Lecture 10: Simulations in Statistical Physics

In these notes we outline a computational algorithm that allows us to simulate the time-dependence of statistical physics systems.

1 The "Dynamics" in Thermodynamics

Although it might not have been apparent in all our analyses, the systems we have been studying have all been dynamic, which is to say they all had properties which varied in time. Previously, we were able to ignore these time varying properties because we computed statistical averages of quantities like spin, energy, or velocity, and by the formalism we developed, these statistical averages are time-independent. However, in the real systems associated with these models (i.e., real magnets or real gases), these quantities actually fluctuate in time about their computed averages.

Take a lattice of N spins denoted $s_1, s_2, \ldots, s_N$. Given the energy of a microstate, we can compute the partition function and then the average total spin $\langle S \rangle$ where $S = \sum_{i=1}^{N} s_i$. But, if we were to let this system evolve in time, we would find S fluctuating about this equilibrium value with a size of fluctuations on the order of $\sigma_{S_{\text{tot}}}$, the standard deviation of S_{tot} (See Fig. 1).

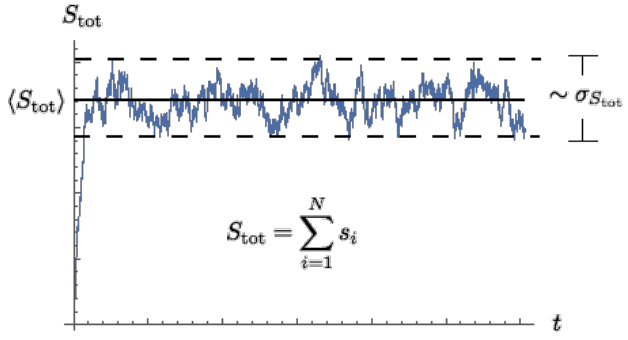

Figure 1: Schematic of time dependence of the total spin in a lattice of spins. There is a short time during which the system is reaching thermal equilibrium and afterwards the average total spin $\langle S_{\text{tot}} \rangle$ and the standard deviation of total spin $\sigma_{S_{\text{tot}}}$ (computed from equilibrium statistical physics) accurately describes the distribution of S_{tot}. We note that S_{tot} is not constant in time, but fluctuates about its average value. Our goal in these notes is to find a way to model this fluctuation.

Averages of physical quantities do provide some information about thermodynamic systems at equilibrium, but it would also be useful if we had a formalism which could model the time-dependent fluctuations in real systems.

Also, up to this point, all of our analyses of thermodynamic systems have been analytic which is to say they have focused on deriving and interpreting equations. Such a focus on analytic methods is all well and good for simple systems[1], but if we were ever to encounter a system which was too complicated to study analytically, we would be in trouble. In theoretical sciences (like theoretical physics), there are two broad classes of methods one can use to solve problems: **analytic methods** like the ones we have been building and applying, and **computational methods** which employ programmed algorithms. When problems become

[1]Here we use "simple" in the tautological way physicists use it: Analytic methods are useful for studying simple systems, and a system is simple if it can be studied analytically.

too difficult to solve analytically—and many, if not most, important physical problems are too difficult to study analytically—scientists turn to computational methods.

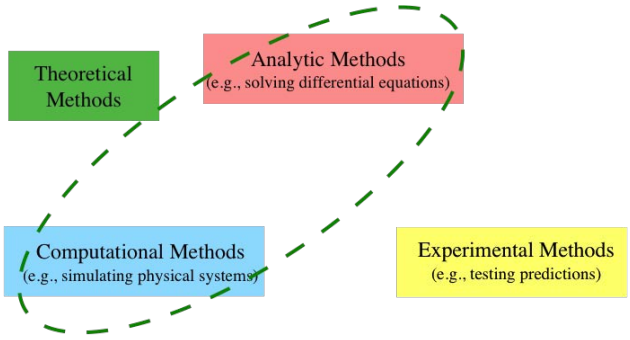

Figure 2: Science applies analytic, computational, and experimental methods to answer questions about nature. Some disciplines only focus on one of the methodological domains. Many life sciences only apply experimental methods. High energy theory (of the kind surrounding string theory) uses only analytic methods. And fluid dynamics uses mostly computational methods extending from an analytic foundation.

