## Physics 4488/6562: Statistical Mechanics http://www.physics.cornell.edu/sethna/teaching/562/ Prelim Spring 2020 Due 10:10am, in class, this Monday March 9 (three days from now) Last correction at March 8, 2020, 5:27 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

Everyone (4488 and 6562)

### 1. Pendulum energy shell. ③

In this exercise, we shall explain why we focus not on the surface of constant energy in phase space, but rather the energy shell. As noted in Fig. 3.1, the energy shell in phase space will typically vary in thickness – causing the microcanonical average to weigh thick regions of the energy surface more heavily than thin regions. (The hyperspheres of the ideal gas are not typical energy shells!) Here we show, for the pendulum, that this weighting by thickness is physically correct.

Figure 1 shows the phase space of the pendulum with Hamiltonian

$$\mathcal{H} = p^2 / 2m\ell^2 + mg\ell(1 - \cos(\theta)) = p^2 / 2 + (1 - \cos(\theta)),$$
 (1)

setting  $mg\ell = m\ell^2 = 1$ . The inner grey ring is an energy shell at a relatively low energy, and the outer ring is at a higher energy where the anharmonic terms in the potential energy are strong.

(a) Why is the inner energy shell roughly circular? For the outer shell, at about what position and momentum is our pendulum at the thinnest point? The thickest? Note that the outer shell comes close to E = 2. What changes topologically in the energy surface at E = 2? Describe physically how our pendulum motion alters when E crosses two.



Fig. 1 Pendulum energy shells. Two energy shells for the pendulum of eqn 1. Both are of thickness  $\delta E = 0.1$ ; the inner one spans from  $E_1 = \frac{1}{2}$  to  $E_1 + \delta E = 0.6$ , the second spans from  $E_2 = 1.88$  to 1.98.

In statistical mechanics, we average observables over the energy shell to get typical behaviors. In particular, we show in Chapter 4 that time averages for a typical initial condition are given by averages over the energy surface. Is the varying thickness of the energy shell important for getting the correct energy-shell average?

(b) Does the pendulum spend extra phase-space time in the regions where the outer energy shell from Fig. 1 is thickest? Explain clearly why you say so. Make sure you explain physically how the two energy shells differ in this regard.

One can use Hamilton's equations 4.1 to show the thickness precisely works to give the correct average in a general Hamiltonian system. Let us check this explicitly for the pendulum.

First calculate the time average. Let us parameterize the phase-space curve of constant energy by its arclength<sup>1</sup> s, where  $ds = \sqrt{dp^2 + d\theta^2}$ .

(c) Argue that the time average of an operator over a period T,

$$\langle O \rangle_t = 1/T \int_0^T \mathrm{d}t \, O(p(t), \theta(t)),$$
 (2)

equals the weighted average

$$1/T \int \frac{\mathrm{d}s}{|\mathbf{v}|} O(p(s), \theta(s)), \tag{3}$$

where  $\mathbf{v} = (\dot{p}, \dot{\theta})$  is the phase-space velocity around the trajectory. Does  $|\mathbf{v}|$  vary significantly around the inner energy shell in Fig. 1?

Next calculate the average over the energy surface.

(d) Argue that the thickness of the energy shell at a point  $(p, \theta)$  is given by  $\delta E/|\nabla \mathcal{H}|$ , where  $\nabla \mathcal{H} = (\partial \mathcal{H}/\partial p, \partial \mathcal{H}/\partial \theta)$ . (Do not use Hamilton's equations yet.) Use eqns 3.5

<sup>&</sup>lt;sup>1</sup>One may note that the units of position and momentum are different! Indeed, there is no natural metric in phase space. Our exercise illustrates a particular case using a convenient set of units (eqn 1). The general case is the focus of Chapter 4.

and 3.6 to argue that the microcanonical average of an operator O acting on the pendulum is

$$\langle O \rangle_{MC} = \int \frac{\mathrm{d}s}{|\nabla \mathcal{H}|} O(p(s), \theta(s)) \bigg/ \int \frac{\mathrm{d}s}{|\nabla \mathcal{H}|}.$$
 (4)

Now we explicitly relate the phase-space velocity  $\mathbf{v}$  to the gradient  $\nabla \mathcal{H}$ .

