Problem 1. Central Limit Theorem and Random Walk

In a random walk, a collegiate drunkard starts at the origin and takes a step of size a, to the right with probability p and to the left with probability $1-p$.

(a) Take $p = 1/2$, i.e. equal probability of right and left steps. Determine the probability of the drunkard having position X, i.e. $P(X)$, after three steps. Plot $P(X)$ where X can be one of $X/a = 0, \pm 1, \pm 2, \pm 3$. Note how your graph begins to approach a Gaussian after just three steps[1]

(b) Now keep p general. What is the mean and variance variance in the drunkard's position X after one step, and after two steps? You can check your reasoning by doing the next part.

(c) After n steps (with $n \gg 1$) find his mean position $\langle X \rangle$, and the std. deviation in his position $\sigma_X = \sqrt{\langle \delta X^2 \rangle}$. Check your result by comparing with the figure below

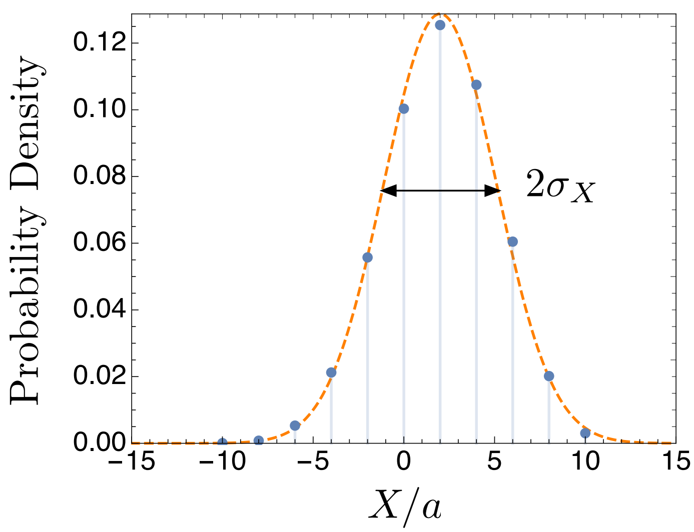


Figure 1: Probability of our drunkard having position X after $n = 10$ steps (the blue points). Of course after 10 steps the drunkard will be between $-10 \ldots 10$, and it is easy to show that he will be only at the even sites, i.e. $-10, -8, -6, \ldots 10$. For $p = 0.6$, I find $\langle X \rangle = 2.0$. Twice the std deviation, $2\sigma_X$, is shown in the figure and is about six in this case. The orange curve is a gaussian (a.k.a the "bell-shaped" curve) approximation discussed in class and approximately agrees with the points – this is the central limit theorem. Recall that the central limit theorm says that if the number of steps n is large, the probability of X (a sum of n independent events) is approximately $P(x)\,\mathrm{d}X \propto \exp(-(X - \langle X \rangle)^2/2\sigma_X^2)$. Evidently the gaussian approximation works well already for $n = 10$.

Hint: X is a sum N independent events x_i where $x_i = \pm a$. Use results from class on the probability distribution of a *sum* of independent events.

[1] The graph should be symmetric. You should find $P_0 = 0$, $P_{\pm 1} = \frac{3}{8}$, $P_{\pm 2} = 0$, $P_{\pm 3} = \frac{1}{8}$. Your graph should look something like the figure below but symmetric around the orgigin.

Random Walk

(a) $$\langle x \rangle = pa - (1-p)a$$

$$\langle x \rangle = a(2p-1)$$

$$\langle x^2 \rangle = pa^2 + (1-p)a^2 = a^2$$

So

$$\langle x^2 \rangle - \langle x \rangle^2 = a^2(1 - (2p-1)^2)$$

$$= a^2(1 - 4p^2 + 4p - 1)$$

$$\langle \delta x^2 \rangle = a^2 4p(1-p)$$

$$\sigma_x = a\sqrt{4p(1-p)}$$

(b) After n steps

$$\langle X \rangle = n\langle x \rangle = n(2p-1)a$$

$$\langle \delta X^2 \rangle = n\langle \delta x^2 \rangle = a^2 4p(1-p)n$$

(c) Then we have to require

$$X > 2\sigma_x$$

Or

$$n \underbrace{(2p-1)\,a} > 2\sqrt{4p(1-p)}\,\sqrt{n}\,a$$

- So

$$\sqrt{n} > \frac{4\sqrt{p(1-p)}}{2(p-1/2)}$$

$p \simeq 1/2$, so the numerator is approx: $4\sqrt{\frac{1}{2}\frac{1}{2}} \simeq 2$

