Problem 1. Big numbers and the Shannon entropy

Here $N_A = 6.0 \times 10^{23}$

(a) Consider the approximation

$$e^S = 100000 \, e^{N_A} \simeq e^{N_A} . \tag{1}$$

What is the percent error in S made by this approximation?

(b) Consider the approximation

$$e^S \simeq e^{N_A} + e^{1.001 N_A} \simeq e^{1.001 N_A} . \tag{2}$$

What is the percent error in S made by this approximation? It may be helpful to recall the Taylor series of the logarithm discussed in previous homework.

(c) Suppose that I have a subsystem which can be in three states, $s = 1, 2, 3$, with probabilities $\mathscr{P}_s$. If I lay down N subsystems drawn from the probability distribution $\mathscr{P}_s$ (see Fig. 1 for examples), then for N large I will have approximately $N_1 \simeq N \mathscr{P}_1$ subsystems in state 1, $N_2 \simeq N \mathscr{P}_2$ subsystems in state two, and $N_3 \simeq N \mathscr{P}_3$ subsystems in state three.

The total number of configurations with specified N_1, N_2 and N_3 that can be generated during this process Ω is exponentially large. So, we study its logarithm $S \equiv \ln \Omega$. We showed in class and in prior homework that

$$S \equiv \ln \Omega = \ln \left(\frac{N!}{N_1! N_2! N_3!} \right) \simeq N S_1 \qquad S_1 \equiv \sum_s -\mathscr{P}_s \ln \mathscr{P}_s \tag{3}$$

where S_1 is known as the Shannon entropy. Thus Ω grows exponentially in the number of subsystems

$$\Omega \simeq e^{N S_1} \tag{4}$$

This formula generalizes straightforwardly to subsystems with more than three states.

(i) If my subsystem has three states that are equally likely, what is its Shannon entropy? How would this change if my subsystem had two states that are equally likely, or six states that are equally likely? Are your results consistent with the graph of the Shannon entropy two state system shown in Fig. 1?