(e) What is the gradient  $\nabla \mathcal{H}$  for our pendulum, in terms of p and  $\theta$ ? Does it agree with **v**? Do the lengths  $|\nabla \mathcal{H}|$  and  $|\mathbf{v}|$  agree? Use Hamilton's equations of motion (eqns 4.1) to check that this also holds for a general Hamiltonian system.

(f) Using your results above, show that  $\langle O \rangle_t = \langle O \rangle_{MC}$  for our pendulum.

Everyone (4488 and 6562)

## 2. Active matter.<sup>2</sup> Active matter ③

'Active matter' is a growing field of statistical mechanics – the description of emergent behavior from systems of self-propelled 'agents' that maintain themselves out of thermal equilibrium. Applications include flocking birds, schools of fish, collective motion of bacterial colonies, manufactured self-propelled colloidal particles, and bio-polymers like microtubules and actin which actively grow and (together with protein molecular motors) can exert forces and move around. Use the exercise as a motivation to also explore the excellent videos and simulations on the Web in this field.

This exercise leverages an active-matter simulation of humans at heavy metal concerts, where loud, fast music, flashing lights, and intoxication lead to segregated regions known as *mosh pits* where participants engage in violent collisional behavior [7, 9, 8, 1]. Here we shall use the simulation to explore both equilibrium behavior and two active matter systems: flocking and self-propelled particles. We shall view the simulator as a kind of experimental system. We shall explore how the system responds to changing the control parameters, and investigate the emergent behavior in different regimes.

First explore the moshpit simulator [2].<sup>3</sup> The simulation has two types of agents – active (red) and passive (black); both interact via a soft repulsive potential, and have a damping force  $-\mu \mathbf{v}$  to absorb kinetic energy. The passive agents prefer to remain stationary, but the active agents are subject to several other types of forces: noise, 'flocking', and 'speed'. In this exercise, we shall explore only the active agents (setting 'Fraction Red' to one).

We shall see in later parts that flocking and speed lead to systems that remain out of thermal equilibrium. For the first three parts we shall explore whether noise and damping instead favor equilibration.

Return the simulation to its Moshpit defaults by reloading the page. Turn all the agents active (Fraction Red to 1), and reduce their number N to 100 (set Particle count and click Change). Set flocking and speed parameters to zero, the damping to 0.05 and the noise to 0.2 (discussed below), and Change. Verify that the the particles are moving in noisy paths between collisions. Adjust the number of frames skipped to speed up the visualization.

The noise and damping implement Langevin dynamics, used for finite-temperature simulations of traditional equilibrium systems. Noise adds an uncorrelated stochastic force  $\eta(t)$  at  $t_n = n\Delta t$  with  $\langle \eta_{\alpha}(t_i)\eta_{\beta}(t_j)\rangle = \sigma^2 \delta_{ij}\delta_{\alpha\beta}$ . This noise might represent the agitation of our agents, who randomly thrash around – or it could represent equilibrium buffeting of red pollen grains by surrounding water molecules. In Exercise 10.7, we

<sup>&</sup>lt;sup>2</sup>This exercise was developed in collaboration with David Hathcock. It makes use of the mosh pit simulator [2] developed by Matt Bierbaum in [9].

<sup>&</sup>lt;sup>3</sup>The current version of the software sometimes stops responding to the user interface. It seems to be more reliable on computers than on phones and tablets; reducing the number of agents may help.

argued that this dynamics could lead to a thermal distribution for the momentum of one particle.

In the first part, we shall check whether our system exhibits a speed distribution compatible with equilibrium statistical mechanics. Return to the settings above (reload, all active, N=100, flocking=speed=0, damping=0.05, noise=0.2, and Change). Show the graph of the speed histogram for the particles.<sup>4</sup>

(a) Examine the shape of the distribution of speeds  $\rho(s)$  for the particles. Derive what the probability distributions of speeds should take for an equilibrium thermal ensemble, and show your work. Does your prediction roughly agree with the speed histogram shown? What qualitative features of the observed distribution does your prediction explain that a Gaussian distribution or the traditional Maxwellian distribution (eqn 1.2) cannot?

