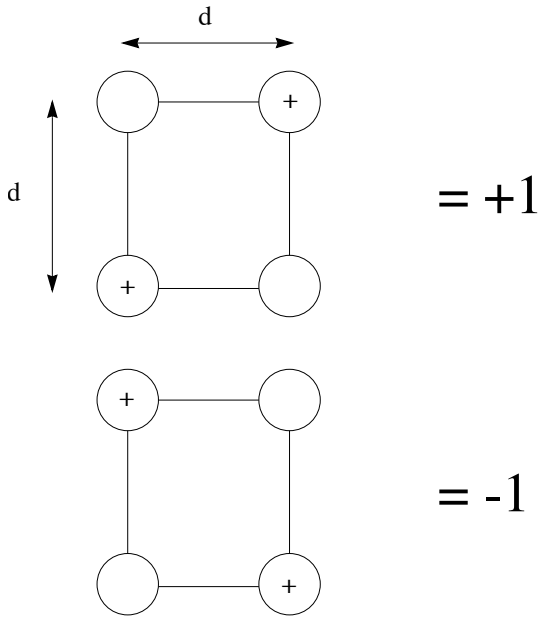
General instructions

1. There are 4 problems. You must do 3 of them for full credit.
2. You are not allowed to discuss this exam with anyone other than Professor Gezelter.
3. You may use books or class notes as long as you clearly cite their contributions to your solutions. *You may not search for solutions on the net*. If you have any questions about whether a source is acceptable, ask Professor Gezelter before using it. You must sign the statement below to affirm your compliance with these rules.
4. You must show all of your work for full credit. This includes printouts of any Mathematica sessions.
5. Your solutions are due in my office (258 Stepan) by 4 p.m. on Wednesday, May 4, 2016.

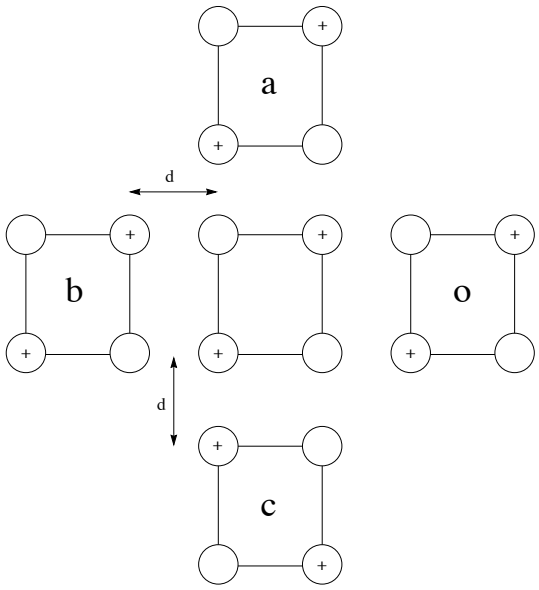
I certify that I have not discussed this exam with anyone other than Professor Gezelter and that I have not used any forbidden or uncited sources in my solutions.

Signature: _____

1. One paradigm for the Quantum Cellular Automata (QCA) computing device is the 4-center, 2-charge device, which has 2 low-lying energetic states,



The "Majority Gate" is a logic device which takes the inputs of three driver cells (a, b, c) and returns in a cell (o) the state that is held by the majority of the a, b, and c cells.



a) How many states are available to the entire system if cells a and b are fixed in the +1 state and cell c is fixed in the -1 state?

b) Use basic electrostatics to determine the energies for two nearest-neighbor cells in the same state and for two nearest-neighbor cells in different states as a function of the cell spacing, d.

c) Using only nearest-neighbor interactions, compute the energies of all of the states of the system you found in part a).

d) Again, using only nearest-neighbor interactions, compute the partition function for the system using the states of the system you found in part a).

e) What is the average polarization of cell o as a function of temperature and cell spacing given your results to the rest of this problem?

f) What have we left out of our treatment of the Majority Gate? How would you improve the treatment of this system?