(ii) Consider a two state subsystem $s = 1, 2$. If the probability of being in the $s = 1$ state is $1/4$ what is the Shannon entropy of two state system. Check your result by comparing to the graph of the Shannon entropy shown on the next page. With no more than a sentence or two, try to qualitatively explain why your result is smaller than the case of equal probability discussed in (i). Perhaps qualitatively comparing Fig. 1(a) and Fig. 1(b) will help.
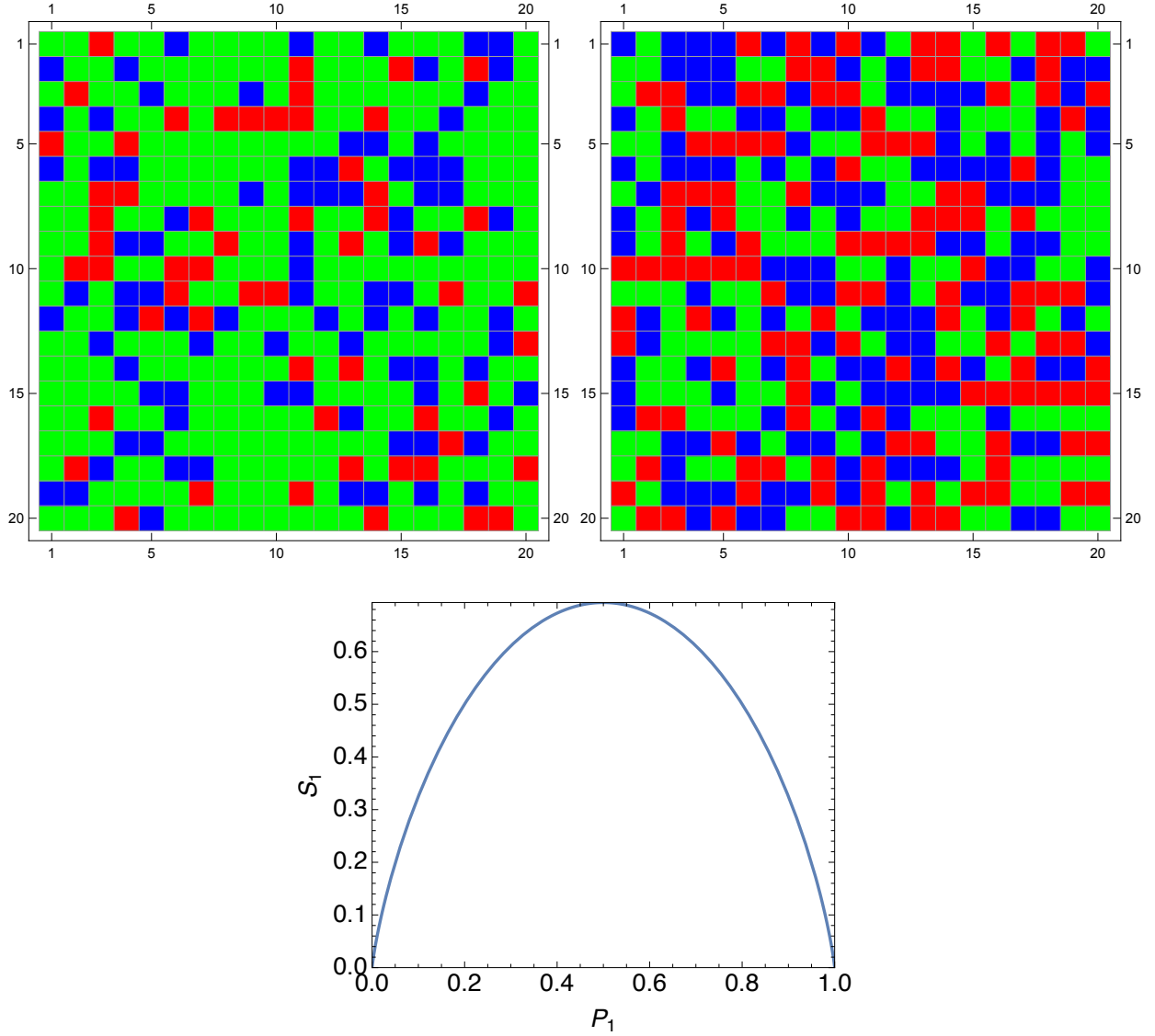
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Figure 1: (a) A configuration generated by laying down 400 subsystems, with probabilities $P_1 = \frac{1}{8}$ (red), $P_2 = \frac{2}{8}$ (blue) and $P_3 = \frac{5}{8}$ (green). $\ln \Omega$ is the number of ways you can shuffle around the red, blue, and green and get a new configuration. (b) A configuration generated by laying down 400 subsystems, with probabilities $P_1 = \frac{1}{3}$ (red), $P_2 = \frac{1}{3}$ (blue) and $P_3 = \frac{1}{3}$ (green). Compared to (a) are more ways to shuffle around the red, blue, and green squares and get a new configuration. (c) The Shannon entropy for a two state system as a function of P_1, with $P_2 = (1 - P_1)$.

(iii) Suppose that the subsystem actually describes two independent subsystems A and B, $\mathscr{P}_s \equiv \mathscr{P}_s^{AB}$. For instance, system A can be in states $a = 1, 2$ with probability $\mathscr{P}_a^A$, and system B can be in states $b = 1, 2, 3$ with probability $\mathscr{P}_b^B$. The probability to be in a state labelled by a and b is

$$\mathscr{P}_{(a,b)}^{AB} = \mathscr{P}_a^A \mathscr{P}_b^B \tag{5}$$

where the six possible states formerly labelled "s" are now labelled by the pair (a, b)

$$(a, b) \in \{(a{=}1, b{=}1); (a{=}1, b{=}2), (a{=}1, b{=}3), (a{=}2, b{=}1), (a{=}2, b{=}2), (a{=}2, b{=}3)\} \tag{6}$$

Show that entropy of the total subsystem is the sum of the entropies of A and B

$$S_1^{AB} = S_1^A + S_1^B \tag{7}$$

where
$$S_1^A = \sum_a -\mathscr{P}_a^A \ln \mathscr{P}_a^A \qquad \text{and} \qquad S_1^B = \sum_b -\mathscr{P}_b^B \ln \mathscr{P}_b^B \tag{8}$$

Problem 2.   Counting

Consider 400 atoms laid out in a row. Each atom can be in one of two states a ground state with energy 0 and an excited state with energy Δ. Assume that 100 of the atoms are excited, so the total energy is $U = 100\,\Delta$.