Langevin dynamics uses the balance between damping and noise to maintain a constant temperature. Exercise 6.18 derives the well known relation  $k_B T = \sigma^2/(2\mu\Delta t)$  (which in turn is related to the fluctuation-dissipation theorem, see Exercise 10.7). But perhaps our definitions of  $\sigma$  and  $\mu$  differ from the adjustable parameters 'Noise strength', 'Damping' used in the simulation (which may differ from the  $\sigma$  and  $\mu$  in the paper).

In the guise of an experimentalists probing the effects of different controls, we shall in the next part check our formula by observing how the speed distribution changes as we change parameters. Return to the settings above.

(b) How much should the speeds increase if we quadruple  $\sigma$ ? How much should they change if we quadruple  $\mu$ ? Double  $\Delta t$ ? Make a table of the measurements you take to check whether these three variables correspond directly to the three experimental controls. (Measuring the peak of a distribution is noisy; try time-averaging the point where the distribution crosses half of the peak value. I used a ruler placed against the screen. Pick values of the parameters allowing for good measurements. If you are really ambitious, you can examine the source Javascript code on github.)

In the third part, we shall explore what happens to the speed distribution when the interactions between particles becomes strong.

Return to the settings above.

(c) Alter the number of particles to 350, where the density is typical of a liquid. Does the final distribution of speeds change from that at lower density? Alter it to 500. Does the distribution change in the crystal formed at this density? Is this a surprise? Explain.

Let us now depart from equilibrium physics, and begin exploring active matter.

Boids may have started the field of active matter. A model for the flocking of birds, boids obey slightly complicated rules to avoid collisions, form groups, and aligning their velocities with their neighbors.

(d) *Find a boids simulation on the Web.* (Currently, the most portable ones are written in javascript, as is the mosh-pit simulator.) *Compare the behavior to a video of starling* 

<sup>&</sup>lt;sup>4</sup>In the current implementation, the speeds are shown on the lower right; the horizontal axis is not labeled, but stays fixed as parameters change. The vertical axis is set by the peak of the distribution.

murmuration. Describe one feature the boids capture well, and one that the boids fail to mimic properly.

Later research on active matter focused on velocity alignment. Toner et al. [11] discuss the behavior of wildebeests (also known as gnu), who graze as individuals for months, but will at some point in the season start stirring around, pick a direction, and migrate as a group – ending some two thousand miles away. How do the wildebeests reach consensus on what direction to go? (Assume a cloudy day on a featureless Serengeti plain. Assume also that they just want to find more water, or better grazing, and do not need to find the Masai Mara where they spend the dry season.)

The mosh pit simulator aligns velocities by pulling each agent toward the average heading of its neighbors,

$$F_i^{\text{flock}} = \alpha \left. \sum_{j=1}^{N_i} \mathbf{v}_j \right/ \left| \sum_{j=1}^{N_i} \mathbf{v}_j \right|, \tag{5}$$

where the sum runs over the  $N_i$  agents within four radii of agent *i* and the flocking strength  $\alpha$  controls the acceleration along the average velocity direction.

Reload, all active, N=40, flocking=speed=0, damping=0.2 and noise=0.2, and Change. Let it equilibrate: the agents should mostly jiggle around without collisions, mimicking wildebeests grazing. Add a flocking force of strength 0.2, and watch the collective behavior of the system. You may increase or decrease the box size and the number of particles (keeping the density fixed), depending on whether your computer is powerful or struggling; if so, report the number and size you used.

(e) Describe the dynamics. Does the flock end up going largely in a single direction? If so, is the direction of motion the same for different simulation runs? Describe the speed distribution. Does the distribution appear to match the equilibrium distribution in part (a)? Observe the bump in the speed distribution at low speeds. Identify the slow particles in the animation. How do the slow particles forming this bump differ from the rest? Increase the noise strength. Estimate the noise level at which the particles stop moving collectively. (Note: If you wait long enough, the flocking direction will shift because of finite-size fluctuations.)

