

Lecture Notes on Statistical Mechanics

Andrew Larkoski

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Lecture 1

This week, we are going to discuss statistical mechanics and numerical methods for simulation of statistical physics. By “statistical physics” I mean simulating the gross, aggregate properties of an ensemble that consists of numerous individual parts. We can’t hope for an accurate description of the individual parts, but we can hope for a description of the collective phenomena.

I should apologize somewhat for the topic this week: I feel that the physics and simulation are important enough that you should be exposed to it, but this will likely require being pushed a bit outside your physics comfort zone. Additionally, I won’t have much opportunity to really deeply motivate the physics we will discuss this week. I have provided a link on Moodle to a statistical physics book that you should look into if you are interested. Nevertheless, if you have heard of “phase transitions”, “Ising Model”, “partition function”, and the like, we will discuss these ideas and be able to visualize with simulation what a phase transition looks like and how to quantify it. For those of you that have taken (or are taking) thermal physics, I hope this is a nice supplement, extending a bit beyond what you learned there.

With that disclaimer out of the way, let’s discuss statistical mechanics.

During this week, I will be very restricted in discussions of thermodynamics quantities, and only discuss what will be relevant for some appreciation of the two-dimensional Ising model. So, first, we must define what systems we are considering.

Our focus will be on systems with N individual entities: molecules, electrons, spins, etc., and we are assuming that N is an extremely large number. When we want to model and understand macroscopic systems, the number of atoms in such a system is of the order of Avogadro’s number, approximately 10^{23} . This is where we imagine N to be.

Our system will be defined by a Hamiltonian, which encodes the total energy of the system by summing over the energy of all individual entities:

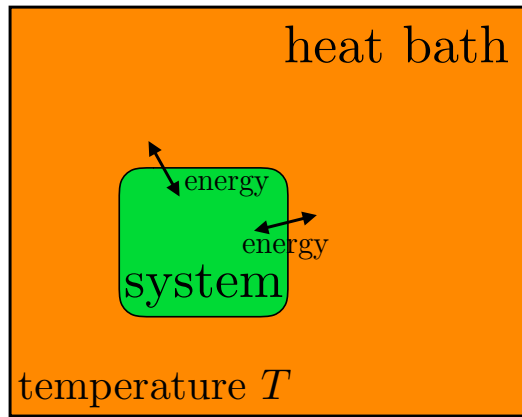
$$H = H(\{q_i, p_i\}_{i=1}^N). \quad (1)$$

Here, we denote the phase space variables by q and p . q_i is the position of the i th particle and p_i is the momentum of the i th particle. For example, for the air molecules in this room, the Hamiltonian is just the sum over the kinetic energies of each molecule:

$$H = \sum_{i=1}^N \frac{p_i^2}{2m_i}. \quad (2)$$

This happens to be a function purely of momentum, but we could also consider systems where the energy is a function of the position (like if the particles were in a potential).

For the systems we want to study thermodynamically, we will assume that they are embedded in a heat bath and are in thermal equilibrium. A heat bath is an infinite energy reservoir that has a single defining quantity: its temperature. The temperature is a measure of the energy available in the heat bath and thermal equilibrium means that the temperature of the heat bath and our system is equal. A picture of this is:



We will assume that energy only is freely shared across the boundary of our system with the heat bath.

If the heat bath has temperature T and our system is in thermal equilibrium, then the energy of the system is a function of T :

$$H = H(T). \quad (3)$$

For our example of the molecules in this room, the total energy is in fact

$$H = \frac{3}{2} N k_B T. \quad (4)$$

This room has a well-defined temperature, and so the average energy per molecule is

$$\langle E \rangle = \frac{3}{2} k_B T. \quad (5)$$

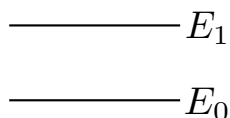
k_B is called Boltzmann's constant and has units of $\frac{\text{energy}}{\text{temperature}}$. In SI units, k_B takes the value

$$k_B = 1.38 \times 10^{-23} \text{ J/K}. \quad (6)$$

The factor of $3/2$ comes from the equipartition theorem: there are 3 momentum degrees of freedom (p_x, p_y, p_z) and in each there is an average contribution to the energy of $\frac{1}{2}k_B T$. (Why the $1/2$ I can't explain here.) Then, the total energy in the room is simply found by summing the energies of all atoms, which gives the factor of N .

Unlike the molecules in this room, later this week we will consider systems with discrete energies (not continuous momenta). Everything we discuss can be generalized to the continuous case, but the discrete energy levels makes the analysis a bit easier.

To provide some motivation for the partition function, let's consider an ensemble of N particles, each of which can only have energy E_0 or E_1 , with $E_1 > E_0$. So, for one particle, the picture is:



Any given particle has either energy $E = E_0$ or $E = E_1$. Note that the total energy of the system is

$$H = \sum_{i=1}^N E_i = N_0 E_0 + N_1 E_1, \quad (7)$$

with N_0 (N_1) the number of particles with energy E_0 (E_1). Note that $N_0 + N_1 = N$. So to find the total energy of the system, we need to determine the number of particles N_0 and N_1 that have energy E_0 or E_1 , respectively. To do this, let's embed the system in a heat bath of temperature T . Can we think about what the total energy is, and how it depends on T ?