(a) Show that there are e^{225} configurations, called microstates, for this energy U. One microstate is shown below.

(b) Suppose that we make a partition of the energy so that the first 200 atoms have an energy of $80\,\Delta$, and the next 200 atoms have an energy of $20\,\Delta$ (see below). The terminology here is that we have specified the "macrostate" (i.e. the 80/20 split), leaving the microstates (exactly which atoms are up are down) to be further specified. How many microstates are there with this macrostate? One microstate for this 80/20 split macrostate is shown below[1]
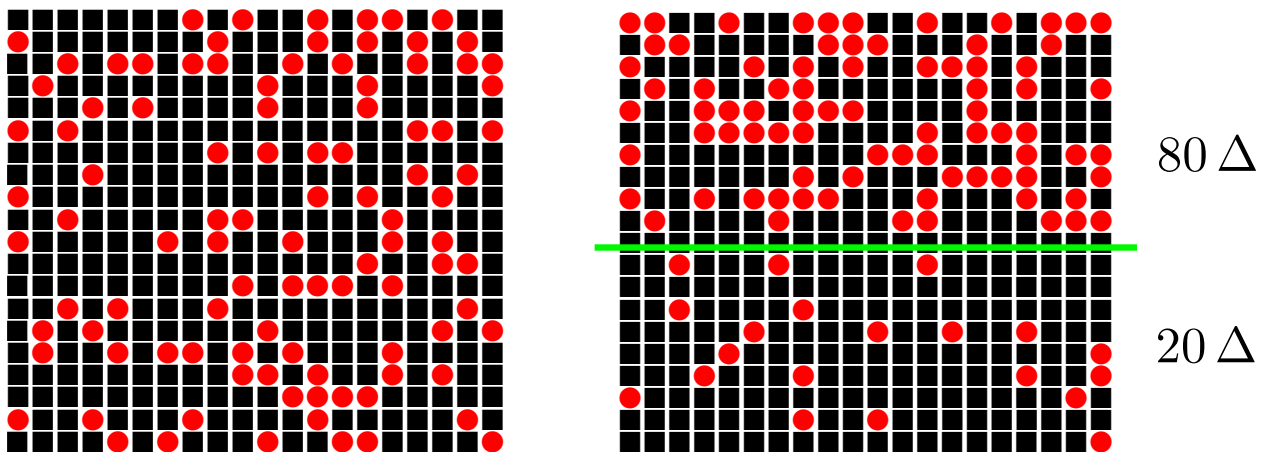
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[1]Answer: e^{200}.

Figure 2: (a) A microstate where the energy is not partitioned. (b) a microstate where the energy is partitioned – 80% on the top and 20% on the bottom.

Problem 3. The Gamma function

The $\Gamma(x)$ function can be defined as[2]

$$\Gamma(x) \equiv \int_0^\infty \mathrm{d}u\, e^{-u} u^{x-1} = \int_0^\infty \frac{\mathrm{d}u}{u}\, e^{-u} u^x \qquad (9)$$

