PH325: Advanced Statistical Mechanics

Centre for Condensed Matter Theory, Physics Department, IISc Bangalore
Semester I, 2014–2015

PROBLEM SET 2, DUE: SEPT. 11, 2014

2/1. **(C/T) Clausius-Clapyron** Verify the Clausius-Clapyron relation along the first order liquid gas line that we obtained in the class for the system of interacting particles. (This is your opportunity reproduce the results of class notes, using Mathematica or otherwise.)

2/2. **(C) Virial coefficient:** Consider the interacting particle model in d dimensions with a potential of interaction

$$V(r) = \begin{cases} \infty, & r < r_0 \\ -u_0 \left(\frac{r_0}{r}\right)^{\alpha}, & r >= r_0 \end{cases}$$

For a given d, what is the range of α for which the second virial coefficient a_2 is well defined?

2/3. **(C) Jellium, the classical variety:** A famous model for a metal is the jellium model. The metal is modeled as a "gas" of electrons of density n_0 (let us focus on 3d - three spatial dimensions), and the ions that make up the solid are considered as a "smooth jelly" with the same density n_0 – in other words, the ions "do nothing"[1] except to provide for a charge neutralising positive background charge density. In this problem we will work out the classical version of this theory. The key question we ask is does the jellium electrons have a gas-liquid transition, and if so what is the critical point.

(a) Write out the Hamiltonian of the jellium model and discuss its symmetries.

(b) Should we *expect* the jellium electrons to have a liquid phase?

(c) Using the procedure that we developed in class (and revisited in the previous problem 2/2), attempt to obtain the phase diagram. You should discover that the procedure fails miserably! Connect the problems you encounter with the results of 2/2, and argue that the long range nature of the Coulomb interaction is the cause of the problem.

(d) Since electrons are very mobile, the long range nature of the Coulomb interaction is mitigated by *screening*. To see best what this means, introduce an external test charge of q into the system. Find out the the electrostatic potential of this charge using the following steps.

i. Let the charge be placed at the origin. This will reorganize the electronic charge density which becomes $n(r)$. Write out an expression for the *total charge density* $n_t(r)$ as a function of r.

ii. Let the electrostatic potential due to the test charge be $\phi(r)$. Use Poisson equation to relate $\phi(r)$ and $n_t(r)$.

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[1] A concept that is very familiar to all of us.

iii. Now, define a *local* chemical potential $\mu(r)$ for the electrons. Argue that $\mu(r)$ as $r \to \infty$ goes to μ_0 (the chemical potential of a non-interacting gas of electrons with density n_0 at temperature T). Based on this result, show that $\mu(r) = \mu_0 - e\phi(r)$, where μ_0 is the chemical potential of an ideal gas of electrons with density n_0 at temperature T.

iv. Next, relate $n(r)$ to $\mu(r)$ using the ideal gas equation of state. Recall as shown in class, for ideal gas with density n_0 at temperature T, $e^{\beta\mu_0} = \lambda^3 n_0$, this is what you need to use in a "local" fashion. Now linearize this equation in $\phi(r)$ and find a linear relationship between $\phi(r)$ and $n(r)$.

v. Use the linear relationship obtained and show that the Poisson equation in standard units reduces to

$$\nabla^2\phi + \xi_D^{-2}\phi = -\frac{q}{\varepsilon_0}\delta(r)$$

where ξ_D is the Debye screening length. What is the expression for ξ_D?

vi. Solve the above equation and show that $\phi(r) \sim \frac{e^{-r/\xi_D}}{r}$, doing everything you need to do to convert the $\sim$ to an $=$. This is the screened Coulomb interaction.

(e) Now use the argument that every electron behaves exactly as a test charge, and produces a screened Coulomb potential. Using this screened interaction, obtain the viral coefficient a_2, and from there on the phase diagram.[2]

2/4. **(C) Properties of Markov Matrix:** Consider the Markov matrix $W(n, m)$ introduced in class. Let λ be a right eigenvalue of W. Show that $|\lambda| \leqslant 1$. Comment on the nature of eigen-probability distributions when $\lambda = 1$ and $0 < \lambda < 1$. Can λ be complex? If yes, what kind of distribution would that correspond to?

2/5. **(C/T) Markov Muscle Flexing:** Consider a set of 2 identical random walkers on a 3 site lattice with periodic boundary conditions. A walker hops to the right with probability p and to the left with $q = 1 - p$.

(a) Enumerate the states of the system (we will use symbols like m and n to count them). The key here is to find a nice numbering scheme.[3]

(b) What is the size of the Markov matrix $W(n, m)$?

(c) Write out a Markov matrix describing the random walk process. Make sure that your matrix you find satisfies the elementary properties of Markov matrices.

(d) Is this process irreducible? Justify.

(e) Find the right eigenspectrum of $W(n, m)$, and the associated probability distributions.

(f) Discuss the physics of your solution for $p = 1/2$. What happens when $p \neq \frac{1}{2}$?