The temperature T of the heat bath ranges from 0 to ∞ . 0 temperature means that the heat bath shares 0 energy with the system. So, when $T = 0$, the system will just be stuck in its lowest energy state. Assuming that $E_0 < E_1$, the the total energy when $T = 0$ is

$$H(T = 0) = N E_0, \quad (8)$$

with no particles that have energy E_1 . Now, let's consider the case when $T = \infty$. The heat bath can share infinite energy with the system. This does not mean that the system has infinite energy, but rather that the energy difference between E_0 and E_1 is totally irrelevant. If a particle has energy E_0 , then it can take a teensy amount from the heat bath and be pushed up to energy E_1 , and vice-versa. From the perspective of the heat bath, the energies E_0 and E_1 are effectively equal. That is, on average, half of the particles will have energy E_0 and half will have energy E_1 . That is, at $T = \infty$, the total energy of the system is:

$$H(T = \infty) = \frac{N}{2} E_0 + \frac{N}{2} E_1. \quad (9)$$

So, to find the energy at a given finite value of T , we want to interpolate between $N E_0$ at $T = 0$ and $\frac{N}{2} E_0 + \frac{N}{2} E_1$ at $T = \infty$.

With a careful analysis, one can derive the energy as a function of temperature for this system to be:

$$H = N \left(\frac{e^{-E_0/(k_B T)}}{e^{-E_0/(k_B T)} + e^{-E_1/(k_B T)}} E_0 + \frac{e^{-E_1/(k_B T)}}{e^{-E_0/(k_B T)} + e^{-E_1/(k_B T)}} E_1 \right). \quad (10)$$

The exponential factor

$$e^{-E/(k_B T)}$$

is called the Boltzmann factor. This can be expressed in the more fundamental object called the partition function. The partition function for this system is:

$$Z = e^{-E_0/(k_B T)} + e^{-E_1/(k_B T)} = e^{-\beta E_0} + e^{-\beta E_1}, \quad (11)$$

with $k_B T = \beta^{-1}$. Note that at $T = 0$, because $E_1 > E_0$, the energy is just $N E_0$ and at $T = \infty$, the energy is $\frac{N}{2}(E_0 + E_1)$. The average energy per particle can be calculated from the partition function by differentiating with respect to β :

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta} = \frac{e^{-E_0/(k_B T)} E_0 + e^{-E_1/(k_B T)} E_1}{e^{-E_0/(k_B T)} + e^{-E_1/(k_B T)}}. \quad (12)$$

Another interesting quantity that we might want to ask is what the entropy of the system is. The entropy is a measure of the amount of information contained in knowing general properties of the system. In this case, we know the total energy of the system. This tells us some information about what state the individual particles are in, but only by a limited amount.

Given the total energy, we only know the number of particles in a given energy state, and not which particles are. Entropy quantifies this information imbalance, this lack of full information about the system. The entropy S is defined as the logarithm of the number of states that correspond to the same observed total energy (or other global quantities). That is,

$$S = k_B \log N_s, \quad (13)$$

where N_s is the number of states.

Let's consider our two-state system. Given a total energy E , what is the entropy? With a total energy E , this defines the number of particles in the ground state. We don't know which particles, so we have to include all possibilities. The number of particles in the ground state with total energy E is:

$$N_0 = N \frac{e^{-E_0/(k_B T)}}{e^{-E_0/(k_B T)} + e^{-E_1/(k_B T)}}. \quad (14)$$

Then for the total energy, I just need to specify that N_0 of the total N particles are in the ground state. The number of possible configurations is then

$$\binom{N}{N_0} = \frac{N!}{N_0!(N - N_0)!}, \quad (15)$$

and so the entropy is

$$S = k_B \log \binom{N}{N_0}. \quad (16)$$

We can massage this to get a more useful expression for the entropy. Note that

$$\log N! = N \log N + \dots, \quad (17)$$

for $N \rightarrow \infty$, which is called Stirling's approximation. Then, using this approximation, the entropy is:

$$S = k_B \log \binom{N}{N_0} \simeq k_B N \log N - k_B N_0 \log N_0 - k_B (N - N_0) \log (N - N_0) \quad (18)$$

$$= -k_B N_0 \log \frac{N_0}{N} - k_B (N - N_0) \log \left(1 - \frac{N_0}{N}\right). \quad (19)$$

Here, note that N_0/N is the probability that a particle is in state with energy E_0 and $1 - \frac{N_0}{N}$ is the probability that the particle is in the state with energy E_1 . Then, the entropy can be written as

$$S = -k_B N (p_0 \log p_0 + p_1 \log p_1) = -k_B N \sum_{i=0}^1 p_i \log p_i, \quad (20)$$

where p_i is the probability to be in the i th state.

While we have just discussed two-state systems, this can be generalized. The general partition function is

$$Z = \sum_i e^{-\beta E_i}, \quad (21)$$

where E_i is the energy of the i th state, summed over all states in the system. The total entropy of the system is

$$S = -k_B \sum_i p_i \log p_i, \quad (22)$$

where p_i is the probability to be in state i .