A plot of $\Gamma(x)$ is shown below. $\Gamma(n)$ provides a unique generalization of $(n-1)!$ when n is not an integer and even negative or complex. It will come up a number of times in this course and is good to know.
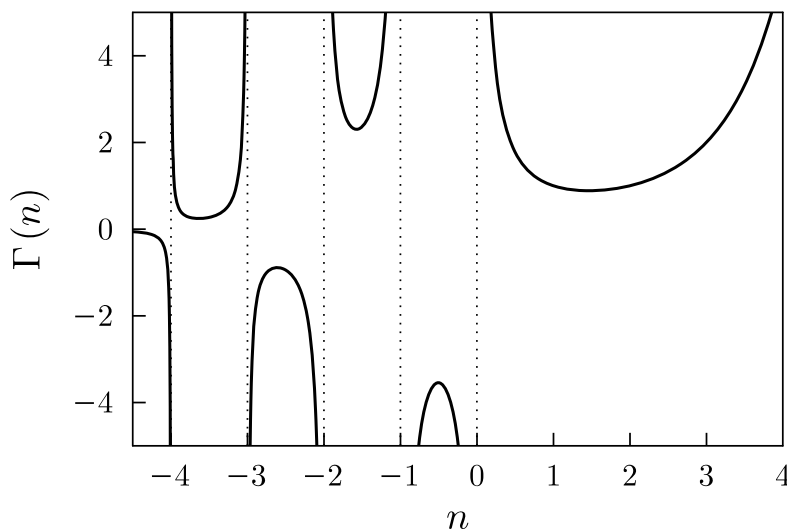

Fig. C.1 The gamma function $\Gamma(n)$ showing the singularities for integer values of $n \leq 0$. For positive, integer n, $\Gamma(n) = (n-1)!$.

Figure 3: Appendix C.2 of our book

(a) Explain briefly why $\Gamma(n) = (n-1)!$ for n integer.

(b) Prove that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. *Hint:* try a substitution $y = \sqrt{u}$.

The following identity is needed below.

$$\Gamma(x+1) = x\Gamma(x), \qquad (10)$$

or

$$x! = x \cdot (x-1)!, \qquad (11)$$

but now x is a real number, and $x!$ is defined by $\Gamma(x+1)$.

(c) (Optional. Dont turn in) Use integration by parts to prove the identity in Eq. (10).

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[2]I like to write $\Gamma(x) = \int_0^\infty \frac{\mathrm{d}u}{u}\, e^{-u} u^x$, which makes the x is more explicit. Also the measure du/u is invariant under a homogeneous rescaling, e.g. under change of variables $u \to u' = \lambda u$ we have $du'/u' = du/u$.

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(d) Use the results of this problem to show that $\Gamma(\frac{7}{2}) = 15\sqrt{\pi}/8$. What is the result numerically? $7/2$ is between two integers. Show that $\Gamma(7/2)$ is between the appropriate factorials related to those two integers?

(e) The "area" (i.e. circumference) of a "sphere" in two dimensions (i.e. the circle) is $2\pi r$. The area of a sphere in three dimensions is $4\pi r^2$. A general formula for the area of the sphere in d dimensions is derived in the book is (the proof is simple, using what we know)

$$A_d(r) = \frac{2\pi^{d/2}}{(\frac{d}{2} - 1)!} r^{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \tag{12}$$

Show that this formula gives the familiar result for $d = 2$ and $d = 3$.

Problem 4.   Two State System

Consider an array of N atoms forming a medium, with each atom possessing two energy states: a ground state with energy 0 and an excited state with energy Δ.

(a) Determine the temperature at which the number of excited atoms reaches $N/4$.

(b) Calculate both the mean energy $\langle \epsilon \rangle$ and the variance of energy $\langle (\delta \epsilon)^2 \rangle$ for an individual atom. Your results should take the following form:

$$\langle (\delta \epsilon)^2 \rangle = \frac{\Delta^2 e^{-\beta \Delta}}{(1 + e^{-\beta \Delta})^2}$$

Additionally, create a graph depicting $\frac{\langle (\delta \epsilon)^2 \rangle}{T^2}$ as a function of $\frac{\Delta}{T}$.