The flocking simulations spontaneously break rotation invariance (see Chapter 9). This is a surprising result, for technical reasons. Toner [11] illustrates this in a contest. He asks whether physicists standing at random on a featureless, cloudy Serengeti plain could all agree to point in the same direction. In analogy with eqn 5, one might imagine each physicist points along the average angle given by its  $N_i$  near neighbors plus a small, uncorrelated angular error  $\xi$ , with  $\langle \xi_j \xi_k \rangle = \epsilon \delta_{ij}$ :

$$\theta_i = (1/N_i) \sum_{j=1}^{N_i} \theta_j + \xi_i \tag{6}$$

We shall model the error as a finite-temperature deviation from a minimum energy state with Hamiltonian given by a spring connecting  $\theta_i$  to each of its neighbors. Let us calculate the behavior of this model for a one-dimensional lattice of physicists:

$$\mathcal{H} = \sum_{i} \frac{1}{2} K(\theta_i - \theta_{i-1})^2.$$

$$\tag{7}$$

(This is a version of the one-dimensional XY model ignoring phase slip.)

(f) Calculate the forces on  $\theta_j$  in eqn 7. Show that the energy is a minimum when  $\theta_j$  points along the average angle of its two near neighbors. Change variables to  $\delta_j = \theta_j - \theta_{j-1}$ , and calculate the thermal average  $\langle \delta_i^2 \rangle$  at a temperature T.

(g) At what temperature will the root mean square error  $\sqrt{\langle \delta^2 \rangle}$  between neighboring physicists be one degree? At that temperature, how large must n be before the root mean square error  $\sqrt{\langle (\theta_n - \theta_0)^2 \rangle}$  is 180°? (Assume K is in units of energy per radian squared.)

What makes wildebeests surprising is that this result also holds in two dimensions. No matter how small the noise  $\xi$ , physicists standing randomly on a plane cannot break rotational symmetry by cooperating with their neighbors! This was proven by Hohenberg [4] and Mermin and Wagner [5] (see note 12 on p. 252). Toner et al. [10] show that this result does not apply to active matter systems, by developing a systematic continuum hydrodynamic theory of flocking. What gives the wildebeests an advantage? The physicists always observe the same neighbors. The active agents (wildebeests) that are not going with the flow of their neighbors keep bumping into new agents – collecting better information about the error in their way.

Finally, let us consider an even more basic class of active matter; particles that are self-propelled but only interact via collisions. We use a propulsion term

$$F_i^{\text{speed}} = \mu (v_0 - v_i) \hat{v}_i, \tag{8}$$

which accelerates or decelerates each particle toward a target speed  $v_0$  without changing the direction. The damping constant  $\mu$  now controls how strongly the target speed is favored; for  $v_0 = 0$  we recover the equilibrium damping.

Such forces plus noise can be a rough model for bacteria propelling themselves in search of food (Exercise 2.19), or for artificially-created 'Janus' particles that have one side covered with a platinum catalyst that burns hydrogen peroxide, pushing it forward.

Reload parameters to default, then all active, N=200, flocking=0, speed  $v_0=0.25$ , damping=0.5 and noise=0, and Change. After some time, you should see most of the particles moving along a common direction. (Increase Frameskip to speed the process.) Again, you can increase the box size and number maintaining the density, but here decreasing the box size below 30 will interfere with the behavior.

(h) Watch the speed distribution as you restart the simulation, turning off skipping frames to see the behavior at early times. Does it get sharply peaked at the same time as

the particles begin moving collectively? Now turn up frameskip to look at the long-term motion. Give a qualitative explanation of what happens. Is more happening than just selection of a common direction? (Hint: Understanding why the collective behavior maintains itself is easier than explaining why it arises in the first place.)

We can study this emergent, collective flow by putting our system in a box – turning off the periodic boundary conditions along x and y. Reload parameters to default, then all active, N=300, flocking=0, speed  $v_0=0.25$ , raise the damping up to 2 and set noise=0. Turn off the periodic boundary conditions along both x and y, set the frame skip to 20, and Change. Again, box sizes as low as 30 will likely work.

After some time, you should observe a collective flow of a different sort. You can monitor the average flow using the angular momentum (middle graph below the simulation).