On Wednesday, we'll apply this partition function formalism to a system of spins in a heat bath, called the Ising Model. For today, I want to make one more observation. The Boltzmann factor for state i

$$e^{-\beta E_i}$$

looks very similar to the time evolution factor of an energy eigenstate in quantum mechanics:

$$e^{-iE_i t/\hbar}.$$

This analogy is very deep, in fact, it is fundamental. The partition function of statistical mechanics is intimately related to the path integral of quantum mechanics/quantum field theory. In fact, one can go back and forth between the partition function and the path integral by taking imaginary temperature/time.

Lecture 2

Last lecture, we introduced/reminded about statistical mechanics. We are considering systems embedded in a heat bath, in thermal equilibrium at temperature T . The system is allowed to freely exchange energy with the heat bath, and so the energy of the system is proportional to temperature T . In general, thermodynamic quantities are defined from the more fundamental object, the partition function Z :

$$Z = \sum_i e^{-\beta E_i}, \quad (23)$$

$k_B T = \beta^{-1}$, where the sum runs over all energy states in the system.

The factor

$$e^{-\beta E_i}$$

is called the Boltzmann factor and encodes the relative probability that the state i is occupied. The average value of a thermodynamic quantity A is found by utilizing the partition function:

$$\langle A \rangle = \frac{\sum_i A_i e^{-\beta E_i}}{Z}. \quad (24)$$

For example, the average energy is

$$\langle E \rangle = \frac{\sum_i E_i e^{-\beta E_i}}{Z} = -\frac{\partial \log Z}{\partial \beta}. \quad (25)$$

We also discussed the entropy which is a measure of the lack of information about the specific phase space configuration of the system, given measured values of thermodynamics quantities. The entropy is

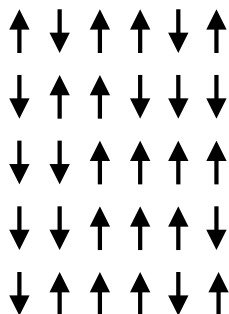
$$S = -k_B \sum_i p_i \log p_i, \quad (26)$$

where

$$p_i = \frac{e^{-\beta E_i}}{Z}. \quad (27)$$

This lecture, we will introduce the Ising model. The Ising model is named after physicist Ernst Ising (pronounced “EE-zing”), who was given the problem to solve as a Ph.D. student by his advisor, Wilhelm Lenz. This Lenz is **not** the Lenz of Lenz’s law (but is the Lenz of the Laplace-Runge-Lenz vector).

The Ising model is one of the simplest statistical mechanics systems, yet manifests highly non-trivial behavior. We’ll study the Ising model for the rest of this week. The Ising model is just a system of spins immersed in a heat bath. For example, the two-dimensional Ising model looks like:

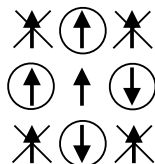


for a system of 6×6 spins at temperature T . Each location of a spin is called a spin or lattice site. The spins of the Ising model can be up or down; that is, $+1$ or -1 . As spins, they correspond to a magnetic moment.

The (source-free) Ising Hamiltonian is

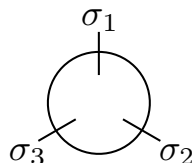
$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j. \quad (28)$$

Here, J is the interaction strength and σ_i is the spin at site i : $\sigma_i = \pm 1$. The sum runs over all nearest neighbor spin sites, e.g., for a 2D spin lattice, the nearest neighbors of the center spin in



don't include the diagonal spins.

To be more explicit and to see how this works, let's consider the 3 spin system in 1D:



We will also choose periodic boundary conditions with $\sigma_4 = \sigma_1$. Then, the Hamiltonian is

$$H = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1). \quad (29)$$

Note that this Hamiltonian encodes our expectation of energy: $\sigma_i\sigma_j$ is positive if the spins align, and so have negative energy if $J > 0$. That is, the spins *want* to align if $J > 0$. Then, we say that the Ising model is ferromagnetic. We'll just study this case in this class, though one can also consider the anti-ferromagnetic case, $J < 0$. The partition function of the Ising model is

$$Z = \sum_{\sigma_i = \pm 1} \exp \left[\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \right]. \quad (30)$$

The outer sum runs over all spins and their value of ± 1 . For our model 1D system, the partition function is:

$$Z = e^{3\beta J} + 3e^{-\beta J} + 3e^{-\beta J} + e^{3\beta J} = 2e^{3\beta J} + 6e^{-\beta J}. \quad (31)$$

The first and last term of the first equality come from the case when all three spins are equal. The middle two cases come from when two spins are up and one is down, or when two spins are down and one is up. There are three configurations for each.