In these notes, we will develop a formalism for studying the time-dependent fluctuations of thermodynamic system and then embed that formalism in a computational algorithm which allows us to simulate these fluctuations. The algorithm falls in a class of computational methods called **Monte Carlo methods** which use random sampling to calculate geometric properties or to generate distributions. In this work, the framing question we pursue is as follows

Framing Questions
How can we use computational methods to simulate the time-dependence of statistical physics systems at equilibrium?

2 Transitions and Equilibria

We are seeking to simulate the time-dependence of statistical physics systems. We will begin by considering these systems on short time scales in which we begin in one microstate at a certain time, and then a short time later we are in another microstate.

Say we have a lattice of N spins each of which can take on the value of $+1$ or -1. The system is initially in a state where all the spins are pointing up. We take a time step (representing, for example, evolving the system forward by 1 second) and this initial microstate transitions to another microstate with some probability. How can we define this transition scheme (i.e., the transition probability and the method of choosing transitions) such that for long times and after the system has reached equilibrium, the probability to be in any particular microstate is given by the Boltzmann distribution? We can view this as our sub-framing question:

Sub-framing Questions
Given that microstates in thermal equilibrium have probabilities dictated by the Boltzmann distribution, how can we model the dynamics of transitions between microstates such that this equilibrium probability distribution is preserved.

To answer this question we will begin with a non-physics example to build intuition before considering the spin-system of interest. Moreover, this non-physics example will be framed as the reversed situation,

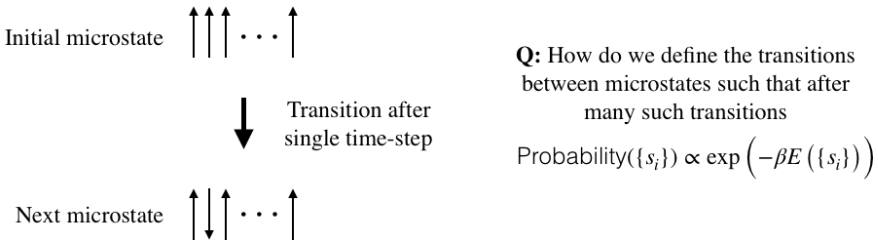

Figure 3: How can we define transitions between microstates such that after long times we obtain the Boltzmann distribution?

where we begin with well-defined transitions and we are seeking the equilibrium probabilities. Analyzing this example will allow us to determine an analytical relationship between transitions and equilibria that is general enough to be applied outside the context of the example.

2.1 From Room to Room

Say we have a floor plan with four rooms arranged as shown in Fig. 4[2]. A person is initially in one of the rooms. We define time in this system as proceeding in steps of size Δt for some Δt. After each time step, the person has equal probability to move through any of the openings leading out of the room. If a room has M openings, the person has a probability $1/M$ of leaving any one of these rooms; the probability of staying in the same room is zero. Thus, for each room there is a **transition probability** defining the probability of moving to one of the adjacent rooms. Now, here is the question:

> After many time steps (i.e., an infinite number of them) what is the probability that the person will be in room j?

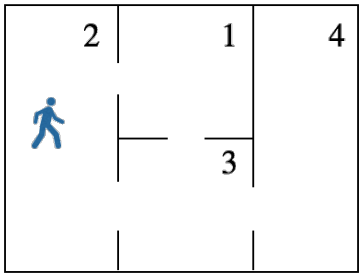

Figure 4: Floor plan for the example. A person is in one of four rooms, and after each time step has a probability $1/M$ of moving to an adjacent room where M is the number of adjacent rooms. In this transition scheme, there is a probability of 0 to remain in the same location