(i) Increase the noise strength. Can you disrupt this collective behavior? Very roughly, a what noise strength does the transition occur? (You can use the angular momentum as a diagnostic.)

A key question in equilibrium statistical mechanics is whether a qualitative transition like this is continuous (Chapter 12) or discontinuous (Chapter 11). Discontinuous transitions usually exhibit both bistability and hysteresis: the observed transition raising the temperature or other control parameter is higher than when one lowers the parameter. Here, if the transition is abrupt, we should have a region with three states – a melted state of zero angular momentum, and a collective clockwise and counterclockwise state.

Return to the settings for part (i), to explore more carefully the behavior near the transition.

(j) Use the angular momentum to measure the strength of the collective motion (taken from the center graph, treating the upper and lower bounds as  $\pm 1$ ). Graph it against noise as you raise the noise slowly and carefully from zero, until it vanishes. (You may need to wait longer when you get close to the transition.) Graph it again as you lower the noise. Do you find the same transition point on heating and cooling (raising and lowering the noise)? Is the transition abrupt, or continuous? Did you ever observe switches between the clockwise and anti-clockwise states? Graduate (6562 only)

#### 3. Quantum measurement and entropy. (Quantum) ③

Here we explore deep analogies between the collapse of the wavefunction during a quantum measurement and the increase of entropy in statistical mechanics.

Entropy is an emergent property in statistical mechanics. There is no place in the microscopic laws where entropy increases (Exercises 5.7 and 7.4). For large numbers of particles, chaos and ergodicity leads to a loss of information that emerges as equilibration and entropy growth (Exercises 5.8 and 5.25).

In quantum mechanics, the process of measurement is also an emergent property. Schrödinger's time evolution has no place where the wavefunction collapses. When a quantum subsystem interacts with a macroscopic object<sup>5</sup> enough to change its state, the quantum system will subsequently behave according to the Born rule. The Born rule describes the interaction as the application of an operator **O**; if the initial quantum state  $\phi$  is decomposed into eigenstates  $\phi = \sum c_o \xi_o$  of **O** then with probability  $|c_o|^2$  the quantum subsystem will behave as if it were in state  $\xi_o$  all along ('collapsing' into that state).

It is natural to describe this measurement without picking one of the observations, treating the quantum subsystem after the interaction as a mixed state. Suppose we begin with a photon in a diagonally polarized state  $\phi_i = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ , and apply an operator  $\mathbf{O} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ . that measures whether the polarization is vertical  $|\phi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  or horizontal  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

(a) What is the density matrix  $\rho_i$  for the photon before the measurement? What is the density matrix  $\rho_f$  after the measurement, according to the Born rule? How much has the entropy changed? (If you write the bra  $\langle \phi_i | as (1/\sqrt{2} 1/\sqrt{2})$  then  $\rho$  naturally forms as a 2 × 2 matrix.)

The Born rule asserts that the measurement process alters the density matrix, changing it from a pure state to a mixed, unpolarized state. It is unsatisfying in two ways. First, it does not keep track of the effect of the quantum state on the measuring device: there is no record of the measurement. Second, it provides no intuition as to why quantum evolution should produce a collapse of this form.

Let us consider including the object's many-body wavefunction  $\Psi(\mathbf{x})$  into the analysis.<sup>6</sup> Before the measurement, the photon is not interacting with the object, so the system (photon plus object) is in a product state

$$\Phi_{i} = \phi_{i} \Psi_{i}(\mathbf{x}) = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \Psi_{i}(\mathbf{x}).$$
(9)

<sup>&</sup>lt;sup>5</sup>This object could be a material which exchanges energy with the quantum subsystem, as for a solid whose phonons cause a qubit to suffer decoherence. It could be a measuring instrument, recording a value stored in the qubit. Or it could be Geiger counter, rigged to a jar of poison gas in a box with a cat.

<sup>&</sup>lt;sup>6</sup>We make the unrealistic assumption that the object starts in a pure state for simplicity: the same argument works for a thermal state, or indeed any macroscopic density matrix for the object.