$$\sqrt{n} \geqslant \frac{1}{p-1/2}$$

$$n \geqslant \frac{1}{(p-1/2)^2}$$

- So if $p = \frac{1}{2} + 0{,}0001$, we have

$$\boxed{n \geqslant 10^8}$$

Problem 2. 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

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

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 p_s. If I lay down N subsystems drawn from the probability distribution p_s (see Fig. 2 for two concrete examples), then for N large I will have approximately $N_1 \simeq N p_1$ subsystems in state 1, $N_2 \simeq N p_2$ subsystems in state two, and $N_3 \simeq N p_3$ 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 is Ω. We study its logarithm $S \equiv \ln \Omega$. We showed in class and in prior homework that

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

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) What is the Shannon entropy for the probability distribution leading to Fig. 2(b))? How would this change if my subsystem had two states that are equally likely, or six states that are equally likely?

(ii) Compute the Shannon entropy for the probability distribution leading to Fig. 2(a)[2]. By comparing Fig. 2(a) and Fig. 2(b) and with no more than a sentence or two, try to qualitatively explain why your result in (ii) is smaller than the case of equal probability discussed in (i).

[2] Answer: 0.9

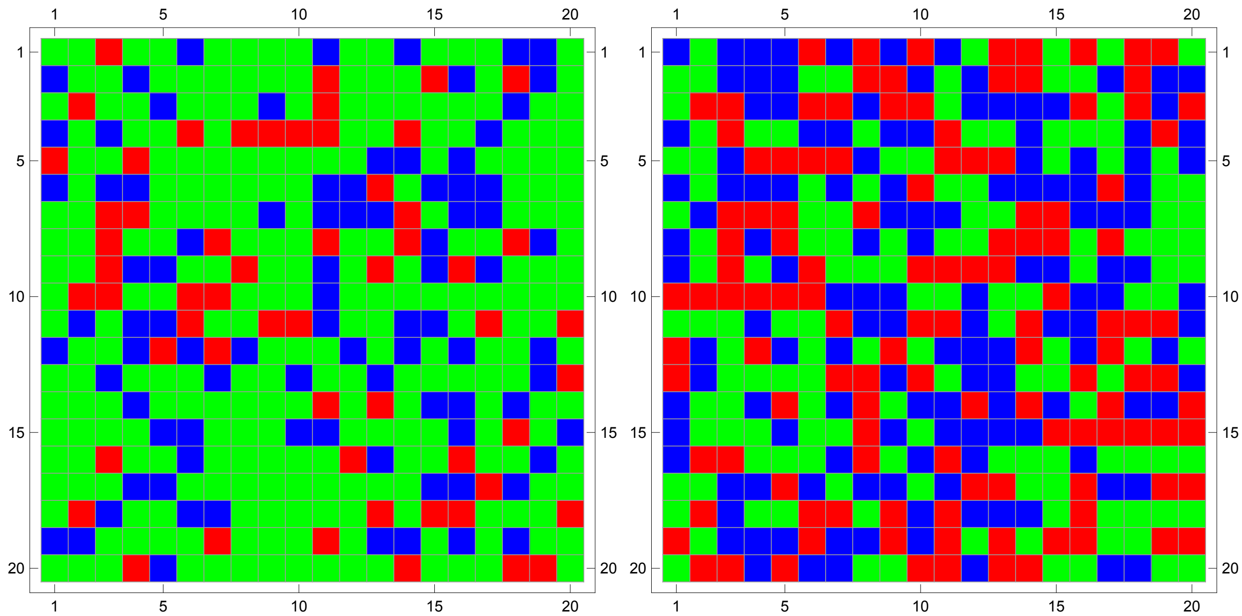


Figure 2: (a) A configuration generated by laying down 400 subsystems, with probabilities $p_1 = \frac{1}{8}$ (red), $p_2 = \frac{2}{8}$ (blue) and $p_3 = \frac{5}{8}$ (green). $\ln \Omega$ is the number of ways you can shuffle around the red, blue, and green and get a new configuration. (b) A configuration 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).