This long-time probability can be seen as the equilibrium probability of this system. In statistical physics, this equilibrium probability would be given by the Boltzmann distribution. Interestingly, the answer to this question is independent of whatever room we started in since considering an infinite number of time steps washes out the subsequent effects of the initial state of the system. Now, to answer this question, we will have to introduce some mathematics. Let $\pi_{i\to j}$ define the probability to move from room i to room j in a single time-step Δt. For this system, the values of $\pi_{i\to j}$ are

[2]This example is taken from Chapter 7 Section 2 of [1].

$$\begin{array}{llll} \pi_{1\to1}=0 & \pi_{1\to2}=1/2 & \pi_{1\to3}=1/2 & \pi_{1\to4}=0 \\ \pi_{2\to1}=1/2 & \pi_{2\to2}=0 & \pi_{2\to3}=1/2 & \pi_{2\to4}=0 \\ \pi_{3\to1}=1/3 & \pi_{3\to2}=1/3 & \pi_{3\to3}=0 & \pi_{3\to4}=1/3 \\ \pi_{4\to1}=0 & \pi_{4\to2}=0 & \pi_{4\to3}=1 & \pi_{4\to4}=0 \end{array} \tag{1}$$

There is one thing we should note about the above array. As we move along a row and sum all of the associated probabilities we will find 1. This should make sense: the probability of moving from one room to *any other* room should be 1. Writing this fact somewhat abstractly we have

$$\sum_j \pi_{i\to j} = 1 \tag{2}$$

where the summation runs over all rooms j and the result is independent of i. Now to determine the probability that the person is in room j after an infinite number of time steps, we will need to define the corresponding probability for a finite number of time steps. Let $p_j(t)$ represent the probability that the person is in room j at time t (or, equivalently, after $t/\Delta t$ time steps). For example, if the person begins in room 2 then we have $p_2(0) = 1$, and $p_j(0) = 0$ for any $j \neq 2$. We want to find a way to relate this probability at adjacent times. For example, given $p_j(t)$, the probability that the person is in room j at time t, we might want to know $p_k(t + \Delta t)$, the probability that the person is in room k at time $t + \Delta t$. If we found such a relationship, we might be able to iterate it many times to find the long-time behavior of the probabilities.

We can find the relationship between room probabilities at adjacent times, by doing a case analysis. Let's say we want to determine $p_3(t + \Delta t)$, the probability that the person is in room 3 at time $t + \Delta t$. And let's say we know $p_j(t)$ for $j = 1, 2, 3, 4$. To get to room 4, at time $t + \Delta t$, the person had to begin in either rooms $1, 2$, or 4 at time t. The person would then have had to transition to room 3 with a probability dictated by a particular entry of Eq.(1). Therefore, the probability to be in room 3 at time $t + \Delta t$ is the sum of the probabilities of transitioning to room 3 from the adjacent rooms *weighted* by the probability to be in each room at time t

$$\begin{aligned} (\text{prob. to be in } 3 \text{ at time } t+\Delta t) = {} & (\text{prob. to be in } 1 \text{ at time } t+\Delta t)(\text{prob. to go from } 1 \text{ to } 3) \\ & + (\text{prob. to be in } 2 \text{ at time } t+\Delta t)(\text{prob. to go from } 2 \text{ to } 3) \\ & + (\text{prob. to be in } 3 \text{ at time } t+\Delta t)(\text{prob. to go from } 3 \text{ to } 3) \\ & + (\text{prob. to be in } 4 \text{ at time } t+\Delta t)(\text{prob. to go from } 4 \text{ to } 3). \end{aligned} \tag{3}$$

In Eq.(3), we include the probability to go from 3 to 3 for completeness, but it does not change our final result because this transition probability is zero. Using our defined notation Eq.(3) becomes

$$p_3(t + \Delta t) = \pi_{1\to3}p_1(t) + \pi_{2\to3}p_2(t) + \pi_{3\to3}p_3(t) + \pi_{4\to3}p_4(t). \tag{4}$$