We then perform a measurement – turning on a time-dependent Hamiltonian coupling the photon to the object, turning it off again, and waiting until the object as a whole received the information. After the measurement, the object is left in one of two distinct many-body wavefunctions,  $\Psi_{\rm v}(\mathbf{x})$  or  $\Psi_{\rm h}(\mathbf{x})$ , depending on whether the photon was measured to be vertically or horizontally polarized. The photon's state is unchanged (we assume the object performed a 'quantum non-demolition' measurement, [12, Section 3.7]). Thus the system after the measurement is in the state

$$\Phi_{\rm f} = \begin{pmatrix} 1/\sqrt{2} \\ 0 \end{pmatrix} \Psi_{\rm v}(\mathbf{x}) + \begin{pmatrix} 0 \\ 1/\sqrt{2} \end{pmatrix} \Psi_{\rm h}(\mathbf{x})$$
(10)

(b) Write the density matrix for the system, both before and after the measurement, as  $a \ 2 \times 2$  matrix of functions. (That is, we use a position-space basis for the object. For example, the density matrix for the *object* before the measurement is  $\rho = |\Psi_i\rangle\langle\Psi_i|$ , which in position space is  $\rho(\mathbf{x}', \mathbf{x}) = \langle \mathbf{x}' | \Psi_i \rangle \langle \Psi_i | \mathbf{x} \rangle = \Psi_i(\mathbf{x}') \Psi_i^*(\mathbf{x})$ . Hint: Both matrices should have off-diagonal terms.)

Since our system obeys Schrödinger's equation, it ought to be still in a pure state. Remember that, in position space, the trace of an operator M(x', x) is given by integrating over the diagonal  $\text{Tr}(M) = \int M(x, x) dx$ , and the square of the density matrix is  $\rho^2(x', x) = \int \rho(x', x'') \rho(x'', x) dx''$ .

(c) Show that your initial density matrix is in a pure state by computing  $Tr(\rho_i^2)$ . Show that your final density matrix  $\rho_f$  is also in a pure state by computing the trace of its square.

(d) What is the entropy change after the measurement, including both the photon and the object? (Hint: You need not calculate anything, given your results of part (c).)

Our calculation so far has followed the microscopic rules – evolving the wavefunctions of the photon and the object via Schrödinger's equation. We now must make the same kind of macroscopic approximations we use in explaining the increase of entropy. The information about the 'coherence' between the two polarizations stored in the object becomes unusable if the object is large and its response to the interaction is complex.

Specifically, the time-dependent Hamiltonian, in making the measurement, has left an indelible imprint on the object. The vector  $\mathbf{x}$  represents the configuration of gigantic numbers of atoms, each of which has shifted in a way that depends upon whether the photon was horizontally or vertically polarized. By the definition of a good measuring apparatus, if the final positions of the atoms  $\mathbf{x}$  has non-zero probability density of arising for a vertical polarization (i.e.,  $|\Psi_{v}(\mathbf{x})|^{2} > 0$ ), then it must have no probability of arising for a horizontal polarization (so  $|\Psi_{h}(\mathbf{x})|^{2}$  must be zero). Otherwise, those shared configurations represent the likelihood us that the object has forgotten which state it measured – that every trace of memory is removed on the atomic level.

It is more drastic even than this. One cannot act on  $\Psi_v$  to make it overlap with  $\Psi_h$  with any sensible, local operator. (Think of the object as including an observer writing down the measurement. What quantum operator<sup>7</sup> could erase that information?) Indeed, for any operator  $\mathbf{B}$  acting on the object,

$$\langle \Psi_{\mathbf{v}} | \mathbf{B} | \Psi_{\mathbf{h}} \rangle = \int d\mathbf{x}' d\mathbf{x} \langle \Psi_{\mathbf{v}} | \mathbf{x}' \rangle \langle \mathbf{x}' | B | \mathbf{x} \rangle \langle \mathbf{x} | \Psi_{\mathbf{h}} \rangle$$

$$= \int \Psi_{\mathbf{v}}^{*}(\mathbf{x}') B(\mathbf{x}', \mathbf{x}) \Psi_{\mathbf{h}}(\mathbf{x}) d\mathbf{x}' d\mathbf{x} \equiv 0.$$

$$(11)$$

The two wavefunctions are not just orthogonal. They are not just with zero overlap. It is sometimes said that the two wavefunctions *live in different Hilbert spaces.*<sup>8</sup>