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

$$p_s^{AB} = p_a^A p_b^B \tag{5}$$

where the six possible states labeled by $s \equiv (a, b)$ are

$$s \equiv (a, b) \in \{(1,1), (1,2), (1,3), (2,1), (2,2), (2,3)\} \tag{6}$$

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

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

where

$$S_1^A = \sum_a -p_a^A \ln p_a^A \qquad \text{and} \qquad S_1^B = \sum_b -p_b^B \ln p_b^B \tag{8}$$

Solution

(a) We have

$$e^S = 100000\, e^{N_A} = e^{11.5} e^{N_A} = e^{11.5+N_A} \simeq e^{N_A}\,. \tag{9}$$

So we have

$$\%\ \text{error} = 100. \times \frac{11.5}{N_A} \simeq 1.9\times 10^{-21} \tag{10}$$

(b) We have

$$e^S = e^{N_A} + e^{1.001N_A} = e^{1.001N_A}(1+e^{-0.001N_A}) \tag{11}$$

So taking the log, noting that $\ln(1+x)\simeq x$

$$S = \ln\left[e^{1.001N_A}(1+e^{-0.001N_A})\right] = 1.001N_A + \ln(1+e^{-0.001N_A}) \simeq 1.001N_A + e^{-0.001N_A} \tag{12}$$

Thus the percent error is

$$\%\ \text{error} = 100\times\frac{e^{-0.001N_A}}{1.001N_A} \simeq e^{-0.001N_A - 50.} \simeq e^{-0.001N_A} = 10^{-2.6\times 10^{20}} \tag{13}$$

(c) (i) We have

$$S_1 = \sum_{i=1}^{3} -\frac{1}{3}\ln(\frac{1}{3}) = \ln(3) \simeq 1.099 \tag{14}$$

For two states we have $S_1 = \ln(2)$, while for six states we have $S_1 = \ln(6)$

(ii) For Fig. 2(a) we have

$$S_1 = -\frac{1}{8}\ln\frac{1}{8} - \frac{2}{8}\ln\frac{2}{8} - \frac{5}{8}\ln\frac{5}{8} = 0.900 \tag{15}$$

So the entropy is lower for the figure (a). Intuitively it is visually less random. If I add another green square this will not increase the number of configurations by much – in the limit it is all green adding another green square will still make it just one state. Adding a red square will increase the number of states, but the probability of this is very low.

(iii) We have

$$\begin{aligned}
S_1^{AB} &= \sum_{(a,b)} -p_s^{AB}\ln(p_s^{AB}) &(16)\\
&= \sum_a\sum_b -p_a^A p_b^B \ln(p_a^A p_a^B) = \sum_a\sum_b -p_a^A p_b^B\ln(p_a^A) - p_a^A p_b^B \ln(p_b^B) &(17)\\
&= \sum_a -p_a^A\ln(p_a^A) + \sum_b -p_b^B\ln(p_b^B) = S_1^A + S_1^B &(18)
\end{aligned}$$

In passing from the second to third line we have used

$$\sum_b p_b^B \times \text{some fcn of } p_a^A = 1\times\text{some function of } p_a^A \tag{19}$$

Problem 3. 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[3]