Eq.(4) can be generalized to represent the probability to be in any room j at time $t + \Delta t$:

$$p_j(t + \Delta t) = \sum_k \pi_{k\to j}p_k(t), \tag{5}$$

where the summation runs over all rooms k. So far so good! We now have an equation relating the transition probability $\pi_{i\to j}$ to the probability $p_j(t)$ of bein in a particular room at a time t. With some additional work we should be able to find a way to relate these transition probabilities to the long-time probability of being in any particular room:

$$\pi_{k\to j} \quad \overset{\text{relationship?}}{\Longrightarrow} \quad \lim_{t\to\infty} p_k(t) \tag{6}$$

In what follows we will go through a few algebraic manipulations which might seem arbitrary but whose purpose will be revealed in time. First, we add zero to the right side of Eq.(5) by adding and subtracting $p_j(t)$:

$$p_j(t+\Delta t) = p_j(t) + \sum_k \pi_{k\to j} p_k(t) - p_j(t) \tag{7}$$

Next, using $\sum_k \pi_{j\to k} = 1$ we multiply the final term by 1

$$p_j(t+\Delta t) = p_j(t) + \sum_k \pi_{k\to j} p_k(t) - \sum_k \pi_{j\to k} p_j(t) \tag{8}$$

which can also be written as

$$p_j(t+\Delta t) = p_j(t) + \sum_k \Big(\pi_{k\to j} p_k(t) - \pi_{j\to k} p_j(t)\Big). \tag{9}$$

Eq.(9) is completely equivalent to Eq.(5), but it has actually brought us closer to finding a relationship between the transition probability $\pi_{i\to j}$ and the long-time probability distribution $\lim_{t\to\infty} p_j(t)$. First, we define the distribution that $p_j(t)$ approaches in long times as p_j^{eq}:

$$p_j^{\text{eq}} = \lim_{t\to\infty} p_j(t). \tag{10}$$

Thus, taking the infinite time limit of Eq.(9) on the left-side and the right-side we have

$$\begin{aligned} \lim_{t\to\infty}\Big[p_j(t+\Delta t)\Big] &= \lim_{t\to\infty}\Big[p_j(t) + \sum_k \Big(\pi_{k\to j} p_k(t) - \pi_{j\to k} p_j(t)\Big)\Big] \\ p_j^{\text{eq}} &= p_j^{\text{eq}} + \sum_k \Big(\pi_{k\to j} p_k^{\text{eq}} - \pi_{j\to k} p_j^{\text{eq}}\Big). \end{aligned} \tag{11}$$

Subtracting p_j^{eq} from both sides we then have

$$0 = \sum_k \Big(\pi_{k\to j} p_k^{\text{eq}} - \pi_{j\to k} p_j^{\text{eq}}\Big) \tag{12}$$

From Eq.(12), we see that the summation is zero (and hence p_j^{eq} is the long-time distribution) if

$$\boxed{\frac{p_j^{\text{eq}}}{p_k^{\text{eq}}} = \frac{\pi_{k\to j}}{\pi_{j\to k}} \qquad \text{[Detailed balance].}} \tag{13}$$

Eq.(13) is called the **detailed balance** condition for transition probabilities; if transition probabilities $\pi_{j\to k}$ satisfy Eq.(13), then the long-time distribution of states is given by p_j^{eq}.

We should note that Eq.(13) is a more specific condition beyond the result Eq.(12). Namely, although Eq.(13) implies Eq.(12), Eq.(12) does not imply Eq.(13)[3] Although, Eq.(13) is less general than its starting point, we can take it to be the condition we were looking for. It relates transition probabilities to equilibrium probabilities and thereby allows us to determine the latter given the former (or vice versa!).

From the transition probabilities in Eq.(1) and Eq.(13), we find

$$\frac{p_1^{\text{eq}}}{p_2^{\text{eq}}} = \frac{\pi_{2\to 1}}{\pi_{1\to 2}} = 1 \quad p_1^{\text{eq}} = p_2^{\text{eq}} \tag{14}$$

[3]This is something that I have not noticed before. It suggests that there is a way to have an equilibrium probability distribution which does not satisfy detailed balance.