2/6. **(C/T) Monte Carlo time!** Extend the code that you wrote in the previous assignment, to perform Monte Carlo calculations of the 1D Ising chain. The code should use temperature T, the uniform magnetic field h, number of sites N as inputs.

(a) Choose $N = 100$, and obtain the magnetization as a function of temperature at $h = 0$ using Monte Carlo simulations. Are you surprised? What happens if you choose $N = 1000$? What happens if you take larger number of Monte Carlo steps?

[2] I have not worked this out myself; there could be something to discover here! Moreover, understanding the concepts of this problem is very important as it forms the basis of many things to come.

[3] Again, I have not worked this out myself.

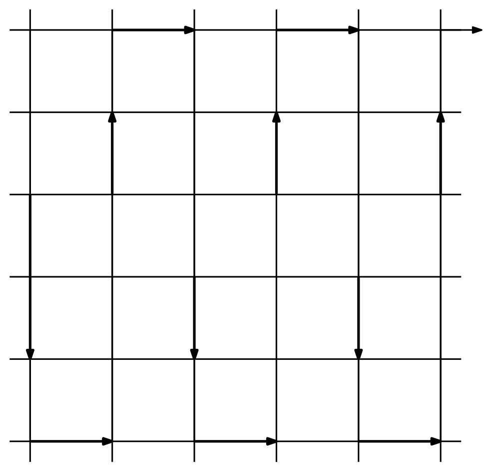
(b) Find the spin-spin correlation function as a function of distance between the spins, and obtain the correlation length as a function of temperature.

(c) Reconcile these results with the exact analytical results obtained in class.[4]

2/7. **(C) Two-Site Ising:** Consider a *two-site* Ising model with Hamiltonian $H = -JS_1S_2$. Prove or disprove the statement: For $J > 0$, the magnetic susceptibility for a uniform magnetic field (equal at both sites) is smaller than the case where $J = 0$. What is the result for $J < 0$?

2/8. **(C/T) Ferro and Anti-Ferro Ising:** Prove or disprove the statement: The partition function of the ferro Ising model with a uniform magnetic field on a d-hypercubic lattice $H = -J\sum_{ij} S_i S_j - h\sum_i S_i$ $(J, h > 0$ is equal to that of the anti-ferro Ising model $(J < 0$, and of equal magnitude as the ferro) with the same uniform magnetic field.

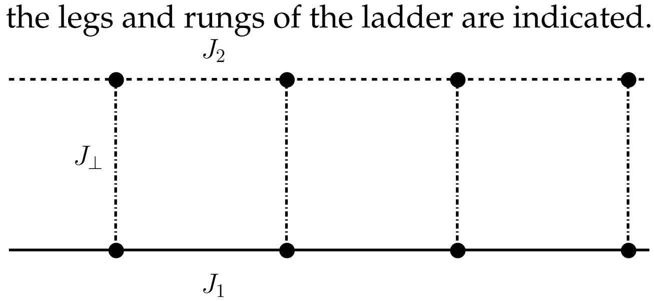
2/9. **(C) Argument shows no order in 2D Ising!** A bright young student argues that the square lattice Ising model is simply a liner chain Ising model that is "curled up"! She says that if one traverses the path on a square lattice as shown in the figure, one sees a linear chain!



Now the 1D Ising model does not have long range order at finite temperature, and hence she insists that the result must be true for the square lattice Ising model as well! She concludes that the square lattice Ising model also does not have long range order. What is wrong with her argument?

2/10. **(C) Long range interactions:** Consider a 1d Ising chain with long range interactions $H = -\frac{1}{2}\sum_{\{i,j\}} J_{ij} S_i S_j$ where $\{i, j\}$ is every pair of sites and $J_{ij} = \frac{J}{|i-j|^\alpha}$. This is a system with long range spin interactions. Does the argument used to conclude that Ising model has no long range order at finite temperatures hold for any α? Explore.

2/11. **(C/T) Ising...on a ladder:** Consider the Ising model on a ladder as shown in the figure. The couplings on the legs and rungs of the ladder are indicated.



[4]This is an opportunity for you to learn thoroughly the transfer matrix method for the 1d-Ising Model.

(a) Find a "clean" way to write out the Hamiltonian of this system.[5]

(b) Assuming $J_1 = J_2 = J_\perp$, find out by qualitative arguments if system would order below a finite temperature.

(c) Use the transfer matrix method to find the free energy of the system for any J_1, J_2 and $J_\perp$. Does your answer agree with the result obtained by physical arguments for the case discussed just above? Discuss.

(d) **(C, and really C) Finding <u>Effective</u> Hamiltonians:** Now let us keep $J_1 = J_2 = J$ and send $J_\perp \to \infty$. Based on *physical arguments*, find the "low-energy" Hilbert space of the problem, write out an *effective Hamiltonian* on this Hilbert space. Now use the general result of the transfer matrix of the previous part when $J_\perp \to \infty$ (with J_1 and J_2 fixed at J), and derive this effective Hamiltonian.

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[5] "Cleaness", like cleanliness, is a subjective idea.