2. Spin Lattice Models

The 3-state Potts model is very much like the Ising model, but has *three* spin states at each lattice site,

$$s_n = \begin{cases} +1 \\ 0 \\ -1 \end{cases}$$

The Hamiltonian looks identical to the Ising model Hamiltonian,

$$\mathcal{H}_{\text{Potts}} = -H \sum_{n=1}^{N} s_n - \frac{J}{2} \sum_{n,n'} s_n s_{n'}$$

where H is the field interacting with all spins, and J is the coupling constant that connects interacting (nearest-neighbor) spins.

a) For the one dimensional Potts model with periodic boundaries, write the 3×3 transfer matrix, $\langle s_n|\mathbf{P}|s_{n+1}\rangle$ that connects one spin to the next one. As we did with the Ising model, you should re-write the field term into an equivalent form so that your transfer matrix is symmetric.

$$\langle s_n|\mathbf{P}|s_{n+1}\rangle = \begin{pmatrix} & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \end{pmatrix}$$

b) Use your transfer matrix in part a) to compute the Partition Function for the 1-d Potts model with periodic boundaries (in the limit of a large number of spins).

c) Compute the free energy for this model.

d) Compute the heat capacity at zero-field.

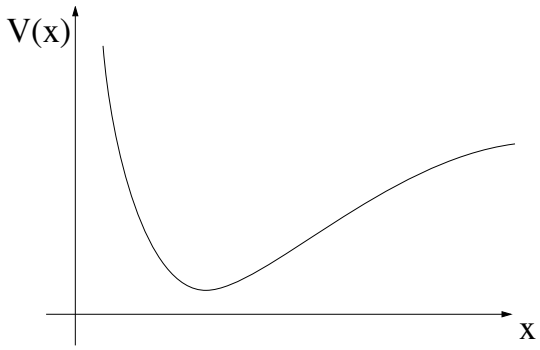
e) Does this model have a phase transition? If so, where is it? If not, why not?

3. The Gibbs-Bogoliubov variational principle is a general principle which tells us that

$$A \leq A_o + \langle \mathcal{H} - \mathcal{H}_o \rangle_o$$

where $\mathcal{H}_o$ is an approximate Hamiltonian to the real Hamiltonian $\mathcal{H}$. (A_o and A are the free energies for the two systems, respectively.)

Consider a general potential $V(x)$ like the one shown below.



The Hamiltonian is

$$\mathcal{H} = \frac{p^2}{2m} + V(x)$$

In order to apply the Gibbs-Bogoliubov variational principle, we're going to use the quantum mechanical harmonic oscillator as the reference Hamiltonian:

$$\mathcal{H}_o = \frac{p^2}{2m_o} + \frac{m_o \omega_o^2}{2}(x-a)^2 .$$

To use the variational principle, we will vary the three parameters: a, m_o and ω_o.

a) To get you started, use the energy levels of the quantum mechanical harmonic oscillator to determine Q_o and from that, determine A_o.

b) Given the statement of the GBVP above, what derivatives would you have to take to find the best values for a, m_o and ω_o?

c) Show that the best value for $m_o = m$.

d) Determine the best values for a and ω_o, and show that they are determined from:

$$\langle V'(x) \rangle_o = 0 \tag{1}$$

$$\langle xV'(x) \rangle_o = \langle \frac{p^2}{m} \rangle_o \tag{2}$$

Here $\langle \rangle_o$ is taken over the states of the reference Hamiltonian, $\mathcal{H}_o$. Eq. (1) comes from the consideration of the fixed location of the system (i.e. a non-zero average force would imply motion), and Eq. (2) corresponds to the virial theorem, which states that

$$\langle xV'(x) \rangle = \langle \frac{p^2}{m} \rangle$$

4. The wave function for a free particle in three dimensions can written (in the spatial representation) as:

$$\langle \mathbf{r}|\mathbf{k}\rangle = \psi_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}},$$

where $\mathbf{k}$ is related to the momentum eigenvalue of that wavefunction:

$$\hat{\mathbf{p}}|\mathbf{k}\rangle = \mathbf{p}|\mathbf{k}\rangle = \hbar\mathbf{k}|\mathbf{k}\rangle$$

(Although I find Dirac notation simpler, if you prefer to work in wavefunction notation, the momentum operator in three dimensions may be written $\hat{\mathbf{p}} = -i\hbar\nabla$ where ∇ is the gradient operator).

a) Prove that the free particle wavefunctions are eigenfunctions of the Boltzman operator, $e^{-\beta\hat{H}}$. What are the eigen*values* of the Boltzman operator?

b) Prove that the density operator between two distinct spatial locations,

$$\rho(\mathbf{r},\mathbf{r}') = \langle \mathbf{r}|e^{-\beta\hat{H}}|\mathbf{r}'\rangle$$

is a Gaussian function of the separation between those two locations with variance $\sqrt{\beta\hbar^2/m}$.

c) Give a physical interpretation of this result. That is, what does the density operator between two locations *mean*? What does changing the free particle's mass and/or temperature do?