From the partition function, we can calculate thermodynamically-averaged quantities. The average spin $\langle \sigma_i \rangle$ is

$$\langle \sigma_i \rangle = \frac{1}{Z} \sum_{\sigma_i = \pm 1} \sigma_i \exp \left[\beta J \sum_{\langle i, j \rangle} \sigma_i \sigma_j \right]. \quad (32)$$

Note that the Hamiltonian is identical if all spins go to minus themselves. Therefore, $\langle \sigma_i \rangle = 0$ for the source-free Ising model. What is more interesting is the spin correlation

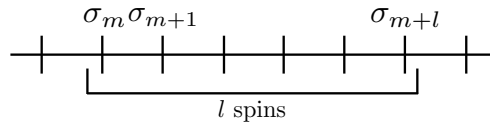
$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z} \sum_{\sigma_i, \sigma_j = \pm 1} \sigma_i \sigma_j \exp \left[\beta J \sum_{\langle i, j \rangle} \sigma_i \sigma_j \right]. \quad (33)$$

This quantity is a measure of long-range order in the Ising model. With periodic boundary conditions, this quantity can only depend on the distance between spin i and spin j , and not the absolute lattice site. That is, the spin correlation can be expressed as

$$\langle \sigma_m \sigma_{m+l} \rangle = \frac{1}{Z} \sum_{\sigma_m, \sigma_{m+l} = \pm 1} \sigma_m \sigma_{m+l} \exp \left[\beta J \sum_{\langle i, j \rangle} \sigma_i \sigma_j \right] \equiv C(\beta, J, l). \quad (34)$$

We want to determine the functional dependence of the spin correlation $C(\beta, J, l)$ on l ; that is, how correlated spins are if they are separated by a distance l on the lattice.

Let's discuss the physics contained in $C(\beta, J, l) = \langle \sigma_m \sigma_{m+l} \rangle$. Note that $\sigma_m \sigma_{m+l} = 1$ if the spins are identical and -1 if the spins are opposite. That is, this is indeed a measure of correlation: $\sigma_m \sigma_{m+l} = 1$ means the spins are correlated and $\sigma_m \sigma_{m+l} = -1$ means the spins are anti-correlated. We are comparing spins separated by l lattice sites:



and $\langle \sigma_m \sigma_{m+l} \rangle$ is a measure of how affected the spin at lattice site $m + l$ is affected by the existence of a $+1$ or -1 spin at lattice site m . It makes some sense that they should be correlated: the spin at site m affects the spin at site $m + 1$ which affects the spin at site $m + 2 \dots$ which will have some effect on the spin at site $m + l$. How large is this effect?

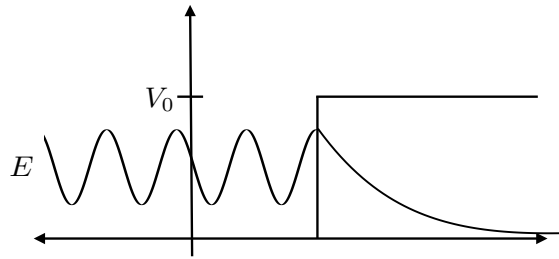
That is, what functional dependence on l of $C(\beta, J, l)$ demonstrates long-range order? We will be interested in the case when the number of lattice sites $N \rightarrow \infty$.

First, if $C(\beta, J, l) = 1$ for all l , then every spin is the same and the full Ising spin system is perfectly correlated. This definitely manifests long-range order, but is an extreme case. The correlation could be exponential:

$$C(\beta, J, l) \propto e^{-l/\xi}, \quad (35)$$

with ξ called the correlation length, as $l \rightarrow \infty$.

Such a functional dependence does not correspond to the existence of long-range order because of the exponential suppression. This is analogous to the finite potential barrier in quantum mechanics:



For an initial free-particle coming from the left with energy $E < V_0$, the potential height, the wave function changes from imaginary to real exponential at the barrier. The amount of the wave function that penetrates to $x = +\infty$ is (the “transmission coefficient” T)

$$T \rightarrow 0, \text{ as the width of the potential barrier goes to } \infty. \quad (36)$$

That is, the probability for the particle to be found arbitrarily far to the right of the edge of the potential barrier is 0. The correlation length in this case would be

$$\xi = \frac{\hbar}{\sqrt{2m(V_0 - E)}}. \quad (37)$$

That is, if the width of the potential barrier was ξ , then the amplitude of the wave function would decrease by a factor of e , with $e^{-1} \simeq 0.368$. In the same way, for spins separated by ξ lattice sites, the correlation decreases by a factor of e . As $l \rightarrow \infty$, the spins become completely decorrelated.

Okay, so no long range order if $C(\beta, J, l) \propto e^{-l/\xi}$. It is also possible that the spin correlation falls off with l as a power law:

$$C(\beta, J, l) \propto l^{-\nu}, \quad (38)$$

with $\nu > 0$. ν is called the “critical exponent” and such a power law fall off is a manifestation of long-range order. This spin correlation is scale-invariant: if the spin lattice distance l is scaled up by a factor a ($l \rightarrow al$), the the power law fall off is identical (up to an overall constant):

$$C(\beta, J, al) \propto l^{-\nu}, \quad (39)$$

This demonstrates that there is effectively equal relative correlation between spins separated by any number of lattice sites l ! Note that this is very different than the exponential decay correlation. In that case, if we scale $l \rightarrow al$, we have

$$C(\beta, J, l) \propto e^{-al/\xi}, \quad (40)$$

which changes the correlation length to ξ/a . This is not scale-invariant.

So, we have two possible behaviors of the system: only short range order, or long range order. The measure of the distance scale over which order is present is the spin correlation:

$$\langle \sigma_m \sigma_{m+l} \rangle = C(\beta, J, l). \quad (41)$$

We call the spin correlation an order parameter because its behavior with l determines the manifestation of order in the system.

