## Final Spring 2020 Physics 4488/6562: Statistical Mechanics

http://www.physics.cornell.edu/sethna/teaching/562/ Due 11:00am, Wednesday May 20, submitted via the course Canvas site Last correction at May 19, 2020, 12:17 pm ©2020, James Sethna, all rights reserved

**Open Book Exam.** Work on your own for this exam. You may consult your notes, homeworks and answer keys, books and published work, or Web pages as you find useful. The problems have been designed to be doable given only material already presented in the course. If you find something in the literature or on the Web that is particularly helpful (*e.g.*, solves the problem), feel free to use it. However, just as in a publication, cite your source.

Some of the parts are as basic as they seem. Our goal here was to present deep and powerful ideas in the simplest possible context.

# Exercises (1-3 for everyone, 4-6 for 6562 only)

Everyone (4488 and 6562) Questions 1-3

1. Crystal defects.<sup>1</sup> (i)

This exercise numerically explores the wide variety of defects formed in crystals. You will either need to be able to write on screenshots of the simulation (either electronically or after printing), or will need to make careful sketches of what you see.

Start up the simulator [2], and select Crystal (one of the Initial Conditions choices under the main simulator window). You should see a collection of atoms moving to lower their energy, 'quenching' to a zero-temperature metastable state each time you hit Restart.<sup>2</sup> The system should settle into a mostly crystalline arrangement with a few vacancies, dislocations, walls, and more complicated defects. The grayscale is a measure of the stresses felt by the particles. The system has periodic boundary conditions, so some defects will stretch past the left or bottom and emerge through the right or top. Generate and admire the variety of defect patterns.

(a) Generate a large crystalline region. Take a snapshot and crop it to show the hexagonal crystal. Draw the three axes along which the crystal has closely-packed rows of atoms. Regenerate other large crystal regions, and sketch the orientations of their axes (no need for screenshots). Are the axis orientations different under different quenches? Does the crystal spontaneously break orientational symmetry?

<sup>&</sup>lt;sup>1</sup>This exercise uses the mosh pit simulator [2], developed to model humans dancing at heavy metal concerts: see [1, 8, 9, 10].

<sup>&</sup>lt;sup>2</sup>You can speed up the relaxation by increasing Frameskip to draw fewer of the steps. You can remove the red 'active' particle by changing 'Fraction Red' to zero.

(b) Generate and crop a simulation showing a vacancy – a missing atom in an otherwise crystalline region.

These vacancies are often quite mobile in crystals (see Exercise 9.12). Their motion allows the atoms in the crystal to diffuse (a vacancy hop to the left is an atom hop to the right). Dopants and impurities can also use vacancies to diffuse through a crystal.

The regions of crystalline order are called *grains*, and two grains are separated by a *grain boundary*. A grain boundary is usually a few atoms thick, separating two regions of fairly undeformed hexagonal crystal with different orientations.

(c) Generate a grain boundary stretching across the simulation, separating two crystals with different orientations. Draw their axes, and measure the misorientation angle – the smallest rotation needed to take one set of crystalline axes to the other. What is the largest misorientation angle possible in a hexagonal crystal?

The grain boundary is an orientational defect. It is not a *topological* defect, because crystalline orientational order is a continuous symmetry – there are crystalline ground states at all angles. Crystals respond to bending with an abrupt wall, rather than with a gradual change in orientation; the translational crystalline order makes gradual changes in orientation energetically expensive.

(d) Generate and crop a dislocation. Note that the dislocations in this simulation are delocalized over a substantial distance along one of the crystal axes. Over roughly how many particle diameters does it extend (as measured by a noticeable skewing of the lattice hexagons, or by the stress measured as the grayscale coloring of the defects)?

Something similar happens in an extreme way in materials like copper, where a dislocation can decompose into *partial dislocations* separated by a stacking fault.

The Burger's vector  $\vec{b}$ , by convention, is the displacement from the start to the end of a path that travels equal numbers of rows of atoms in a clockwise path around the defect.

(e) Find and indicate the direction and magnitude of the Burger's vector of your dislocation in part (d), by tracking the atomic layers along a curve encircling the defect. On the square lattice (Fig. 9.11), the Burger's vector was perpendicular to an extra row of atoms that ended at the dislocation. How is this different from the atomic configuration near your hexagonal-crystal dislocation?

#### 2. Unicycle. ③

We model a person pedaling a unicycle as a three-state Markov chain (Fig. 1). Let the three states of the Markov chain depict the pedal when the right foot is Up, Front, or Back in the cycle, 120° apart. Please use the convention that the vector of probabilities of her being in the three states is  $\boldsymbol{\rho} = \begin{pmatrix} \rho_{\rm U} \\ \rho_{\rm B} \\ \rho_{\rm B} \end{pmatrix}$ . Assume she pedals steadily, at 120° per time step, as shown by the arrows in Fig. 1.

(a) Write the Markov matrix P for a single time step. Find its eigenvalues and eigenvectors. If she starts cycling in state  $\mathbf{U}$ , how long will it take to reach a time-independent steady state? Explain how this relates to the eigenvalues of P.

The Markov matrix for our unicycle in part (a) thus has a cycle (Section 8.2).