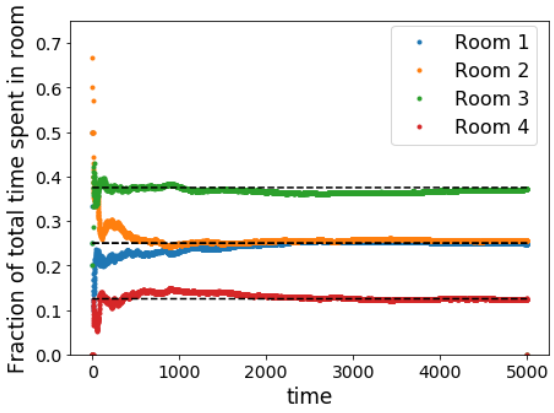

Figure 5: Plot of time evolution of the "room-to-room" system for 5000 time steps. Figure is the result of a python implementation of the Transition Scheme 1. We see that the after the system reaches equilibrium, the fraction of time spent in each room matches the results computed in Eq.(18).

$$\frac{p_1^{\text{eq}}}{p_3^{\text{eq}}} = \frac{\pi_{3\to1}}{\pi_{1\to3}} = \frac{2}{3} \quad p_1^{\text{eq}} = \frac{2}{3}p_3^{\text{eq}}. \tag{15}$$

$$\frac{p_3^{\text{eq}}}{p_4^{\text{eq}}} = \frac{\pi_{4\to3}}{\pi_{3\to4}} = 3 \quad p_3^{\text{eq}} = 3p_4^{\text{eq}} \tag{16}$$

Now, with the probability normalization condition

$$p_1^{\text{eq}} + p_2^{\text{eq}} + p_3^{\text{eq}} + p_4^{\text{eq}} = 1, \tag{17}$$

we can use Eq.(14), Eq.(15), and Eq.(16) to find

$$p_1^{\text{eq}} = \frac{1}{4}, \qquad p_2^{\text{eq}} = \frac{1}{4}, \qquad p_3^{\text{eq}} = \frac{3}{8}, \qquad p_4^{\text{eq}} = \frac{1}{8}. \tag{18}$$

Thus, the transition probabilities defined in Eq.(1) have allowed us to determine the equilibrium probabilities Eq.(18). The key equation in this calculation was the detailed balance condition Eq.(13). We can check the results in Eq.(18) computationally by simulating these room-to-room transitions. First we need to define a transition scheme. Following the prompt, we can choose the following transition scheme to define the time evolution of our system for each time step:

Transition Scheme 1

1. Start in room j.
2. Number the adjacent rooms from 1 to M. (Ordering of rooms is not important).
3. Draw a random real number u between $[0, 1)$.
4. If $u \in [(k-1)/M, k/M)$, then move to the kth adjacent room.
5. Return to step 1

This transition scheme is simply a computational representation of the description in Eq.(**??**). If, after sufficiently long times, we were to tally up the amount of time (i.e., the number of time steps) the person

spent in each room and then divide the result by the total time (i.e., total number of time steps), we would find probabilities given in Eq.(18). We did just that in Fig. 5[4]

Although, we derived Eq.(13) result using the toy example of a person in a room, our mathematical presentation was sufficiently general to carry over wholesale to statistical physics. In this carry over, we take the indices j and k to denote microstates, p_j^{eq} is the equilibrium probability for microstate j, and $\pi_{k\to j}$ is the transition probability to move from k to j in one time step.

2.2 Transition probabilities in statistical physics

Now, we return to the question that opened this section: Given the equilibrium probabilities of a statistical physics system, how can we choose a scheme for transitioning between microstates such that the equilibrium probability distribution is preserved for long times? In the above example, we answered the converse of this question. That is, given transition probabilities and a scheme for transitioning from room to room, we determined the equilibrium probabilities. To answer the desired question, we have to achieve the reverse of this. Is this possible?