Now, how does this depend on temperature? Well, at $T = 0$, all spins must be aligned (for $J > 0$), as this is the minimum energy configuration. So, we have

$$C(\beta = \infty, J, l) = 1, \quad (42)$$

with $k_B T = \beta^{-1}$. At $T \rightarrow \infty$, the spins are now completely randomized because a tiny amount of energy can be taken from the heat bath and flip the spin. Therefore, if the temperature is large enough, then

$$C(\beta \rightarrow 0, J, l) \propto e^{-l/\xi}, \quad (43)$$

which is no long range order. Then, on general grounds, we expect that there is some temperature T_c where the ordered system changes into the unordered system. This is called the critical temperature and manifests the power-law long-range order:

$$C(\beta_c = \frac{1}{k_B T_c}, J, l) \propto l^{-\nu}. \quad (44)$$

The temperature T_c marks the temperature between the ordered phase ($T < T_c$) and the unordered phase ($T > T_c$). The behavior of the order parameter $C(\beta, J, l)$ defines what phase the system is in.

The 1D Ising model was solved by Ising himself and he explicitly showed that there was no phase transition in 1D. The 2D Ising model, which we will discuss next lecture, does exhibit a phase transition, and we will talk about how to simulate it and find the critical temperature.

Finally, I want to mention a couple of things about the Ising model. What makes it so relevant even still today is that the Ising model manifests properties shared by a huge number of other systems. In particular, the phase transition exhibits similar properties to many other systems; i.e., the critical exponent ν of the order parameter is the same in Ising as in other systems. This property is called universality. The Ising model is still an active area of research: the 3D Ising model has been studied in the context of conformal field theory (using a technique called the “conformal bootstrap”). See arXiv:1203.6064 for more details. A pedagogical review is arXiv:1602.07982.

Lecture 3

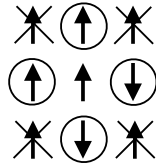
Last lecture, we introduced the Ising model, which is a system of spins on a lattice defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (45)$$

where σ_i is the spin (± 1) at lattice site i . The symbol $\langle i, j \rangle$ means that i and j are nearest neighbors. In 1D this would be



while in 2D this is



i.e., neighbors directly left, right, up and down, but not diagonal. With $J > 0$, the Ising model is ferromagnetic: the energy is minimized if the spins are aligned. The partition function of the Ising model is

$$Z = \sum_{\sigma_i = \pm 1} \exp \left[\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \right]. \quad (46)$$

We also discussed long-range order in the Ising model. The spin correlation

$$\langle \sigma_m \sigma_{m+l} \rangle = C(\beta, J, l), \quad (47)$$

is an order parameter for the Ising model, and exhibits different dependence on l if there is long-range order in the system. The order in the system depends on temperature, and we argued generally that at low temperature the system is ordered and at high temperature the system is disordered. Thus at some intermediate temperature T_c , called the critical temperature, the system manifests long-range order in a scale-invariant way:

$$C(\beta_c, J, l) \propto l^{-\nu}, \quad (48)$$

where ν is the critical exponent. In this lecture we will discuss the simulation of the Ising model.

As I mentioned last lecture, Ising solved the 1D, uh, Ising model for his Ph.D. thesis. By “solved”, I mean that he was able to derive a closed-form expression for the partition

function, in the limit that the length (or number of spins) goes to ∞ . This is actually quite easy to derive directly. The partition function for the 1D Ising model is

$$Z = \sum_{\sigma_1, \sigma_2, \dots, \sigma_N = \pm 1} e^{\beta J \sigma_1 \sigma_2} e^{\beta J \sigma_2 \sigma_3} \dots e^{\beta J \sigma_{N-1} \sigma_N}. \quad (49)$$

Here, we assume “free” boundary conditions (σ_1 has no left neighbor and σ_N has no right neighbor). We can call

$$\sigma'_i = \sigma_{i-1} \sigma_i, \quad 2 \leq i \leq N, \quad (50)$$

and then the partition function dramatically simplifies:

$$Z = 2 \prod_{j=2}^N \sum_{\sigma'_j = \pm 1} e^{\beta J \sigma'_j} = 2(e^{\beta J} + e^{-\beta J})^{N-1} = 2^N \cosh^{N-1}(\beta J). \quad (51)$$

The spin correlation can also be calculated similarly. I’ll just sketch the details here. We want to compute

$$\langle \sigma_m \sigma_{m+l} \rangle = \frac{1}{Z} \sum_{\sigma_i = \pm 1} \sigma_m \sigma_{m+l} \exp \left[\beta J \sum_{\langle i, j \rangle} \sigma_i \sigma_j \right]. \quad (52)$$

Note that, in terms of $\sigma'_i = \sigma_{i-1} \sigma_i$, we have

$$\sigma_m \sigma_{m+l} = (\sigma_m \sigma_{m+1})(\sigma_{m+1} \sigma_{m+2}) \dots (\sigma_{m+l-1} \sigma_{m+l}) = \sigma'_{m+1} \sigma'_{m+2} \dots \sigma'_{m+l}. \quad (53)$$

The product of spins consists of l factors and the spins for $j < m$ or $j > m+l$ cancel between the partition function in the numerator and denominator. So, there are only two possibilities: the product of the spins is ± 1 , multiplied together l times. Therefore,

$$\langle \sigma_m \sigma_{m+l} \rangle = \left(\frac{e^{\beta J} - e^{-\beta J}}{e^{\beta J} + e^{-\beta J}} \right)^l = \tanh^l(\beta J). \quad (54)$$