The Markov matrix is a linear evolution law for the probability distribution. Schrödinger's equation, the diffusion equation, and the wave equation are other examples of linear systems. If a linear evolution law has a symmetry, then its solutions can be chosen from the eigenstates of that symmetry operator (see Section A.4). All three of our other examples all have a translation invariance  $x \to x + \Delta$ , and thus have solutions of the form  $f_k(t) \exp(ikx)$ , where  $\exp(ikx)$  for various k are the eigenstates of the translation operator.



#### Fig. 1 Three-state unicycle.

(b) What symmetry does our unicycle Markov chain have? Show that your Markov eigenstates are also eigenstates of the unicycle's symmetry. Our three examples with translation symmetry also have real (non-complex) solutions of the form  $f(t)\sin(kx)$ . Can your eigenstates be combined into real solutions of this form? What extra symmetry possessed by these two systems above guarantees that they have sine and cosine solutions?

Now our cyclist starts up a steep hill. With probability p she succeeds in pushing uphill at each time step; with probability 1 - p she stays in the same state.

(c) Write the transition matrix  $P^{\text{Hill}}$ . Does it have the same symmetry as P? What are the new eigenvectors and eigenvalues? Will it approach a stationary state  $\rho^*$  as time goes to infinity? (Solving for the motion is not an efficient method for deriving the answer.) Does  $P^{\text{Hill}}$  satisfy detailed balance? Why or why not?

Our probability distribution may be in a stationary state, but our cyclist is not – she is moving uphill, doing work. A Markov chain satisfying detailed balance evolves into a statistical mechanical equilibrium state (Exercise 8.12) that can do no work. One might think that the converse is true: if the steady state has a net flow of probability between two states, one could extract work from the imbalance in the transitions as one might use a paddle wheel in flowing water to make electricity or mill grain. But magnetic fields and such can break detailed balance (Exercise 9.13) without allowing work to be done in equilibrium.

### 3. Pandemic.<sup>3</sup> ③

Perhaps the most substantive contribution to public health provided by physics is the application of statistical mechanics ideas to model disease propagation. In this exercise, we shall introduce a few categories of epidemiological models, discuss how they can inspire and inform public health strategies (once adapted to real-world data), and then study one model as a continuous phase transition. You should leave this exercise empowered to think about the public health responses and modeling of potential pandemics – Ebola, SARS, and now COVID-19. Perhaps a few of us will contribute to the field.

Pandemics can undergo a phase transition. For diseases like measles, a single contagious child in an environment where nobody is immune will infect between twelve and eighteen people before recovering, depending on details like population density. For influenza, this number is around two to three. We define the 'basic reproduction number'  $R_0$  to be the ratio of infected people per contagious person in a fully susceptible community: 12–18 for measles, 2–3 for influenza. For a new pathogen, where nobody is immune,  $R_0 < 1$  will mean that an outbreak will eventually die out, and  $R_0 > 1$  means that a large initial outbreak will spread globally until reaching a significant fraction of the entire population. Much effort is spent during a pandemic to lower  $R_0$  into the safe range.

This transition is a continuous phase transition, with fluctuations on all scales near the critical threshold  $R_0 = 1$ . In this exercise, you will briefly consider three types of epidemic models (compartmental models, network models, and lattice models), compare different social interventions designed to lower  $R_0$ , and explore the fluctuations and critical behavior very close to threshold.

Compartmental models use coupled differential equations to model the disease spread between different 'compartments' of the population. The classic SIR model (see Exercise 6.25) involves three coupled compartments,

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\beta IS, \quad \frac{\mathrm{d}I}{\mathrm{d}t} = \beta IS - \gamma I, \quad \frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I, \tag{1}$$

where S(t), I(t), and R(t) are the proportions of the population that are susceptible, infected, and recovered. The parameter  $\beta$  measures the rate of infection spreading contact between people and  $\gamma$  is the rate at which people recover.

Network models treat people as nodes, connected to their contacts with edges. They assume a *transmissibility* T, the average probability that a victim will infect each of their contacts. For low T the epidemics die out; there will be a critical  $T_c$  above which a large outbreak will continue to grow exponentially. There are a variety of networks studied: fully connected networks (where SIR models become valid), loopless branching tree networks where everyone has k neighbors, real-world networks gleaned

<sup>&</sup>lt;sup>3</sup>This exercise was developed in collaboration with David Hathcock. Computer hints can be found at the book Web site [7].

from data on households and school attendance [4], and scale-free networks with a power-law distribution  $p(k) \propto k^{-\alpha}$  for the probability that a person has k contacts (has *degree k*). (Scale-free networks have been found to approximate the pattern of interactions between proteins in cells and nodes on the Internet, and serve as our model for populations with wide variation in the number of social contacts with potential for disease transmission.)

Lattice models – networks in two dimensions where only near neighbors are contacts – are sometimes used in agricultural settings, where the plant victims are immobile and the disease is spread only by direct proximity.

(a) Write  $R_0$  for the SIR model in terms of  $\beta$  and  $\gamma$ , for an initially nearly uninfected population ( $S \approx 1$  and  $I \ll 1$ ).