Yes! As long as our transition probabilities satisfy the detailed balance result Eq.(13), then for sufficiently long times the probability distribution to be in a mircostate j will converge to p_j^{eq}. In statistical physics the equilibrium distribution is the Boltzmann distribution normalized by the partition function: $p_j^{\text{eq}} = e^{-\beta E_j}/Z$ where E_j is the energy of microstate j. Therefore, by Eq.(13), in order to simulate a statistical physics system, we need to choose the single-step transition probability $\pi_{j\to k}$ such that

$$\frac{\pi_{j\to k}}{\pi_{k\to j}} = e^{-\beta(E_k - E_j)}. \tag{19}$$

Eq.(19) is the only condition we need: If our transition probabilities satisfy it and we perform sufficiently many transitions between microstates, then over time, our states will be Boltzmann distributed. Moreover, we note that there is no mention of the initial microstate in this discussion. This is because the equilibrium distribution for this type of process is independent of the initial microstate. This means we can begin in any initial microstate and if we step forward in time for a long enough time, then we will reach the Boltzmann distribution. These two facts are sufficiently important to deserve their own bullet points. If the transition probabilities satisfy Eq.(19), then...

- ...we will always get Boltzmann distributed equilibrium distributions.
- ...the equilibrium distribution is independent of the initial microstate.

We are now prepared to devise a scheme to simulate the transitions between microstates in a statistical physics system. We will return to our example of a lattice of spins where each spin can take on the value $+1$ or -1. Here are the steps of our transition procedure.

Simulating a lattice of spins at a temperature T and energy $E(\{s_j\})$

1. Start in an initial spin microstate with N spins given by $s_1, s_2, \ldots, s_N$; This microstate is denoted $\{s_j\}_0$.
2. Randomly select a spin j, and flip it to -1 if it is $+1$ or to $+1$ if it is -1; The potential microstate is denoted $\{s_j\}_{\text{new}}$.
3. Determine whether to accept or reject transition in 2. according to the following:

[4]We should mention that there is some ambiguity in defining this transition scheme. As long as our transition probabilities are related to the equilibrium probabilities through the detailed balance relation Eq.(13), then *any* time evolution of the system will, for long-times, lead to the equilibrium probability distribution. Namely, the ratio of transition probabilities is important, rather than their exact magnitude.