This spin correlation is fascinating, and tells us a huge amount about the 1D Ising model. First, when $\beta \rightarrow \infty$ or $T \rightarrow 0$, we find

$$\langle \sigma_m \sigma_{m+l} \rangle_{\beta \rightarrow \infty} = 1, \quad (55)$$

which is perfect correlation, as expected. However, for $\beta < \infty$, $\tanh^l(\beta J) \rightarrow 0$ as $l \rightarrow \infty$. Thus, except at $T = 0$, there is no long range order in the 1D Ising model! That is, the spin correlation exponentially decays with l :

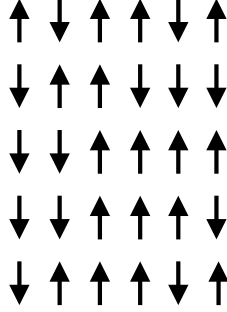
$$C(\beta, J, l) = \exp \left[-l \log \frac{1}{\tanh(\beta J)} \right], \quad (56)$$

with correlation length

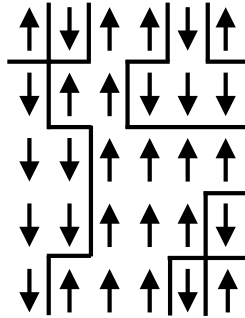
$$\xi = \frac{1}{\log \frac{1}{\tanh(\beta J)}}. \quad (57)$$

As $\beta \rightarrow 0$ ($T \rightarrow \infty$), $\xi \rightarrow 0$. So, no phase transition in the 1D Ising model!

The first phase transition occurs in 2D. Rudolph Peierls first gave the argument that a phase transition should occur in 2D. His argument is quite detailed, so we won't discuss it in detail here, but I'll just provide a flavor of how to think about it. In 2D, we have a collection of spins



We can equivalently think of this instead as domains of $+1$ or -1 spin, and define the system by the boundary of those regions:



One can express the partition function either as a sum over spins or as a sum over regions. This is called a duality, as one system (the 2D Ising model) has two different, yet equivalent, descriptions. Comparing these descriptions, one is able to find the critical temperature of

$$k_B T_c = \frac{2}{\log(1 + \sqrt{2})} J \simeq 2.27J. \quad (58)$$

Below this temperature, the system exhibits long-range order, while above this temperature the long range order disappears.

An exact solution to the 2D Ising model was found by Lars Onsager in 1944. This is one of the “heroic” physics calculations of history, which opened up the field of two-dimensional conformal field theories. While Onsager’s solution is elegant and insightful, we won’t study it more. We want to simulate the 2D Ising model and see if we can observe the phase transition ourselves.

To describe the Monte Carlo techniques we will use to simulate the 2D Ising model, first a bit of organization. We will define a lattice site on an $N \times N$ grid by an ordered-pair of

integers (i, j) . This lattice site has four neighbors: $(i+1, j)$, $(i-1, j)$, $(i, j+1)$, and $(i, j-1)$, which are included in the Hamiltonian via:

$$H \supset -J\sigma_{i,j}(\sigma_{i+1,j} + \sigma_{i-1,j} + \sigma_{i,j+1} + \sigma_{i,j-1}). \quad (59)$$

The first algorithm we define for solving the 2D Ising model is called the “heat bath” algorithm. It is:

1. Pick a lattice site (i, j) at random.
2. Calculate how many of its neighbors are pointing up, and assign a value to this according to the terms in the Hamiltonian:

$$m_k = \sum_{\text{neighbors of } (i,j)} \sigma_k = \begin{cases} 4 \text{ (4 up)} \\ 2 \text{ (3 up)} \\ 0 \text{ (2 up)} \\ -2 \text{ (1 up)} \\ -4 \text{ (0 up)} \end{cases} \quad (60)$$

3. Set the spin at lattice site (i, j) to be up (+1) with probability

$$p_+ = \frac{e^{\beta J m_k}}{e^{\beta J m_k} + e^{-\beta J m_k}}. \quad (61)$$

Otherwise, set it to be down (−1).

4. Go to step 1, and repeat many time until the system reaches equilibrium.

The heat bath algorithm is a relaxation method, similar to what we discussed for solving the Poisson problem on a grid. So, it isn’t so elegant, and can take significant time to thermalize. Here, what we mean by “equilibrium” and “thermalize” is that the probability for a spin to be set up (+1) settles and becomes fixed as the algorithm continues.

A more elegant algorithm for solving the 2D Ising model is the Metropolis algorithm, named after Nicholas Metropolis. Metropolis worked at Los Alamos during World War 2. After the war, he lead the computing group at Los Alamos, building the MANIAC 1 machine. However, as is typical of these sorts of things, there is significant controversy over who created the Metropolis algorithm. Roy Glauber, the only remaining living scientist who was on the Manhattan Project, credits Fermi with the original algorithm.

Whoever came up with it, the Metropolis algorithm is a Markov Chain Monte Carlo and the algorithm is the following:

1. Pick a lattice site (i, j) at random.
2. Calculate the energy with the current spin, E_i , and the energy with the spin flipped, E_f .
3. If $E_f < E_i$, flip the spin.