Network models usually ignore the long-range correlations between nodes: except for real-world networks, the contacts are usually picked at random so there are very few short loops. In that limit, Meyers et al. [4] express  $R_0$  in terms of the moments  $\langle k^n \rangle = \sum k^n p(k)$  of the degree distribution, which they solve for using generating functions (see Exercise 2.23):

$$R_0 = T\left(\frac{\langle k^2 \rangle}{\langle k \rangle} - 1\right). \tag{2}$$

People like nurses and extroverts with a lot of contacts can act as 'super-spreaders', infecting large numbers of colleagues. Scale-free networks explore what happens with a range of contacts: the smaller the exponent  $\alpha$ , the larger the range of variation.

(b) What is the critical transmissibility  $T_c$  predicted by the network model in eqn 2? Show that, for a scale-free network with  $\alpha \leq 3$  the critical transmissibility  $T_c = 0$ ; no matter how unlikely a contact will cause disease spread, there are rare individuals with so many contacts that they (on average) will cause exponential growth of the pathogen. If our population had  $\alpha = 3$ , what percentage of the people would we need to vaccinate to immunize everyone with more than 100 contacts? What would the resulting  $T_c$ , the maximum safe transmissibility, be? (If you find that the first percentage is small, use that fact to simplify your calculation of  $T_c$ . Hint:  $\sum_{1}^{\infty} k^{-z} = \zeta(z)$ , the Riemann zeta function, which diverges at z = 1.)

An important limitation of these network results is that they assume the population is structureless: apart from the degree distribution, the network is completely random. This is not the case in a 2D square lattice, for example. It has degree distribution  $p_k = \delta_{k,4}$ , but connections between nodes are defined by the lattice, and not randomly assigned. As you might expect, disease spread is closely related to percolation. In the mean-field theory, percolation predicts that the epidemic size distribution exponent is  $\tau = 3/2 = 1.5$ ; you will explore this in parts (e) and (f). In 2D, the lattice structure changes the universality class, the epidemic sizes are given by the cluster-size distribution exponent  $\tau = 187/91 \approx 2.055$ .

Besides exhibiting different power-law scaling, the value of the critical transmissibility can be quite different in structured populations. (c) What is  $T_c$  for a tree with k = 4 branches at each node (so  $p(k) = \delta_{k,4}$ )? Compare that to the critical transmissibility for a 2D square lattice,  $T_c = 0.5384$  [11]. Which is more resistant to disease spread?

One might imagine that a lattice model would mimic the effect of travel restrictions to prevent disease spread. Travel restrictions reduce the contact numbers, but do not change the qualitative behavior. This is due to the 'small world phenomenon': a surprisingly small number of long-range contacts can change the qualitative behavior of a network (see Exercise 1.7). Only a few long-distance travelers are needed to make our world well connected.

Finally, let us numerically explore the fluctuations and scaling behavior exhibited by epidemics at their critical points. We shall assume (correctly) that our population is well connected. We shall also assume that our population does not have system-scale heterogeneities: we ignore cities, subpopulations of vulnerable and crowded people, and events like the Olympics. Given these assumptions, one can argue that the qualitative behavior near enough to the critical point  $R_0 = 1$  is *universal*, and controlled not by the details of the network or SIR model but only by the distance  $1 - R_0$  to the critical point.

Let us organize our victims in 'generations' of infected people, with  $I_{n+1}$  the number of victims infected by the  $I_n$  people in generation n; we shall view the generation as roughly corresponding to the time evolution of the pandemic. The mean  $\langle I_{n+1} \rangle = R_0 I_n$ , but it will fluctuate about that value with a Poisson distribution, so  $I_{n+1}$  is a random integer chosen from a Poisson distribution with mean  $R_0 I_n$ .

(d) Write a routine pandemicInstance, that returns the evolution vector  $[I_0, I_1 \dots I_n \dots]$ and the total size  $S = \sum_n I_n$ . Iterate your routine with with  $R_0 = 0.9999$  and  $I_0 = 1$ in a loop until you find an epidemic with size  $S \ge 10^5$ . Plot the trajectory of this epidemic,  $I_n$  vs. n. Does your epidemic nearly halt during the time interval? Do the pieces of the epidemic before and after this near halt appear statistically similar to the entire epidemic?

One might presume that these large fluctuations could pose a real challenge to guessing whether social policies designed to suppress a growing pandemic are working. We must note, however, that the fluctuations are important only near  $R_0 = 1$ , or when the infected population becomes small.

At  $R_0 = 1$ , the size of the epidemic S has a power-law probability density  $P(S) \propto S^{-\tau}$  for large avalanches S.

(e) Write a routine pandemicEnsemble that does not store the trajectory, but instead runs N epidemics at a given value of  $R_0$ , and returns a list of their sizes. Plot a histogram of the sizes of  $10^4$  epidemics with  $R_0 = 0.99$ , with, say, 100 bins.

Regular histograms here are not useful; our distribution has a long but important tail of large events. Most epidemics subside quickly at this value of  $R_0$ , but a few last for hundreds of generations and infect tens of thousands of people. We need to convert to *logarithmic binning*.

(f) Change the bins used in your histogram to increase logarithmically, and be sure to normalize so that the counts are divided by the bin 'width' (the number of integers in that bin) and the number of epidemics being counted. Present the distribution of sizes for  $10^4$  epidemics at  $R_0 = 0.99$  on log-log plots. On the same plot, show the power-law prediction  $\tau = 3/2$  at the critical point.

