

Problem 1. Counting

(Optional, But Please Read!) 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 $U = 100 \Delta$.

- Show that there are e^{255} configurations, called microstates, for this energy U . One microstate is shown below.
- Suppose that we make a partition of the energy so that the first 200 atoms have an energy of 80Δ , and the next 200 atoms have an energy of 20Δ (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.

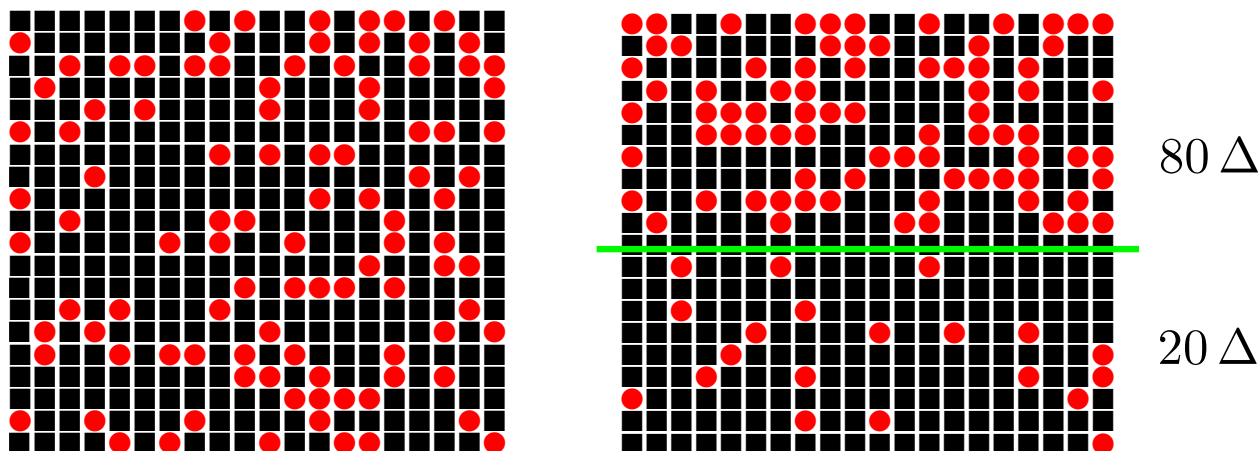


Figure 1: (a) A microstate where the energy is not partitioned. (b) a microstate where the energy is partitioned – 80% on the top and 20% on the bottom.

Problem 2. The Gamma function

The $\Gamma(x)$ function can be defined as¹

$$\Gamma(x) = \int_0^\infty du e^{-u} u^{x-1} \quad (1)$$

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

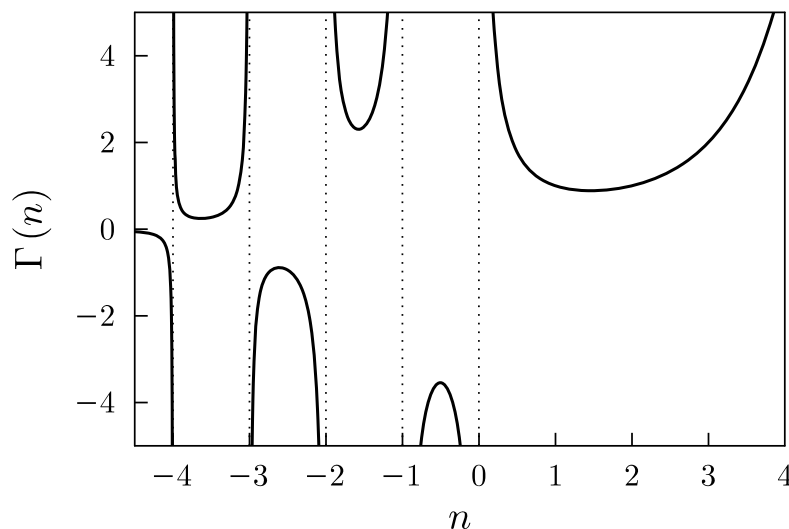


Fig. C.1 The gamma function $\Gamma(n)$ showing the singularities for integer values of $n \leq 0$. For positive, integer n , $\Gamma(n) = (n-1)!$.

