PH325: Advanced Statistical Mechanics

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Semester I, 2014–2015

PROBLEM SET 1, DUE: AUG. 25, 2014

Reading: Chaikin and Lubensky, Appendix of Chapter 2.

1/1. **(C) Hypercubic lattice:** Consider the hypercubic lattice in d dimensions introduced in class.

(a) How many nearest neighbours does a site have?

(b) How many *unique* bonds emanate from a site? A bond is a link between a site and its nearest neighbour.

1/2. **(T, C for some!) Fourier this!** Consider the Ising model on d-hypercubic lattice with

$$H = -J \sum_{\langle ij \rangle} S_i S_j, \tag{1}$$

$\langle ij \rangle$ is on nearest neighbour bonds. The system is a lattice with lattice parameter a in a box of size $N = L^d$ (L is large positive integer), with periodic boundary conditions. Define the Fourier transform of S_i as

$$S(\mathbf{k}) = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} S_i,$$

where $\mathbf{R}_i$ are the position vectors of lattice sites. Please note that this definition is slightly different from what we did in class.

(a) What are the allowed values of $\mathbf{k}$? Show that for two allowed values $\mathbf{k}$ and $\mathbf{k}'$

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} e^{i\mathbf{k}'\cdot\mathbf{R}_i} = N\delta_{-\mathbf{k},\mathbf{k}'}$$

(b) Show that, since S_i is real, $S(-\mathbf{k}) = S^*(\mathbf{k})$.

(c) Show that

$$S_i = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} S(\mathbf{k})$$

(d) Show that, in the thermodynamic limit

$$H = \left(\frac{a}{2\pi}\right)^d \int_{BZ} d^d\mathbf{k}\, f(\mathbf{k}) S^*(\mathbf{k}) S(\mathbf{k})$$

where BZ is the first Brillouin zone of the d-hypercubic lattice (what is it?). What is $f(\mathbf{k})$?

1/3. **(C) Ising symmetry:** Consider a *square* lattice (2d) system, which will be the arena of our system. The dofs are Ising spin variables. The Hamiltonian is known to have Ising Z_2 symmetry.

(a) Assuming that there are only the usual nearest neighbour interactions, write out a Hamiltonian that *does not* have translational symmetry. (Hint- Ask yourself: where did we use lattice translation symmetry in writing down eqn. (1)?)

(b) Assuming that there are only nearest neighbour interactions, write out a Hamiltonian that *has* lattice translation symmetry, but *does not* have point-group symmetry of the square lattice.

(c) Assuming that the system has all the symmetries like translation and lattice point group. Write a Hamiltonian that involves *only* four spin plaquette interactions (a plaquette consists of four site from the square of area a^2, a is the lattice parameter).

1/4. **(C) Top brass!** β-Brass is a "solid solution" of copper and zinc that shows interesting order-disorder transitions. The arena of this system is the BCC lattice (body-centred cubic, 3d). *Equal* numbers of Cu and Zn atoms occupy the BCC lattice (one atom per site), with only nearest neighbour interactions. If the nearest neighbours are both Cu the interaction energy is $-E_{CC}$, while if they are Zn, then it is $-E_{ZZ}$. If one of them is Cu and the other is Zn, then it is $-E_{CZ}$. All Es are positive, and $E_{CZ} > E_{CC}$ and $E_{CZ} > E_{ZZ}$.

(a) Show that the physics of order disorder transition can be studied using the Ising model. What is the value of J?

(b) What is the ground state of the system? What is its degeneracy?

Note: Similar considerations can be used to study the liquid-gas transition with a related model called the **lattice gas model**. Think about how such a model can be obtained.

1/5. **(C) Ferro is Antiferro?** Show that on a bipartite lattice, the partition function of the ferro Ising model is equal to that of the anti-ferro Ising model.

1/6. **(C) Frustration:** Prove or disprove the statements

(a) The anti-ferro Ising model (interaction between nearest neighbours only) possessing all the "usual" symmetries, on a honeycomb lattice (find out what this is, hint- graphene) is frustrated.

(b) A model with Ising symmetry with pairwise interactions is always *un*frustrated on a d-dimensional hypercubic lattice.

1/7. **(C) Exciting Ising!** Consider an infinite 1d ferro Ising chain $H = -J\sum_i S_i S_{i+1}$

(a) What is the ground state of this chain? Is it degenerate?

(b) What is the first excited state of the chain? What is its energy? Is it degenerate?