In Exercise 12.28 we derived the universal scaling form for the avalanche size distribution in the random-field Ising model. This calculation also applies to our pandemic model. It predicts that the probability P(S) of an epidemic of size S for small distances  $r = (1 - R_0)$  below the critical point is given by

$$P(S) = CS^{-3/2} e^{-Sr^2/2},$$
(3)

where the nonuniversal constant C is around 0.4 to 0.5 (depending on the small S cutoff). Note that this gives the predicted power law  $\tau = 3/2$ , and is cut off above a typical size that grows quadratically in 1/r.

(g) Multiply your data by  $S^{3/2}$  to make it near constant for small sizes. Plot it and the scaling prediction (eqn 3) on a log-log plot. Does the universal scaling function describe your simulated epidemic ensemble?

The tools we learn in statistical mechanics – generating functions, universality, power laws, and scaling functions – make tangible predictions for practical models of disease propagation. They work best in the region of greatest societal importance  $R_0 \approx 1$ , where costly efforts to contain the pandemic are minimized while avoiding uncontrolled growth.

## Graduate (6562 only) Questions 4 - 6

### Warning: the version of exercise 4 in the text until recently was quite different.

### 5. Telegraph noise in nanojunctions. (Condensed matter) ③

Many systems in physics exhibit *telegraph noise*, hopping between two states at random intervals (like a telegraph key going on and then off at different intervals for dots and dashes). The nanojunction in Fig. 2 has two states,  $\alpha$  and  $\beta$ . It makes transitions at random, with rate  $\Gamma_{\beta \leftarrow \alpha} = \Gamma_{\beta \alpha}$  from  $\alpha$  to  $\beta$  and rate  $\Gamma_{\alpha\beta}$  from  $\beta$  to  $\alpha$ .



Fig. 2 Telegraph noise in a metallic nanojunction. Resistance versus time R(t) for a copper constriction, from [6]. We label  $\alpha$  the state with low resistance  $R_{\alpha}$ , and  $\beta$  the state with high resistance  $R_{\beta}$ . The two states probably represent a local shift of an atom or a small group of atoms in the constriction from one metastable state to another.

Master equation. Consider an ensemble of many identical copies of this system. Let the state of this ensemble at time t be given by  $\rho(t) = (\rho_{\alpha}, \rho_{\beta})$ , a vector of probabilities that the system is in the two states. This vector thus evolves according to the master equation

$$\mathrm{d}\boldsymbol{\rho}/\mathrm{d}t = M \cdot \boldsymbol{\rho}.\tag{4}$$

(a) What is the 2 × 2 matrix M for our system, in terms of  $\Gamma_{\alpha\beta}$  and  $\Gamma_{\beta\alpha}$ ? At long times, when the system is in a stationary ensemble  $\rho^*$ , what fraction of the time  $\rho^*_{\alpha}$  will our system be in the  $\alpha$  state? (Notice that, unlike the Markov chains in Section 8.2, we now evolve continuously in time (making this a Markov process). Remember also that  $\Gamma_{\alpha\beta}$  increases  $\rho_{\alpha}$  and decreases  $\rho_{\beta}$ .)

(b) Find the eigenvalue-eigenvector pairs for M.<sup>4</sup> Which eigenvector corresponds to the stationary state  $\rho^*$  from part (a)? Suppose that at t = 0 the system is known to be in the  $\alpha = 1$  state,  $\rho(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ . Write this initial condition in the basis of eigenvectors, and hence give a formula for the subsequent time evolution  $\rho(t)$ . What is the rate of decay to the stationary state?

Let us define the Green's function  $G_{\delta\gamma}(\tau)$  to be the probability of being in the  $\delta$  state at time  $t + \tau$ , given that it is in the  $\gamma$  state at time t. Thus in part (b),  $\rho(t) = \begin{pmatrix} G_{\alpha\alpha}(t) \\ G_{\beta\alpha}(t) \end{pmatrix}$ . (c) Solve for  $G(\tau)$ . Check that (i) probability is conserved,  $\sum_{\delta} G_{\delta\gamma}(\tau) = 1$ ; (ii) evolution for zero time does not change the state,  $G_{\delta\gamma}(0) = \delta_{\delta\gamma}$ ; (iii) the stationary state is stationary  $\sum_{\gamma} G_{\delta\gamma}(\tau) \rho_{\gamma}^* = \rho_{\delta}^*$ ; and (iv) the evolution goes at late times to the stationary state, independent of where it starts:  $G_{\delta\gamma}(t) \to \langle \rho_{\delta}^* \rangle$  as  $t \to \infty$ .

<sup>&</sup>lt;sup>4</sup>More specifically, the right eigenvectors  $M \cdot \rho_{\lambda} = \lambda \rho_{\lambda}$ .

