Physics 114 **Statistical Mechanics** **Spring 2021**

Week 9 Reading and Problem Assignment

Overview:

Magnets! This week, we will envision magnets as lattices populated by *spins*, with *magnetic moments*. Spins are distinguishable objects which, in the simplest model of magnetism, can point either "up" or "down" along a chosen axis. Each spin's energy is lower when it is parallel to an applied magnetic field. If these spins do not interact with one another, we have a *paramagnetic material*, possible to treat with the kind of statistical mechanics we have applied to Einstein solids, ideal gasses, and other noninteracting systems.

If the magnetic moments interact, as they will in a *ferromagnet*, there can be a *phase transition*. This transition is highly analogous to the gas-to-liquid transition in a real fluid, which we will meet in a future week. The simplest ferromagnet model is the *Ising model*, in which nearest neighbors lower their energy by aligning. They will align even in the absence of an external magnetic field, if $T < T_c$, a critical temperature. We will study this "paramagnetic-to-ferromagnetic" phase transition, finding that in 1D the critical temperature is $T_c = 0$. Other properties like the magnetization and magnetic susceptibility are readily calculated in 1D. In 2D finding an exact solution is much tougher, and in 3D it's impossible. For these reasons, we will learn other fruitful approaches to magnetic phase transitions, like *mean field theory* and *Monte carlo simulation*.

Suggested Reading:

G&T Sections

- Sections 5.1-5.7
  Note: Syllabus says read through Section 5.9 but you can stop at 5.7. 5.8: Wang-Landau sampling and 5.9: The Lattice Gas are each interesting topics, but totally optional.

B&B Sections

- Section 28.8

Some good readings in Schroeder:

- Schroeder Section 8.2 is an excellent treatment of the Ising Model, including mean field theory, and the Metropolis Monte Carlo algorithm for the Ising Model.

- Schroeder Section 3.3 is an accessible and complete discussion of paramagnetism.

Old reading about noninteracting spin, which you could revisit:

- B&B Example 20.5 is a review of the spin 1/2 paramagnet
- B&B Section 3.5 pages 134-137 is a review of Bernoulli processes applied to magnetic spins
- B&B Example 4.1 is a review of Microcanonical stats for N noninteracting spins.

Warmup Problems:

1: Thermodynamics of noninteracting spins G&T Problem 5.3

2: Mean field critical temperature and exponents
i) In your own words, define the concepts "critical temperature" and "critical exponents" as they pertain to the reading this week (about the Ising model).

ii) What does mean field theory predict for the critical temperature, T_c, and the critical exponents β, γ and δ for a 2d square lattice of spins.

iii) Does mean field theory care about the shape of the lattice of spins? To answer this question concretely: What would mean field theory predict for T_c and the critical exponent β for the triangular and hex lattices shown below?

iv) Also below are exact and simulated data (S. Eltinge, 2015) on T_c and the critical exponent β. What similarities and differences are there between Eltinge's data, and what you got using mean field theory?

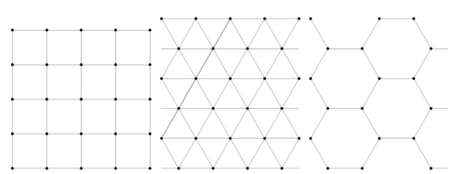

FIG. 1: The square, triangular, and hexagonal lattices.

Lattice	z	$T_{c,\text{exact}}$	$T_{c,\text{measured}}$	β_{exact}	β_{measured}
Hexagonal lattice	3	1.519	1.678 ± 0.002	0.125	0.129 ± 0.009
Square lattice	4	2.269	2.409 ± 0.007	0.125	0.129 ± 0.008
Triangular lattice	6	3.641	3.782 ± 0.007	0.125	0.121 ± 0.006

Problems to discuss in our meeting

Note: The * means that these problems are to be handed in. They are due the day after we meet.

1: Magnetic susceptibility
i) G&T Problem 5.2
ii) Demonstrate that your result for susceptibility makes sense by doing the following:

- Show that your answer to i) plus the expression for χ in G&T Eq. (5.19) imply that

$$\bar{M^2} - \bar{M}^2 = N\mu^2 sech^2(\mu\beta B) \tag{1}$$

- In Ch. 3 when we studied the Binomial distribution, G&T Eq. (3.78) claimed that:

$$\bar{M^2} - \bar{M}^2 = N(4pq) \quad (with \ \ \mu \equiv 1) \tag{2}$$

  Show that Eqs. (1) and (2) above are equivalent, when Eq. (2) is applied to spins in equilibrium at temperature T.

2*: Thermodynamics of 1d Ising model G&T Problem 5.6

3: Classical paramagnet G&T 5.32

4*: Mean field (Landau) free energy G&T Problem 5.18

5: Transfer matrix solution of 1d Ising chain

i) Show that the definition $\mathbf{T} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$ implies G&T Eq. (5.76). In other words, that $Z_N = Tr(\mathbf{T}^N)$.

ii) Find the eigenvalues of $\mathbf{T}$ which are given in Eq. (5.80).

iii) Show that Eq. (5.81) follows, so that only the larger eigenvalue λ_+ is important in the thermodynamic limit.

iv) Do the algebraic manipulations necessary to find $m(T)$ as in Eq. (5.83). Plot f this function: $m(T)$ $vs.$ T for cases $H = 0$ and $H = 1$. For each case, use $J = 0, 0.5, 2.0$,and 4.0 to show us how this function looks.

6: 2d Ising model via MC simulation
Use the "Ising model: Square lattice" program - or write your own in Python - to do parts (a) - (d) of G&T Problem 5.13. You can do fewer temperatures than they say in part (c); it's fine to do $T = 3.6, 3.1, 2.6, 2.3, 2.1, 1.9$ and 1.6.

7*: Counting states with small magnetic systems
i) Do G&T Problem 5.7 . Compare your data (admittedly only two points) for $G(r)$ with the infinite chain result : $G(r) = tanh(\beta J)^r$
ii) G&T Problem 5.36

8: Playing around with the Onsager solution

Though our texts don't, a few undergraduate books quote the famous "Onsager solution" Z_N for the 2d Ising model. It is:

$$Z_N(H=0) = [2cosh(\beta J)e^I]^N$$

where

$$I = \frac{1}{2\pi}\int_0^\pi ln[\frac{1}{2}(1+(1-\kappa^2 sin^2\phi)^{1/2})]d\phi$$

and

$$\kappa(\beta J) = 2sinh(2\beta J)/cosh^2(2\beta J)$$

a) This is a familiar form for Z_N if one sets $I = 0$ ... what other system has this partition function? If $I = 0$ for the 2d Ising ferromagnet, what temperature does this correspond to?

b) Using Z_N above, find an expression for F/N, the free energy per spin.

c) We could differentiate the result of b) ourselves to find the energy E, but let's trust that G&T have done their math right; assume that E is given by G&T Eq. (5.88). Use Mathematica's `EllipticK` function to show that the needed "elliptic integral of the first kind" indeed has a divergence at $\kappa = 1$.

d) Show that $\kappa = 1$ when $T = T_c$ is equivalent to saying $sinh(2J/kT_c) = 1$. Then solve numerically to find T_c and confirm Eq. (5.86).

e) Again using Mathematica if you wish, try to reproduce the plot on p. 264 of Eq. (5.90), which is $C(kT/J)\ vs.\ kT/J$.

f) Your experience of specific heats from earlier seminars tell you that $C(T)$ peaks at a temperature T where lots of modes are becoming available for energy to inhabit. Extend this understanding to the 2d Ising model ... what is happening to the system near the critical temperature?