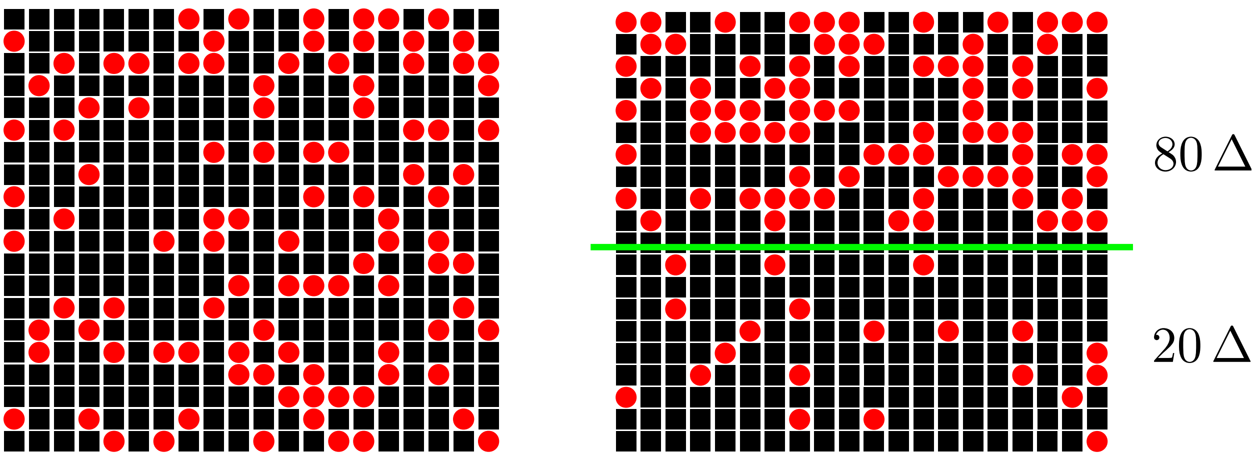


Figure 3: (a) A microstate where the energy is not partitioned. (b) a microstate where the energy is partitioned – 80% on the top and 20% on the bottom.

[3] Answer: e^{200}.

Solution:

(a) We are making a selection of $N_1 \simeq 100$ atoms out of $N = 400$ to be excited, with $N_2 = 300$ not excited:

$$\begin{aligned}
\ln \Omega =& \ln \frac{N!}{N_1! N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (20)\\
=& 400 \left[-\frac{1}{4} \ln(\frac{1}{4}) - \frac{3}{4} \ln(\frac{3}{4}) \right] && (21)\\
\simeq& 225; && (22)
\end{aligned}$$

Thus there e^{225} microstates.

(b) The reasoning is similar for top half, we are selecting 80 out of 200. So for the first half

$$\begin{aligned}
\ln \Omega_1 =& \ln \frac{N!}{N_1! N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (23)\\
=& 200 \left[-\frac{80}{200} \ln(\frac{80}{200}) - \frac{120}{200} \ln(\frac{120}{200}) \right] && (24)\\
\simeq& 135.; && (25)
\end{aligned}$$

While the bottom half we are selecting 20 out of 200

$$\begin{aligned}
\ln \Omega_1 =& \ln \frac{N!}{N_1! N_2!} \simeq -N_1 \ln(N_1/N) - N_2 \ln(N_2/N) && (26)\\
=& 200 \left[-\frac{20}{200} \ln(\frac{20}{200}) - \frac{180}{200} \ln(\frac{180}{200}) \right] && (27)\\
\simeq& 65.; && (28)
\end{aligned}$$

So the total number of configurations is a product

$$\ln(\Omega_1 \Omega_2) = \ln(\Omega_1) + \ln(\Omega_2) \simeq 200. \quad (29)$$

Problem 4. The Gamma function

The $\Gamma(x)$ function can be defined as[4]

$$\boxed{\Gamma(x) \equiv \int_0^\infty \mathrm{d}u e^{-u} u^{x-1} = \int_0^\infty \frac{\mathrm{d}u}{u}\, e^{-u} u^x} \tag{30}$$

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.