Let R(t) be the resistance as a function of time, hopping between  $R_{\alpha}$  and  $R_{\beta}$ , as shown in Fig. 2, and let  $\overline{R}$  be the time average of the resistance. In analogy to eqn 10.19 for equilibrium systems, the connected correlation function for the resistance fluctuations can be written as

$$C(\tau) = \left\langle (R(t+\tau) - \overline{R})(R(t) - \overline{R}) \right\rangle_{\text{ev}} = \left\langle (R(\tau) - \overline{R})(R(0) - \overline{R}) \right\rangle_{\text{ev}} = \left\langle ([R(\tau)]_{\gamma} - \overline{R})(R_{\gamma} - \overline{R}) \right\rangle_{\text{eq}}.$$
(5)

in the (daunting) notation for different ensembles used in Section 10.4. Here  $[R(\tau)]_{\gamma}$  is the noise average of  $R(\tau)$  given initial state  $\gamma$ .

(d) Argue directly that

$$C(\tau) = \sum_{\gamma,\delta} G_{\delta\gamma}(\tau) (R_{\delta} - \overline{R}) (R_{\gamma} - \overline{R}) \rho_{\gamma}^{*}.$$
 (6)

Calculate  $[R(\tau)]_{\gamma}$  in terms of G; use it and conservation of probability (part (c)) to derive eqn 6 from the last line of eqn 5.



#### Fig. 3 Telegraph noise with three metastable states, from [5].

Nanojunctions, especially at higher temperatures, often show more than two metastable states in the experimental bandwidth.<sup>5</sup> Usually these form independent two-level fluctuators (atomic rearrangements too far apart to interact substantially), but sometimes more complex behavior is seen. Figure 3 shows three resistance states, which we label  $\alpha$ ,  $\beta$ , and  $\gamma$  from lowest resistance to highest. We notice from Fig. 3 that the rates  $\Gamma_{\gamma\beta}$ and  $\Gamma_{\beta\gamma}$  are the highest, followed by the rates  $\Gamma_{\alpha\gamma}$  and  $\Gamma_{\gamma\alpha}$ . There are no transitions seen going between states  $\alpha$  and  $\beta$ .

There is a large current flowing through the nanojunction, allowing the resistance to be measured. Whether these transitions are equilibrium fluctuations, perhaps with a field-dependent effective temperature, or whether they are non-equilibrium transitions mostly induced by the external current, could be tested if these last two rates could be measured. If detailed balance is violated, the system is out of equilibrium.

(e) Detailed balance. Approximate the master equation rates  $\Gamma_{\alpha\beta}$  as a discrete-time Markov chain with a tiny step  $\Delta t$  and transition matrix  $P: P_{\alpha\beta} \approx \exp(\Gamma_{\alpha\beta}\Delta t)$ . What does the cyclic detailed balance condition (eqn 8.22) imply about the rates  $\Gamma$ ? Assuming that the system satisfies detailed balance, what is the difference between the two unmeasured rates  $\Gamma_{\alpha\beta}$  and  $\Gamma_{\beta\alpha}$  in terms of the other four rates?

<sup>&</sup>lt;sup>5</sup>A junction is outside the bandwidth if it fluctuates either too fast or too slowly to measure with the experimental set-up.

## 6. Entanglement of two spins.<sup>6</sup> (Quantum) ③

How does entropy increase in a quantum system? The typical way is through the loss of coherence – information lost to the environment (Exercise 7.25). A measurement through an operator **O** can cause a pure state wavefunction (entropy zero) to split into an ensemble<sup>7</sup> of eigenstates of **O** (entropy  $-k_B \sum_o |c_o|^2 \log |c_o|^2$ ). Here we focus on a different mechanism; *Entropy can increase when we ignore or throw away information*. In this exercise, we will concentrate on a quantum system with two spins, an example of *entanglement* and entropy. In Exercise 7 we shall discuss the entanglement of larger systems, and explore both entanglement entropy and *eigenstate thermalization*.

Consider first the spin singlet<sup>8</sup> state of positronium: an electron-positron pair with opposite spins in an antisymmetric spin wave function

$$(1/\sqrt{2})\left(\left|\uparrow_{e}\right\rangle\left|\downarrow_{p}\right\rangle-\left|\downarrow_{e}\right\rangle\left|\uparrow_{p}\right\rangle\right).$$
(7)

#### (a) What is the entropy of this spin singlet wavefunction?

What happens if we separate the two particles with an electric field (without disturbing their spins), and throw away<sup>9</sup> the electron?

To study this, we introduce the *reduced density matrix*. Suppose  $\rho$  is the density matrix of a system composed of two subsystems A and B with bases  $\{|\psi_a\rangle\}$  and  $\{|\phi_b\rangle\}$ . Suppose we consider experiments solely involving A (since we are ignoring B or have thrown it away). Then these experiments will involve observables  $\mathbf{O}$  that do not act on the variables in B, so  $\mathbf{O}|\phi_b\rangle = |\phi_b\rangle\mathbf{O}$  and  $\langle\phi_b|\mathbf{O} = \mathbf{O}\langle\phi_b|$ . We can write the expectation value of  $\mathbf{O}$  in terms of the density matrix for the entire system with the usual trace

$$\begin{aligned} \operatorname{Tr}_{a,b}(\mathbf{O}\rho) &= \sum_{a,b} \langle \psi_a | \langle \phi_b | \mathbf{O}\rho | \phi_b \rangle | \psi_a \rangle \\ &= \sum_a \langle \psi_a | \mathbf{O} \left( \sum_b \langle \phi_b | \rho | \phi_b \rangle \right) | \psi_a \rangle \\ &= \operatorname{Tr}_a \mathbf{O}\rho^{[A]}, \end{aligned} \tag{8}$$

where the reduced density matrix

$$\rho^{[A]} = \sum_{b} \langle \phi_b | \rho | \phi_b \rangle \tag{9}$$

<sup>&</sup>lt;sup>6</sup>This exercise was developed in collaboration with Jaron Kent-Dobias. Computer hints can be found at the book Web site [7].