4. If $E_f > E_i$, flip the spin with the probability

$$p_f = e^{-\beta(E_f - E_i)} . \quad (62)$$

5. Return to step 1 and continue until the system reaches equilibrium.

Note that this is indeed a Markov Chain: to determine if the spin should flip, you only need to know the current state of the system.

Also, importantly, nothing in this algorithm specified the number of dimensions. We will focus on $D = 2$, but you could also consider $D > 2$. Also, only the case when $D = 2$ is solved exactly (by Onsager), and the $D > 2$ Ising model remains unsolved. Monte Carlos are our only tool for understanding the 3D Ising model, which could be a model for a real system. (This isn't quite true; there have been recent advances in using something called the "operator product expansion" and the "conformal bootstrap", which does not rely on Monte Carlos. These techniques exploit conditions on the system to self-consistently solve it.)

Note that the Metropolis algorithm is very general in other ways: the Metropolis algorithm is the same if the Hamiltonian is changed by adding new interactions, adding an external magnetic field, etc. We just need to be able to calculate the change in energy it takes to flip a spin.

For the rest of this class, we will discuss the implementation and results of simulating the 2D Ising model with the heat bath algorithm. You will code up and study the Metropolis algorithm in homework.

The code for the heat bath algorithm is below. We first initialize all spins to be up, then we randomly choose a lattice site (x, y) somewhere on the grid. Imposing periodic boundary conditions, we have to identify nearest neighbors carefully if they lie at the boundary. We then calculate the spin sum of the neighbors and correspondingly, the probability for the spin at site (x, y) to be up (+1). We choose the spin accordingly, and then repeat, picking a new site.

```

heatbath[Nspins_, T_, J_, Nev_] := Module[{spinstab, i, j, x, y, leftn,
rightn, upn, downn, mval, rand, pup, plottab},

(*Initialize the lattice of spins to be all up (+1)*)
spinstab = Table[1, {i, 1, Nspins}, {j, 1, Nspins}];
plottab =
ArrayPlot[spinstab, ColorFunction -> (If[# == 1, Blue, Yellow] &)];

(*Run over all iterations*)
Monitor[
For[i = 1, i <= Nev, i++,

(*Find a random lattice site*)
x = RandomInteger[1, Nspins];
y = RandomInteger[1, Nspins];

(*Determine the neighbors. Need to consider if the chosen spin is at
the boundary. If so, we impose periodic boundary conditions.*)
leftn = If[x != 1, x - 1, Nspins];
rightn = If[x != Nspins, x + 1, 1];
upn = If[y != 1, y - 1, Nspins];
downn = If[y != Nspins, y + 1, 1];

(*Calculate the neighbors' spin sum*)
mval = spinstab[[leftn, y]] + spinstab[[rightn, y]] + spinstab[[x, upn]]
+ spinstab[[x, downn]];

(*Calculate the probability to have up (+1) spin*)
pup = Exp[J mval/T]/(Exp[J mval/T] + Exp[-J mval/T]);
rand = RandomReal[];
If[rand < pup, spinstab[[x, y]] = 1, spinstab[[x, y]] = -1];

If[Mod[i, 100000] == 0,
plottab =
ArrayPlot[spinstab, ColorFunction -> (If[# == 1, Blue, Yellow] &), PlotLabel
-> i]; ], plottab];
Print[plottab];
Return[spinstab];
];