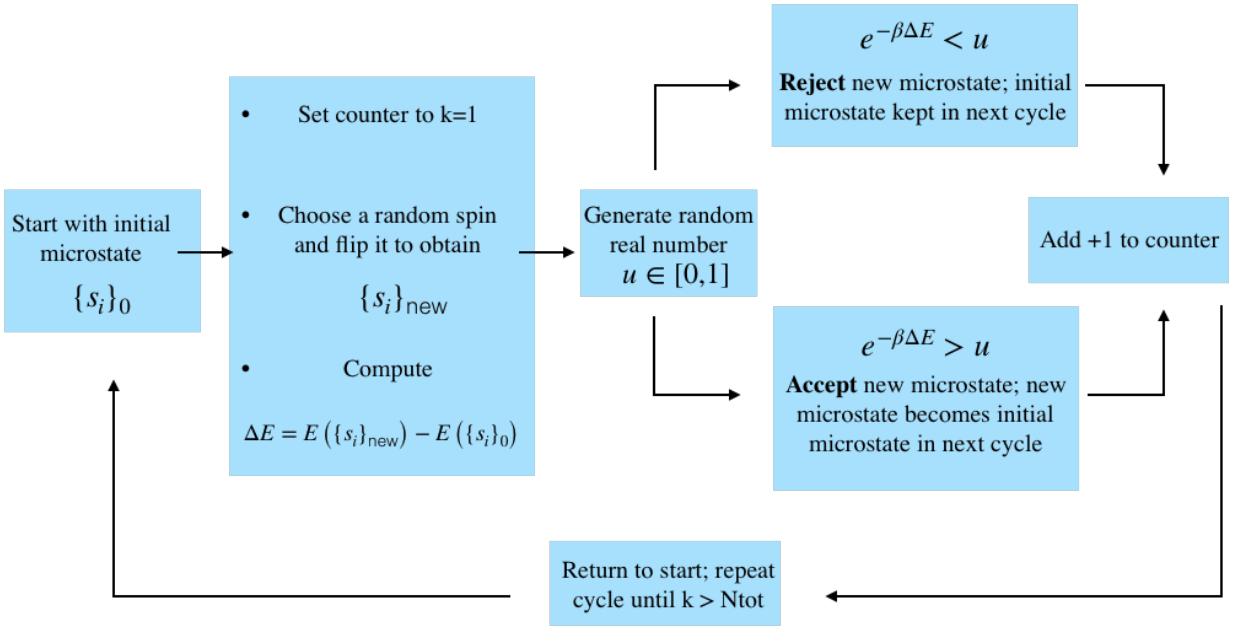

Figure 6: Algorithm for simulating lattice of spins in statistical physics. This simulation assumes a chosen temperature T (related to β through $\beta = 1/k_B T$) and a given energy of a microstate $E(\{s_i\})$. Simulation iterates for N_{tot} time steps.

(a) Compute the energies of the initial microstate and the potential microstate (i.e., $E(\{s_j\}_0)$ and $E(\{s_j\}_{\text{new}})$, respectively) and calculate the energy difference

$$\Delta E = E(\{s_j\}_{\text{new}}) - E(\{s_j\}_0) \tag{20}$$

(b) Draw a random real number u between $[0, 1]$.

(c) If $u < e^{-\beta\Delta E}$ then accept the potential microstate; If $u > e^{-\beta\Delta E}$ then reject the potential microstate.

4. If the transition is accepted, then $\{s_j\}_{\text{new}}$ becomes the new $\{s_j\}_0$. If the transition is rejected, then $\{s_j\}_0$ remains as $\{s_j\}_0$ for the next iteration.

5. Return to step 1; cycle through procedure until stopping time.

The scheme we have just outlined is formally called a **Markov Chain Monte Carlo** (MCMC) algorithm. When studying time-dependent probability distributions, "Markov" is the label applied when the probability to move to a new state depends *only on the current state* and not any other state in the far past; such probability distributions are called "memory-less". "Chain" refers to the fact that we are considering discrete time steps. And "Monte Carlo" is the label for a class of computational methods which uses random sampling to generate results.

The best way to develop an understanding of this simulation algorithm is to implement it yourself programming software like *Python* or *Mathematica*. In class we will implement an example of this algorithm using the relatively simple energy $E(\{s_i\}) = -\mu H \sum_i s_i$. And because this algorithm generates an ensemble of microstates whose probabilities are consistent with those given by the Boltzmann distribution, we can compute the average of any quantity that depends on these microstates and we should find results which match those computed from the partition function.

3 Final Remarks

The simulation algorithm presented above is fairly simple to write, but its power is immense. There are many systems in statistical physics which are difficult to solve analytically but which yield to a computational analysis through the MCMC algorithm. The **two-dimensional Ising Model** falls in this class of models and there are many online applications[5] which implement the algorithm above in order to represent how this model evolves in time.

We can see this algorithm as the main result of these notes. However, the result Eq.(9) is also quite important. It can allow us to move in a new direction along our previous search for analytical methods in statistical physics. It serves as an entry point into domain of **non-equilibrium statistical physics** which we turn to in the final notes.

References

[1] M. Plischke and B. Bergersen, *Equilibrium Statistical Physics*. World Scientific Publishing Company, 1994.

[5] Assuming these links aren't dead, here are two: https://mattbierbaum.github.io/ising.js/, https://physics.weber.edu/schroeder/software/demos/IsingModel.html

Resource: Introduction to Statistical Physics

Mobolaji Williams