 $<sup>^{7}</sup>$ Exercise 7.25 describes microscopically how this arises; the wavefunctions of the environment split into pieces for each possible observation that differ so much that no operator can connect them.

<sup>&</sup>lt;sup>8</sup>This is a classic system for exhibiting 'spooky action at a distance' and disproving hidden variables theories [3, III.18-3].

<sup>&</sup>lt;sup>9</sup>Or, more realistically, what happens if we let the positronium decay into two photons of correlated polarization, and let one escape into outer space [3, III.18-3].

is the trace over the basis states in B. The reduced density matrix is thus a partial trace. Indeed, one often talks of partial traces in classical systems where one has integrated out over some degrees of freedom to get an effective free energy (see note 5 on page 141).

(b) Calculate the reduced density matrix  $\rho_P$  for the positron portion of the spin-singlet wavefunction of eqn 7, which can be used to describe subsequent experiments on the positron not involving the electron. Show your steps. What is the entropy if we ignore or discard the electron?

(c) Now consider the positronium in a triplet state  $|\uparrow_p\rangle|\uparrow_e\rangle$ . After discarding the electron, what is its entropy?

We say that the singlet state is *entangled*, while the triplet state is not. Some speculate the growth of quantum entanglement with time is equivalent to the growth of entropy with time; that all loss of information rests upon quantum entanglement with unobservable degrees of freedom (either information escaping to far places as in part (b), or information escaping into many-body correlations in quantum wavefunctions of macroscopic objects, as in Exercise 7.25). This speculation would seem at odds, however, with the observation that chaotic classical systems also lose information and have entropies that grow with time.

## 7. Heisenberg entanglement.<sup>10</sup> (Quantum) ③

Here we introduce the quantum Heisenberg antiferromagnet, and use it to explore how entropy, temperature, and equilibration can emerge through the entanglement of two portions of a large system – closely related to the *eigenstate thermalization hypothesis* (see Exercise 7.17). We saw in Exercise 6 that ignoring part of a system can take a quantum pure state into a mixture of states on the remaining subsystem. This should remind you of the way we derived the canonical ensemble by splitting a system in the microcanonical ensemble into a subsystem and a bath, and ignoring the bath (Section 6.1, Fig. 6.1). We can make this analogy much more powerful by using a larger quantum system, here a one-dimensional chain of spin  $\frac{1}{2}$  particles.

The one-dimensional Heisenberg antiferromagnet has Hamiltonian

$$\mathcal{H}_{N_{\rm spins}} = \sum_{m=1}^{N_{\rm spins}-1} \mathbf{S}_m \cdot \mathbf{S}_{m+1}, \tag{10}$$

where we have set the strength of the coupling J to 1 – positive, and hence favoring antiparallel spins. Here the quantum spins  $\mathbf{S} = (\sigma_X, \sigma_Y, \sigma_Z)$  have spin  $\frac{1}{2}$ , and are written in terms of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(11)

Let us begin with an analytical calculation of the Hamiltonian and the eigenstates for  $N_{\text{spins}} = 2$ , considered already in Exercise 6. We work in the four-dimensional  $\sigma_z$  basis

$$\begin{pmatrix} |\uparrow_1\rangle|\uparrow_2\rangle\\ |\uparrow_1\rangle|\downarrow_2\rangle\\ |\downarrow_1\rangle|\uparrow_2\rangle\\ |\downarrow_1\rangle|\downarrow_2\rangle \end{pmatrix}.$$
(12)

(a) Show analytically that

$$\mathcal{H}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
 (13)

Find the eigenvalues and eigenstates for this Hamiltonian. Is the ground state the triplet or the singlet? Does this make sense for an antiferromagnet? (Hint: The spin  $\mathbf{S}_1$  commutes with the kets  $|\uparrow_2\rangle$  and  $|\downarrow_2\rangle$  and vice-versa. The tensor discussion below may also be helpful.)

 $<sup>^{10}</sup>$ This exercise was developed in collaboration with Jaron Kent-Dobias. Computer hints can be found at the book Web site [7].

Implementing this calculation elegantly on the computer demands that we understand how the single-spin  $\sigma$  operators and the dot product  $\mathbf{S}_m \cdot \mathbf{S}_{m+1}$  act on the entire  $2^{N_{\text{spins}}}$ dimensional Hilbert space. The fact that they commute with the parts of the wavefunction that only involves other spins says that they act as identity matrices on those parts of the Hilbert space. That is,  $\sigma_x[1]$  for the first spin needs to be promoted to  $\sigma_x[1] \otimes \mathbf{1}_{2^{N_{\text{spins}}-1}}$ , and  $\sigma_x[2]$  for the second needs to be turned into  $\mathbf{1}_2 \otimes \sigma_x[1] \otimes \mathbf{1}_{2^{N_{\text{spins}}-2}}$ , ...