(c) Suppose you have a collection of 16 such atoms (shown below). Calculate the average values of $\langle E \rangle$, $\langle (\delta E)^2 \rangle$ and $\langle E^2 \rangle$, where E represents the total energy of all 16 atoms. What approximately is the probability distribution for the energy E?
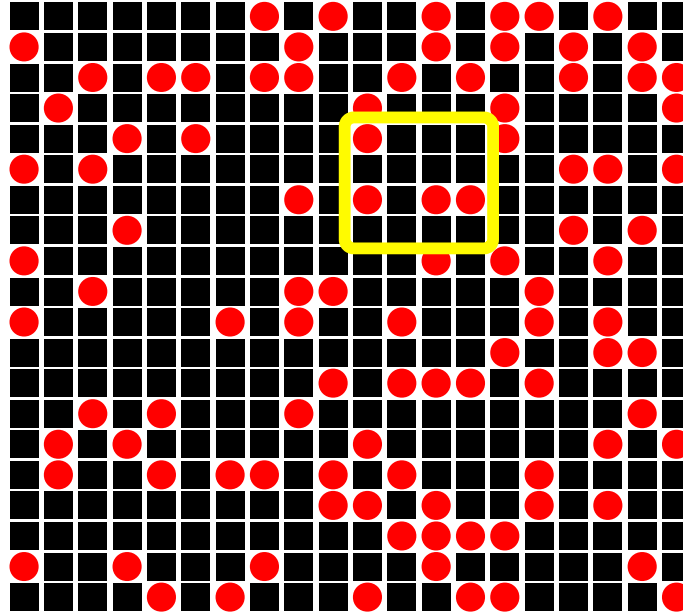
Problem 5. Classical distribution of two potentials

Consider a classical harmonic oscillator in one dimension interacting with a thermal environment. This could be for example a single atom attached to a large molecule in a gas.

The potential energy is $U = \frac{1}{2}kx^2$. At some point in physics we stop using the spring constant k (for some unknown reason) and start expressing k in terms of the oscillation frequency $\omega_0 = \sqrt{k/m}$. Thus, I will (usually) write the potential as

$$U = \frac{1}{2}m\omega_0^2 x^2 \tag{13}$$

The energy is the kinetic and potential energies and the Hamiltonian[3] is

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 \tag{14}$$

The oscillator is in equilibrium with an environment at temperature T.

(a) What is the normalized probability density $P(x,p)$ to find the harmonic oscillator with position between x and $x+dx$ and momentum between p and $p+dp$, i.e. the probability per phase space volume $dx\,dp$:

$$d\mathscr{P}_{x,p} = P(x,p)\,dx\,dp \tag{15}$$

Your final result for $P(x,p)$ should be a function of ω_0, p, x, m and kT. You can check your result by doing part (b). Check that your result for $P(x,p)$ is dimensionally correct.

What is the probability of finding position between x and $x + dx$ without regards to momentum

$$d\mathscr{P}_x = P(x)\,dx \tag{16}$$

Hint: Change variables to $u_1 = x/\sigma_x$ and $u_2 = p/\sigma_p$ before doing any integrals. You need to look at the integrand (like the exponent) and decide what the appropriate length scale, σ_x, and momentum scale, σ_p, are.

(b) Compute the $\langle x^2 \rangle$ and $\langle p^2 \rangle$ by integrating over the probability distribution. (Don't do dimensionful integrals.)

You should find $\langle x^2 \rangle = kT/m\omega_0^2$ and $\langle p^2 \rangle = mkT$.

(c) The equipartition theorem precisely says that, for a classical system, the average of each quadratic form in the Hamiltonian is $\frac{1}{2}kT$. The quadratic forms here are the kinetic energy $p^2/2m$, and the potential energy, $m\omega_0^2 x^2/2$. Are your results of the part (b) consistent with the equipartition theorem. What is the average total energy of the oscillator and the number of "degrees of freedom" of the oscillator?

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[3]The Hamiltonian is the energy *as a function of* x and p.

(d) Now consider a classical particle of mass m in a potential of the form

$$V(x) = \alpha|x| \tag{17}$$

at temperature T.

Write down the Hamiltonian and determine the normalized probability density $P(x, p)$. You can check your result by doing the next part.

What is the probability of finding position between x and $x + dx$ without regards to momentum

$$d\mathscr{P} = P(x)\,dx \tag{18}$$

Sketch the $P(x)$ from part (a) and the $P(x)$ from (d).

(e) Determine the mean potential energy and mean kinetic energy of the particle in the potential by integrating over the coordinates and momenta. Does the equipartition theorem apply here? Explain.

You should find that the average potential energy and average kinetic energy are kT and $\frac{1}{2}kT$ respectively.