PHYS CS 5: Non-Equilibrium Statistical Mechanics - Problem Set 1

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1 Instructions

The problems are divided into two categories: Foundations and Applications. The problems in Foundations are more don't come with fun stories. They would be good to do if you are feeling uncertain about the basic mechanics of the calculations we did in lecture. The problems in applications demonstrate some of the real world systems these methods can be applied to. Pick your poisons and have fun!

You are welcome to use computational aids to assist in the computation of eigenvectors of matrices, and such. You should not need them for any of the integrals that need to be done. Please don't outsource your thinking to language models, large or small.

2 Foundations

1. ($\star$) **A Periodic Random Walker** *(5 pts)*

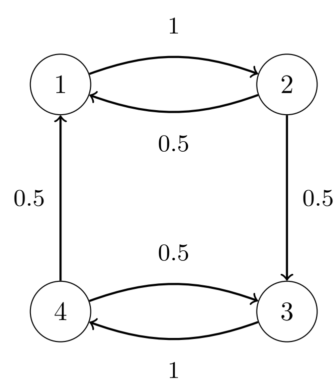

Figure 1: A variant of the random walker

Consider the random walker in the figure.

(a) *(3 pts)* Write down the transition matrix for this Markov process.

(b) *(2 pts)* Does this system equilibrate? If so, identify the distribution that things converge to.

2. ($\star\star$) **Solving the Diffusion Equation** *(15 pts)*

   This problem is designed to give you more practice with the diffusion equation.

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}$$

   We will solve the diffusion equation for some arbitrary initial condition, $P(x,0) = f(x)$.

   (a) *(5 pts)* Starting from the diffusion equation, take the spatial Fourier transform of both sides to rewrite the diffusion equation in k-space. You should get

$$\frac{\partial \hat{P}(k,t)}{\partial t} = -Dk^2\hat{P}(k,t)$$

   where the hats indicate that we are discussing the Fourier transform of the probability density.

   (b) *(5 pts)* You will note from the prior part that by converting to Fourier space, the diffusion equation has transformed from a partial differential equation to an ordinary differential equation. Solve this ODE to determine the general solution to our Fourier transformed equation. Again, the solution should be

$$\hat{P}(k,t) = h(k)e^{-Dk^2t}$$

   Apply the initial condition to get

$$\hat{P}(k,t) = \hat{f}(k)e^{-Dk^2t}$$

   (c) *(5 pts)* To proceed, we need to specify an initial condition. Say our particle starts at $x = 0$. That is, $P(x,0) = \delta(x)$. Then, using this initial condition, solve the diffusion equation and show that

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}}$$

   Food for thought: Now that you have determined the probability density for a delta source, can you use that to solve for the time evolution for any arbitrary initial distribution? (yes!)

3 Applications

3. ($\star\star$) **Road Rage** *(15 pts)*

   An antisymmetric simple exclusion process (ASEP) is a class of Markov processes that is useful in modeling a wide range of physical processes, like ribosomes traveling down mRNA strands or vehicles on a single lane highway. In this problem, we will treat a simple example of an ASEP.

   The key idea is that we have some set of lattice sites arranged in a line, and particles are trying to travel down it in a particular direction (like a ribosome trying to read the mRNA, or a car driving down the road). Say we have two sites, L(eft) and R(ight).

   Cars (or ribosomes) enter from the left, and exit from the right, but *multiple cars cannot be in the same place.* It is a single lane road after all. The rules are as follows:

- At each time step t, if L is empty, then a car enters onto the highway with probability α. If L is already occupied, then no car can enter.
- If L is occupied, but R is empty, then the car moves to R with probability β. If R is already occupied, the car is blocked.
- If R is occupied, the car in R exits the highway with probability γ.

(a) *(2 pts)* List out the possible states for the system.

(b) *(6 pts)* Calculate the transition matrix. In the simple case where $\alpha = \beta = \gamma$, calculate the stationary distribution.

(c) *(7 pts)* Now, using the stationary distribution, calculate the rate at which cars pass through the highway. That is, calculate, at each time t, what is the probability that a car exits the highway. Since we are at steady state, this tells us the average throughput of the highway.

Would the current be higher if multiple cars were allowed to be in the same spot? Justify your answer either with explicit calculation of the current (not recommended) or just with a short explanation.

4. ($\star\star$) **Based on a True Story** *(15 pts)*

Jack and Ji(ll)hoon went to a Physics department event to fetch a cup of water. Unfortunately, the physics department places the plastic cups next to the boiling water. When Jack fills his cup with water, the boiling water begins to melt the plastic, but to their surprise, the base of the cup rises up, not down! In this problem, we will discover why.