(b) Implement this numerically for the two-spin system. Calculate the Heisenberg Hamiltonian, and verify the answer of part (a). (Hint: Many modern programming languages have support for tensor data structures. These efficient routines will be important in later steps, so use them here.<sup>11</sup> See the hints files at [7].)

In this exercise, we shall discuss how pure energy eigenstates states in a system AB become mixed states when we split the system into a subsystem A and a bath B, and study the properties of these mixed states. We shall index operators acting on the subsystem A with Latin letters i, j, operators on the bath B with Greek letters  $\alpha, \beta$ , and operators on the total system AB with capital letters I, J, or sometimes with pairs of indices  $i\alpha, j\beta$ .

(c) If  $\rho_{i\alpha,j\beta}$  is the density matrix for the whole system AB, show analytically that the sum  $\sum_{\alpha} \rho_{i\alpha j\alpha}$  gives the reduced density matrix for the subsystem (e.g., as defined in *Exercise* 6).

We can use the two-spin problem of part (a) to preview the rest of the exercise, in a context where you know the answer from Exercise 6. Here we view the first spin as the the 'subsystem' A, and the second spin as the 'bath' B.

(d) Select the singlet eigenstate, and normalize it if necessary. Generate the pure-state density matrix, and reshape it into the four index tensor  $\rho_{i\alpha,j\beta}$ . Trace over the bath as in part (c), and verify that the reduced density matrix  $\rho_{ij}^A$  describes an unpolarized spin. Calculate the entropy by taking the suitable matrix trace.

To generate the Heisenberg Hamiltonian for multiple spins, we can save steps by noting that we already know the Hamiltonian for two spins from eqn 13 So the term  $\mathbf{S}_m \cdot \mathbf{S}_{m+1}$  in eqn 10 becomes<sup>12</sup>

$$\mathbf{1}_{2^{m-1}} \otimes \mathcal{H}_2 \otimes \mathbf{1}_{2^{N_{\text{spins}}-(m+1)}}$$
(14)

(e) Use this to write a function that returns the Heisenberg Hamiltonian  $\mathcal{H}_{N_{\text{spins}}}$  (eqn 10) as a  $2^{N_{\text{spins}}} \times 2^{N_{\text{spins}}}$  matrix. Check, for  $N_{\text{spins}} = 2$  it returns  $\mathcal{H}_2$  (eqn 13). Check also for  $N_{\text{spins}} = 3$  its eigenvalues are (-4, -4, 2, 2, 2, 2, 0, 0), and for  $N_{\text{spins}} = 4$ that its distinct eigenvalues are  $\{-3 - 2\sqrt{3}, -1 - 2\sqrt{2}, 3, -1 + 2\sqrt{2}, -1, -3 + 2\sqrt{3}\} \approx$  $\{-6.46, -3.8, 3, 1.8, -1, 0.46\}.$ 

<sup>&</sup>lt;sup>11</sup>One subtle point. In combining an operator  $L_{ij}$  acting on subsystem A with  $M_{\alpha\beta}$  acting on subsystem B, we want an operator O which labels rows using  $i\alpha$  and columns with  $j\beta O_{i\alpha j\beta}$ . We can then use O as a two-index matrix to compute eigenvectors and eigenvalues. In some implementations, this demands that we swap the two inner axes of the naive product  $L_{ij}M_{\alpha\beta}$ .

<sup>&</sup>lt;sup>12</sup>In the C and Python convention where indices start with zero, this would be  $\mathbf{1}_{2^m} \otimes \mathcal{H}_2 \otimes \mathbf{1}_{2^{N_{\text{spins}}-(m+2)}}$ .

We shall work with a system of  $N_{\text{spins}} = N_{AB} = 10$  spins in the chain; we shall primarily study a subsystem with  $N_A = 4$  spins, so the bath has  $N_B = N_{AB} - N_A = 6$  spins. We shall use a particular eigenstate  $\psi$  of  $\mathcal{H}_{N_{AB}}$  in a sequence of four steps: (i) to calculate the reduced density matrix  $\rho_A$  for  $N_A$ , (ii) to investigate the entanglement between A and the bath B, (iii) to calculate the entanglement entropy, and (iv) to illustrate eigenstate thermalization. For the last, we want to choose  $\psi$  with an energy that is lower than average, but not near zero.

(f) Create  $\mathcal{H}_{AB} = \mathcal{H}_{10}$ . Find its energy eigenvalues and eigenstates, and (if necessary) sort them in increasing order of their energy. Pick the energy eigenstate  $\psi$  of the full system that is 1/4 the way from the bottom (the  $K = 2^{N_{AB}-3}$  entry). Calculate the pure density matrix  $\boldsymbol{\rho}^{\text{pure}}$ , reshape it into the four index tensor  $\rho^{AB}_{i\alpha,j\beta}$ , and trace over the bath to give the reduced density matrix  $\rho^{A}_{ij}$ . Check that  $\boldsymbol{\rho}^{A}$  has trace one (as it must), and calculate  $\text{Tr}[(\boldsymbol{\rho}^{A})^{2}]$ . Is it is a mixed state?

The entanglement entropy between A and B for a pure state  $\psi$  of AB is the entropy of the reduced density matrix of A.