```

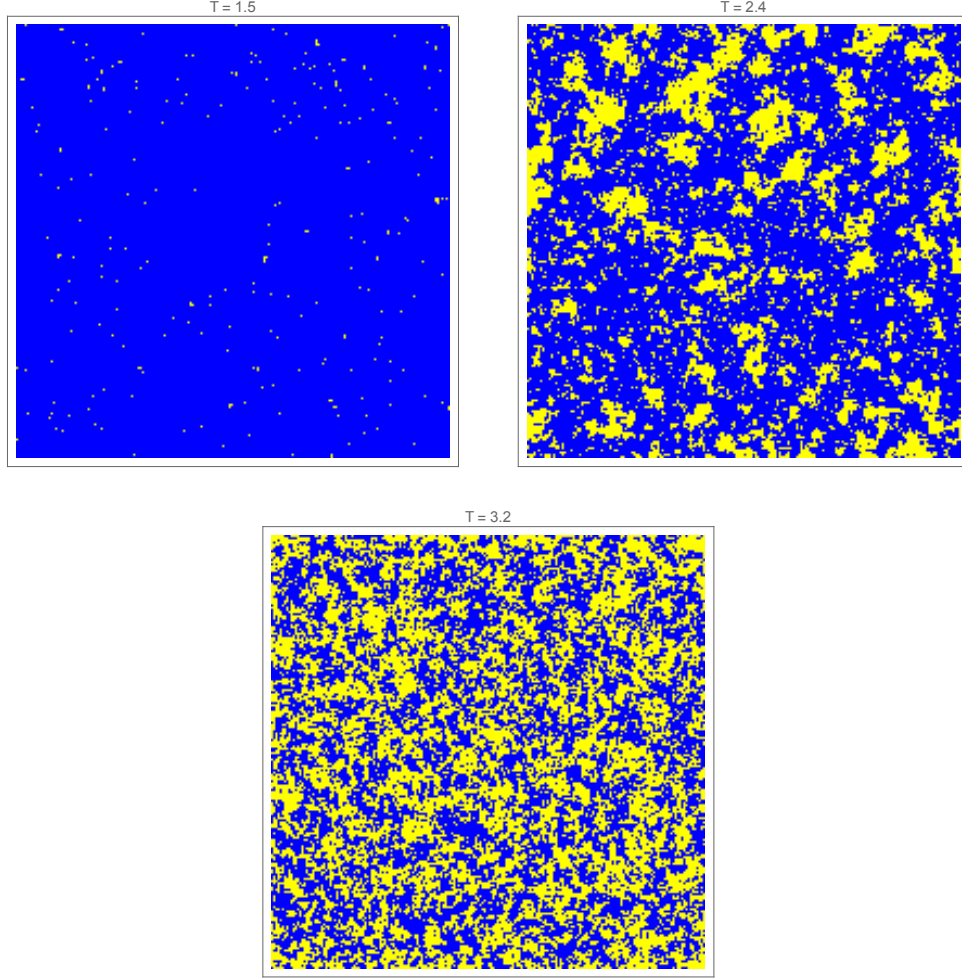



Figure 1: Plots of the 2D Ising model of a grid of 200×200 spins simulated with the heat bath algorithm. Blue denotes up spins and yellow are down spins.

Let's look at some plots of this. We will consider a 200×200 spin lattice system with the Ising coupling strength $J = 1$. For the system to thermalize (i.e., look similar after updating again), we will take millions of updates, so we set the numbers of updates to 10 million. We can then set the temperature, and watch it go.

Let's consider the temperatures $T = 1.5$, 2.4 , and 3.2 . Plots of the system at these temperatures are given in Fig. 1. $T = 1.5$ is well below the critical temperature, 2.4 is near the critical temperature, and 3.2 is above the critical temperature. First, consider $T = 1.5$. With all spins initially up, the temperature is too low for many down spins to exist. So, we see just a few yellow dots on a field of blue. For $T = 3.2$, now the temperature is high and it is much more likely that the spins are flipped at random. Thus, we see a picture that almost looks like static on a TV screen. The correlation length is small, too, as spins are being flipped everywhere. Finally, let's look at $T = 2.4$, near the critical point. Let's even

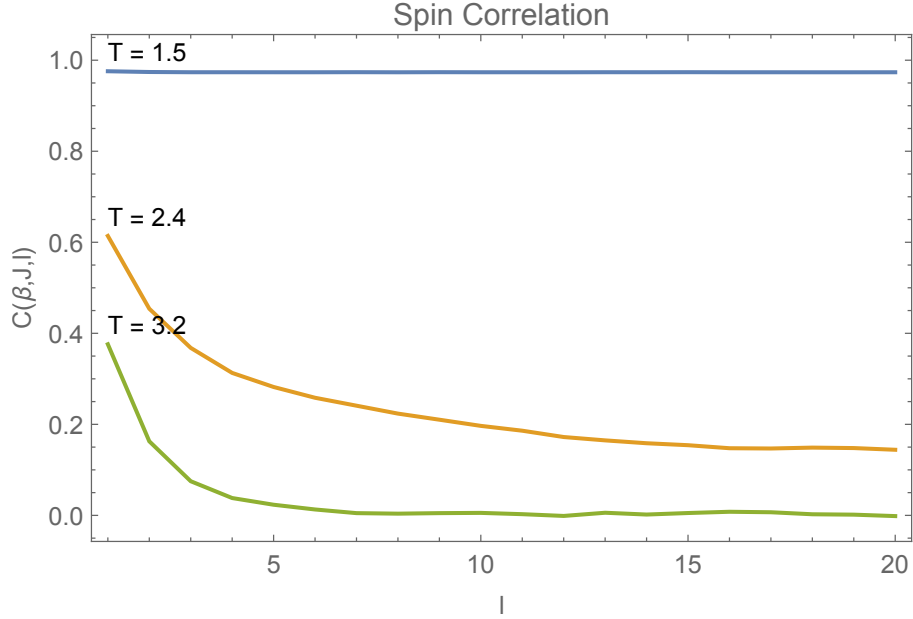


Figure 2: Estimates of the spin correlation as a function of separation l for the systems illustrated in Fig. 1.

let this run for a bit (in class!), so you can see the evolution of the system. Note that as it runs, patches of yellow are produced of “all” sizes. If you zoomed in on the plot it would look self-similar, or exhibit fractal properties. Indeed, this is a consequence of the power law spin correlation at the critical point. This is what we mean when we say “scale-invariant”: if the scale is changed (zoomed in or out) the system appears the same.

We can see these effects more quantitatively by calculating the spin correlation at each of these temperatures. I’ve also provided some simple code in the supplemental Mathematica notebook that estimates the spin correlation as a function of the distance l . The spin correlations at $T = 1.5$, $T = 2.4$, and $T = 3.2$ are plotted in Fig. 2. At $T = 1.5$, there is really only the default correlation (all spins up), which is why when the correlation is about 1. At $T = 3.2$, there is more correlation, but the most correlation is visible at $T = 2.4$, near the critical temperature. The spin correlation at $T = 2.4$ falls off the most slowly with l of the temperatures shown here.