(c) Is the system *gapped* or *gapless*? A system is said to be *gapped* if a *finite* amount of energy separates the first excited state from the ground state. On the other hand, if the first excited state can be reached with excitation energies that can be made arbitrarily small, we say that the system is *gapless*. (Exercise: Give examples of gapped and gapless systems from elementary quantum mechanics.)

1/8. **(C) Exciting XY!** Read problem 1/7. Now, consider an 1d XY-chain with $H = -J\sum_i \cos(\theta_{i+1} - \theta_i)$ with N lattice sites and periodic boundary conditions.

(a) What is the ground state of this chain (described by θ_i^g)? Is it degenerate? Are any symmetries broken in the ground state?

(b) Now consider excitations above the ground state. We can describe this by $\theta_i = \theta_i^g + \phi_i$. Assuming that ϕ_i are small (compared to what?), find the Hamiltonain in terms of ϕ_i – call this H_ϕ.

(c) Let $\phi(q)$, be the Fourier transform of ϕ_i. Find H_ϕ in terms of $\phi(q)$.

(d) Is this system gapped or gapless in the thermodynamic limit?

(e) Repeat all the steps above for the 1-D classical ferro Heisenberg chain. What is your conclusion about gaplessness or gapfulness?

(f) Repeat the steps above the the 1-D classical Anti-Ferro Heisenberg chain. What is your conclusion about gaplessness or gapfulness?

(g) What did you learn from this (and the last) problem?

1/9. **(C) Frustrating XY?** What is the ground state of the classical anti-Ferro XY model on a triangular lattice? Is it degenerate?

1/10. **(C) Heisenberg's quantum avatar:** Consider the *quantum* Heisenberg chain in 1d. Prove or disprove each part of statements:

(a) For the ferro-Heisenberg model: (i) The fully polarized state ($|... \uparrow\uparrow\uparrow\uparrow ...\rangle$) is the ground state of the system, (ii) This ground state is non-degenerate, (iii) This ground state breaks no symmetry of the Hamiltonian.

(b) For the antiferro-Heisenberg model: (i) The Neél state ($|... \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow ...\rangle$) is the ground state, (ii) This ground state is non-degenerate, (iii) This ground state breaks no symmetry of the Hamiltonian.

1/11. **(C) Ising...in your computer:** In this problem, we will start a short project on the computer simulation of the Ising model. Write a programme in your favourite language to simulate a 1D Ising chain that will

- Take the following inputs:
  (a) Number of lattice sites N
  (b) Value of temperature (to be used later)
  (c) Periodic or open boundary conditions
  (d) Random seed
- Create a random spin configuration
- Evaluate the energy of a given spin configuration
- Plot out the spin configuration for visualization

Use the programme you have developed and

(a) For the ferro Ising model find the energy of the Neel state with both periodic and open boundary conditions. Check your answer with a calculation.

(b) Take $N = 10$. Generate a random configuraiton – print out the energy calculated by the computer, and plot out the spin configuration. Using the plot hand calculate the energy. Does it match with what the computer finds? Do this both for periodic and open boundary conditions. (For your own satisfaction: Repeat this for 10 different random configurations.)

1/12. **(C/E)** Z_3 **Symmetry:** Consider a triangular lattice. On the sites of this lattice we attach fields s_i which can take values $1, 2, 3$. In addition to the usual symmetries, the system has Z_3 symmetry in the s_i variables.

(a) Assuming nearest neighbour pairwise interactions, write out a Hamiltonian.

(b) Why on earth would you want to study such a model?

1/13. **(E) non-Abelian model:** Try this out:

(a) What is the smallest discrete non-Abelian group G?

(b) Find a system with G-symmetry on the d-hypercubic lattice.

(c) Do you think this model will have any interesting physics?

1/14. **(E/C) Liquid crystals:** Liquid crystals are made up of molecules that are "rod shaped" – somethings like Basmati rice grains. The interaction between these favour their parallel orientation. One can have phases where the orientations of all grains order in a particular direction – this is called a "nematic" phase. Note that it is not necessary for the grains themselves form a regular array of some sort – only their orientations need to be ordered for it to be a nematic.

(a) Assuming that the arena is a 3d continuum, what are the dofs of a system of N grains in volume V. (Focus on the "positional" degrees of freedom, ignore the "momentum" degrees of freedom for the moment.)

(b) What would be an appropriate "internal symmetry" for the system? Write out a simple Hamiltonian (only the "potential energy") that respects this symmetry.

(c) Using the answer(s) of the previous questions, find a quantity that will serve as a "nematic order parameter"?

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