(g) Calculate the entanglement entropy  $S = -\text{Tr} \rho_A \log \rho_A$ .<sup>13</sup> Check that it has the same entropy as subsystem B. See how the entanglement entropy changes with the size of the subsystem, by looping over  $N_A$  from zero to  $N_{AB}$ . Plot S as a function of  $N_A$  for our particular eigenstate  $\psi$ . Where is the entanglement entropy largest? Explain why it goes to zero for the two endpoints.

The term 'entanglement' sounds mutual; A and B are entangled together, rather than the bath B has perturbed A. This nomenclature is not an accident. As you checked numerically, the entanglement entropies of the two subsystems is the same, as can be shown using the *Schmidt decomposition* (not described here).

In statistical mechanics, a large ergodic system AB in the microcanonical ensemble at energy E, when restricted to a relatively small subsystem A, will generate an equilibrium thermal ensemble at the corresponding temperature. The *eigenstate thermalization hypothesis* says that many systems<sup>14</sup> take this to an extreme: for each eigenstate  $\psi$ , the reduced density matrix  $\rho_A$  of the subsystem will converge to a Boltzmann equilibrium thermal ensemble

$$\rho_{jk}^{\beta} = \delta_{jk} \mathrm{e}^{-\beta E_k^A} \left/ \sum_{\ell} \mathrm{e}^{-\beta E_{\ell}^A} \right.$$
(15)

as the system size goes to infinity.

<sup>&</sup>lt;sup>13</sup>Note:  $\rho_A$  will have some zero eigenvalues, which may confuse a matrix logarithm. Remember that diagonalizing  $\rho$  also diagonalizes log  $\rho$ , and the trace is invariant under a change of basis. Hence, you can define your own function pLogp which returns zero if  $p \leq 0$  and  $p \log p$  otherwise, and sum it over the eigenvalues of  $\rho_A$ .

<sup>&</sup>lt;sup>14</sup>Systems exhibiting, for example, many-body localization (of considerable current interest) do not exhibit eigenstate thermalization.

Let us calculate the probability  $p_k$  that our subsystem is in eigenstate  $\psi_k^A$ ,  $p_k = \text{Tr}(|\psi_k^A\rangle\langle\psi_k^A|\boldsymbol{\rho}_A)$ . We are simulating a rather small system, so fluctuations will be large.

(h) Make a log plot of  $p_k$  vs.  $E_k^A$ . Do a fit to the predicted form eqn 15 to find  $\beta$ , and plot the result with your data.

In particular, the reduced density matrix is predicted to be at the temperature of the microcanonical ensemble at the energy E of the original pure state  $\psi$ .

(i) Write a function  $\text{EbarAB}(\beta)$  returning the average energy of the entire system as a function of  $\beta$ . Take a sampling of eigenstates  $\psi_K$  of the total system, fit  $p_k$  vs  $E_k^A$  as in part (h), and plot  $\beta$  vs. E along with your prediction  $\beta(\text{EbarAB})$ . Do you achieve a rough agreement?

# References

- [1] Bierbaum, M. K., Silverberg, J. L., Sethna, J. P., and Cohen, I. (2013). Collective motion of mosh pits: Bierbaum web site. http://hey.runat.me/pages/science/moshpits\_project.html.
- [2] Bierbaum, M. K., Silverberg, J. L., Sethna, J. P., and Cohen, I. (2013). Moshpits simulation. http://mattbierbaum.github.io/moshpits.js/.
- [3] Feynman, R. P., Leighton, R. B., and Sands, M. (1963). *The Feynman lectures on physics*. Addison-Wesley, Menlo Park, CA.
- [4] Meyers, Lauren Ancel, Pourbohloul, Babak, Newman, M.E.J., Skowronski, Danuta M., and Brunham, Robert C. (2005). Network theory and sars: predicting outbreak diversity. *Journal of Theoretical Biology*, 232(1), 71 – 81.
- [5] Ralls, K. S. and Buhrman, R. A. (1991). Microscopic study of 1/f noise in metal nanobridges. *Physical Review B*, 44, 5800–17.
- [6] Ralls, K. S., Ralph, D. C., and Buhrman, R. A. (1989). Individual-defect electromigration in metal nanobridges. *Physical Review B*, 40, 11561–70.
- [7] Sethna, J. P. and Myers, C. R. (2020). Entropy, Order Parameters, and Complexity computer exercises: Hints and software. http://www.physics.cornell.edu/sethna/ StatMech/ComputerExercises.html.
- [8] Silverberg, J. L. (2015). Moshing with physics. TED talk at https://www.youtube. com/watch?v=rjvaiiXIySc.
- [9] Silverberg, J. L., Bierbaum, M. K., Sethna, J. P., and Cohen, I. (2013). Collective motion in mosh pits: Cohen group web site, links to press. http://cohengroup.lassp. cornell.edu/projects/collective-motion-mosh-pits.
- [10] Silverberg, J. L., Bierbaum, M. K., Sethna, J. P., and Cohen, I. (2013, May). Collective motion of humans in mosh and circle pits at heavy metal concerts. *Physical Review Letters*, **110**, 228701.
- [11] Tomé, Tânia and Ziff, Robert M. (2010, Nov). Critical behavior of the susceptibleinfected-recovered model on a square lattice. *Phys. Rev. E*, 82, 051921.