Figure 2: 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.

$$\Gamma(x+1) = x\Gamma(x), \quad (2)$$

or

$$x! = x \cdot (x-1)!, \quad (3)$$

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. (2).

¹I like to write $\Gamma(x) = \int_0^\infty \frac{du}{u} e^{-u} u^x$, which makes the x is more explicit. Also the measure du/u is invariant under a homogeneous rescaling, e.g. under change of variables $u \rightarrow u' = \lambda u$ we have $du'/u' = du/u$.

- (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)

$$A_d(r) = \frac{2\pi^{d/2}}{(\frac{d}{2} - 1)!} r^{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \quad (4)$$

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

Problem 3. Two State System

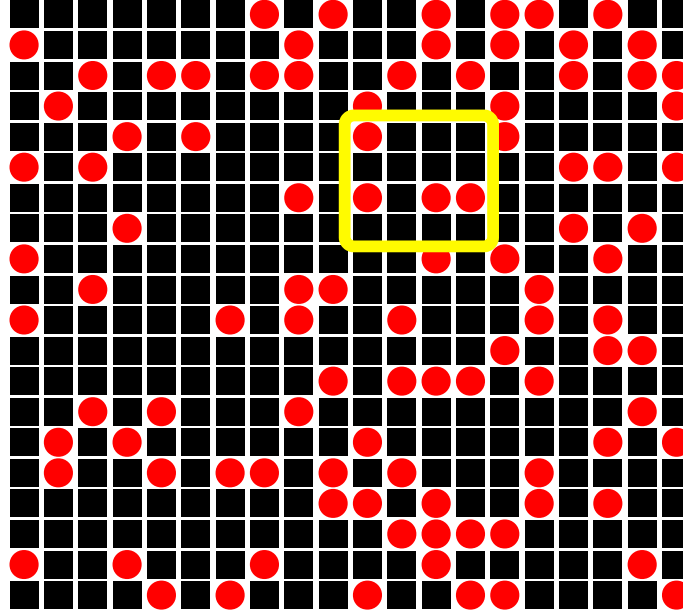
Consider an array of N atoms forming a medium, with each atom possessing two energy states: a ground state with energy 0 and an excited state with energy Δ .

- (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 $\langle E \rangle$ and $\langle (\delta E)^2 \rangle$, where E represents the total energy of all 16 atoms. What approximately is the probability distribution for the energy E ?



Problem 4. 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

$$U = \frac{1}{2}m\omega_0^2x^2 \quad (5)$$

The energy is the kinetic and potential energies and the Hamiltonian² is

$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2x^2 \quad (6)$$

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 $dx dp$:

$$d\mathcal{P}_{x,p} = P(x, p) dx dp \quad (7)$$

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

$$d\mathcal{P}_x = P(x) dx \quad (8)$$

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, $m\omega_0^2x^2/2$. 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?

²The 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

$$V(x) = \alpha|x| \tag{9}$$

at temperature T .

Write down the Hamiltonian and determine the normalized probability density $P(x, p)$. What is the probability of finding position between x and $x + dx$ without regards to momentum

$$d\mathcal{P} = P(x) dx \tag{10}$$

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.

Problem 5. Distribution of energies

The speed distribution is

$$d\mathcal{P} = P(v) dv \quad (11)$$

where $P(v) = (m/2\pi kT)^{3/2} e^{-mv^2/2kT} 4\pi v^2$.

- (a) Show that the probability distribution of energies $\epsilon = \frac{1}{2}mv^2$ is

$$d\mathcal{P} = P(\epsilon) d\epsilon \quad (12)$$

where

$$P(\epsilon) = \frac{2}{\sqrt{\pi}} \beta^{3/2} e^{-\beta\epsilon} \epsilon^{1/2} \quad (13)$$

Note: that the distribution of energies is independent of the mass, and recall $\beta = 1/kT$.

- (b) Compute the variance in energy using $P(\epsilon)$. Express all integrals in terms $\Gamma(x)$ (as given in the previous homework) – it is helpful to change to a dimensionless energy $u = \beta\epsilon$. You should find (after evaluating these Γ functions as in the previous homework) that

$$\langle (\delta\epsilon)^2 \rangle = \frac{3}{2} (k_B T)^2 \quad (14)$$