(a) *(4 pts)* Plastic cups are made of polymers. At some point during manufacturing process, the polymers get stretched out, so we model the cup as a single 1D chain of N links, each of length $a = 1$. Initially, the cup is fully stretched, so all links point down ($s_i = -1$) and the bottom of the cup is at height $h(0) = -N$.

When Jack fills the cup, the water reaches a height d above the bottom of the cup. We assume that only the links in contact with the boiling water are hot enough to flip. This creates an "active zone" of height d at the bottom of the chain. Links above this zone are frozen in the down state. For simplicity, assume that once a link is active, it is never deactivated.

Let n_{up} be the number of *active* links pointing up, and n_{down} be the number of *active* links pointing down.

Write a geometric constraint equation relating n_{up}, n_{down}, and the water level d. (Hint: The vector sum of the links in the active zone must bridge the vertical distance d).

(b) *(6 pts)* First, assume the thermal energy is high compared to the energy required to flip a link either way. Then, we can approximate the rate of flipping in each direction as equal. A link in the active zone flips from Down→Up with probability rate p, and from Up→Down with the same rate p.

We are interested in the average drift velocity of the cup's bottom, $v = \langle \frac{dh}{dt} \rangle$. Note that $h(t)$ increases by $+2$ if a link flips Up, and decreases by -2 if a link flips Down.

i. Write the master equation for the average drift velocity v in terms of n_{up}, n_{down}, and p.

ii. Using your constraint from Part (a), show that in this specific regime, the velocity v is constant (independent of n_{up}).

iii. Calculate the average time τ it takes for the cup to shrink to half its original size (i.e., for $h(t)$ to go from $-N$ to $-N/2$).

(c) *(5 pts)* Now, let's refine the model. In reality, gravity acts on the polymer, making it slightly harder to flip a link up than down. We model this by perturbing the rates with a small parameter ϵ:

$$\text{Rate}(Down \to Up) = p - \epsilon$$

$$\text{Rate}(Up \to Down) = p + \epsilon$$

i. Derive the new expression for the drift velocity v. Does it still depend only on d?

ii. Show that as the cup shrinks (and the chain in the active zone becomes more "crumpled" or entropically favorable), the upward velocity decreases.

iii. Find the critical number of upward links, n^*_{up}, at which the cup stops shrinking entirely.

5. ($\star\star\star$) **Do Ising Machines Dream of Parallel Updates?** *(25 pts)*

The Ising model of ferromagnetism is one of the canonical problems in statistical mechanics. In this problem, we will model its dynamics using a simple discrete-time Markov chain.

Consider two spin-$\frac{1}{2}$ particles, m_1 and m_2. Each spin can be in one of two states: up ($\uparrow$) or down ($\downarrow$), corresponding to magnetizations $m_i = +1$ and $m_i = -1$, respectively.

The Ising Hamiltonian in the absence of an external magnetic field is given by

$$H = -\frac{1}{2}\sum_i \sum_{j \neq i} J\, m_i m_j.$$

For our two-particle system, this simplifies to

$$H = -J m_1 m_2.$$

In the ferromagnetic case, the coupling constant $J > 0$ (for example, let $J = 1$).

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(a) *(2 pts)* List all possible states of the system.

(b) *(17 pts)* Suppose the spins evolve according to the following stochastic update rule:

$$m_i(t+1) = \text{sign}\big(\tanh(Jm_j(t)) + x\big), j \neq i$$

where x is a random variable drawn uniformly from the interval $[-1, 1]$.

Consider two different update schemes:

i. At each time step, choose one of the two spins at random and update its state according to the rule above.

ii. At each time step, update both spins simultaneously using the rule above.

For each scheme, write down the corresponding transition matrix.

Hint: You should not need to compute 16 probabilities for each matrix. There are really only a few cases, depending on if the spins are flipping from pointing in the same direction to opposite, or vice versa.

(c) *(6 pts)* The transition matrices obtained in part (b) will differ. However, if both algorithms are valid, each should converge to the Boltzmann distribution. Determine whether they do. If they do, explain physically why both update rules lead to the same equilibrium distribution. If not, provide an initial condition for which one of the schemes either fails to equilibrate or converges to an incorrect equilibrium distribution.

Remark: Incorrect equilibration in parallel update schemes is not just a theoretical curiosity. One practical example of a problem like this is in the design of *Ising machines*—hardware systems that attempt to find low-energy configurations of the Ising Hamiltonian. These machines can be used to solve problems in quantum simulation, logistics, optimization, and machine learning by running a class of algorithms called *Markov Chain Monte Carlo* algorithms. See Fig. 4 in this paper for an example of a similar pathology leading to incorrect equilibration.