How does this allow us to simplify the final density matrix you derived in part (c)? Suppose we subject our photon and our object to a second observation operator  $\mathbf{Q}$ , which we represent in complete generality as a 2 × 2 matrix of operators in the polarization space

$$\mathbf{Q} = \begin{pmatrix} A(\mathbf{x}', \mathbf{x}) & B(\mathbf{x}', \mathbf{x}) \\ B^*(\mathbf{x}', \mathbf{x}) & C(\mathbf{x}', \mathbf{x}) \end{pmatrix}.$$
 (12)

We know from eqn 7.5 that  $\langle \mathbf{Q} \rangle = \text{Tr}(\mathbf{Q}\rho)$ .

We now demonstrate that the pure-state density matrix  $\rho_{\rm f}$ , if the object is a good measuring instrument, is equivalent to a mixed state  $\hat{\rho}_{\rm f}$ .

(e) Using eqn 11 and your final density matrix from part (b), show that  $\langle \mathbf{Q} \rangle$  is equal to  $\text{Tr}(\mathbf{Q}\hat{\rho}_{f})$ , where

$$\widehat{\boldsymbol{\rho}}_{f} = \begin{pmatrix} \frac{1}{2} \Psi_{v}(\mathbf{x}') \Psi_{v}^{*}(\mathbf{x}) & 0\\ 0 & \frac{1}{2} \Psi_{h}(\mathbf{x}') \Psi_{h}^{*}(\mathbf{x}) \end{pmatrix}.$$
(13)

What terms changed between  $\rho_{\rm f}$  from part (c) and  $\hat{\rho}_{\rm f}$ ? How do these changes represent the loss of coherence between the two polarizations, stored in the object? Explain in words how  $\hat{\rho}_{\rm f}$  represents a photon and an object which has recorded the polarization.

(f) How much has the entropy changed after the measurement, using the emergent density matrix  $\hat{\rho}_{\rm f}$  eqn 13 that reflects the loss of coherence? (Warning: The entropy of a state described by a wavefunction  $\psi(x)$  is zero (since it is a pure state). The entropy is not  $-k_B \int |\psi(x)|^2 \log |\psi(x)|^2$ . That would be the entropy of the ensemble of states generated after the position of the particle was observed. Hint:  $\Psi_{\rm v}$  and  $\Psi_{\rm h}$  are pure states describing the object.)

We can now connect our discussion to the Born rule, by considering an effective theory for the photon valid for any observable not also involving the object. This allows us to 'integrate out' the object's degrees of freedom to get an effective 'reduced' density

<sup>&</sup>lt;sup>7</sup>The operator  $\mathbf{U}(-t)$  that evolves the photon and the object backward in time would get them to overlap perfectly, erasing all memory. Of course, reversing time would also allow entropy to decrease. Such operators are declared not sensible.

<sup>&</sup>lt;sup>8</sup>For the sophisticated, one could build an entire Fock space by applying (sensible, local) creation and annihilation operators to the two states; the resulting Hilbert spaces would never overlap, in the limit of an infinite-sized object.

matrix just for the photon, as we do in classical statistical mechanics to derive free energies (see note 5 on p. 141 and Section 6.7).

After the measurement, the object no longer interacts with the photon. Equation 12 still describes a general operator for our system. Operators which do not involve the object will be independent of  $\mathbf{x}$  and  $\mathbf{x}'$ , the coordinates describing the object's degrees of freedom.

(g) Show that our density matrix  $\hat{\boldsymbol{\rho}}_{f}$  reflecting decoherence is equivalent to the unpolarized density matrix  $\rho_{f}$  given by the Born rule, for any operator that does not involve the object. (Hint: Integrate out  $\mathbf{x}$  and  $\mathbf{x}'$  in the trace.)

Thus the collapse of the wavefunction emerges naturally from the complexity and size of macroscopic objects interacting with microscopic quantum subsystems. There remain deep questions about quantum measurement (see Weinberg [12, Section 3.7]), but the wavefunction 'collapse' is an emergent property of macroscopic observing systems, much like the entropy.

# References

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