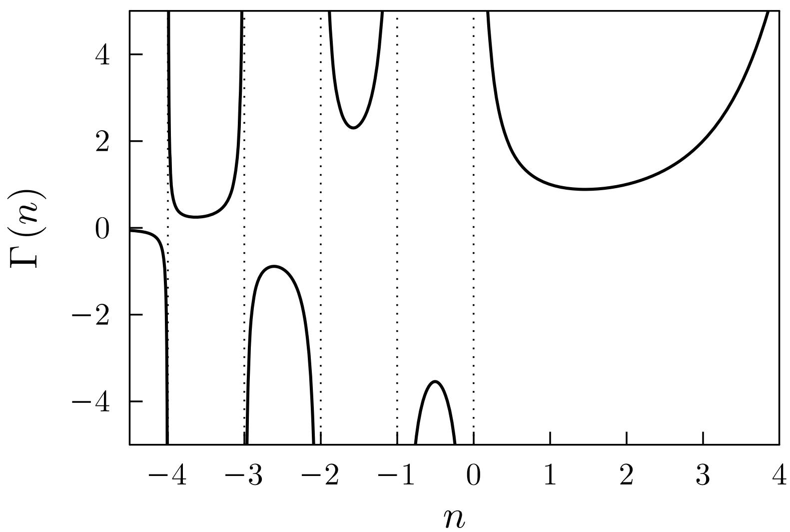


Fig. C.1 The gamma function $\Gamma(n)$ showing the singularities for integer values of $n \leq 0$. For positive, integer n, $\Gamma(n) = (n-1)!$.

Figure 4: Appendix C.2 of our book

(a) Using notions of generating functions, briefly explain 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.

$$\boxed{\Gamma(x+1) = x\Gamma(x)\,,} \tag{31}$$

or

$$x! = x \cdot (x-1)!\,, \tag{32}$$

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. (31).

[4] 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 $du'/u' = du/u$.

(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)

$$A_d(r) = \frac{2\pi^{d/2}}{(\frac{d}{2}-1)!} r^{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \tag{33}$$

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

Gamma Fcn

(a) According to the previous problem

$$n! = \int_0^\infty dx\ e^{-x}\ x^n$$

$$= \underbrace{\int_0^\infty \frac{dx}{x}\ e^{-x}\ x^{n+1}}_{\text{definition of } \Gamma(n+1)} = \Gamma(n+1)$$

(b) So

$$\Gamma(1/2) = \int_0^\infty \frac{dx}{x}\ e^{-x}\ x^{1/2}$$

- writing $y = \sqrt{x}$, $dy = \frac{1}{2\sqrt{x}}\,dx$, or

$$2\frac{dy}{y} = \frac{dx}{x}$$

- So we find

$$\Gamma(1/2) = 2\int_0^\infty \frac{dy}{\cancel{y}}\ e^{-y^2}\ \cancel{y} = \int_{-\infty}^{\infty} dy\ e^{-y^2}$$

- This is a gaussian integral, $\int_{-\infty}^{\infty} dx\ e^{-\frac{1}{2}\frac{x^2}{\sigma^2}} = \sqrt{2\pi\sigma^2}$,

with $\sigma^2 = 1/2$, so $\boxed{\Gamma(1/2) = \sqrt{\pi}}$

• Then (this is optional):

$\boxed{c)}$ $$\Gamma(x) = \int_0^\infty \frac{du}{u} e^{-u} u^{x+1}$$

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

$$= \int_0^\infty - de^{-u} u^x$$

$$= e^{-u} u^x \Big|_0^\infty + \int_0^\infty e^{-u} x u^{x-1}$$

$$= 0 + x \int_0^\infty e^{-u} u^{x-1}$$

$$= x \Gamma(x)$$

$\boxed{d)}$ So if $$\Gamma(7/2) = \frac{5}{2} \Gamma\left(\frac{5}{2}\right) = \frac{5}{2} \cdot \frac{3}{2} \Gamma\left(\frac{3}{2}\right)$$

$$= \frac{5}{2} \cdot \frac{3}{2} \cdot \frac{1}{2} \Gamma\left(\frac{1}{2}\right)$$

$$= \frac{15}{8} \sqrt{\pi} \simeq 3.3$$

Now $3 < \frac{7}{2} < 4$ so we expect (and find)

$$2! < \frac{15\sqrt{\pi}}{8} < 3! \quad \text{or} \quad 2 < 3.3 < 6$$

e) $$A_2 = \frac{2\pi^{2/2}}{\Gamma(1)} r = 2\pi r$$

$$A_3 = \frac{2\pi^{d/2}}{\Gamma\left(\frac{3}{2}\right)} r^2 = \frac{2\pi^{3/2}}{\frac{1}{2}\Gamma(1/2)} r^2$$

using $\Gamma(1/2) = \sqrt{\pi}$ we have:

$$A_3 = 4\pi r^2$$

Problem 5. Two State System

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

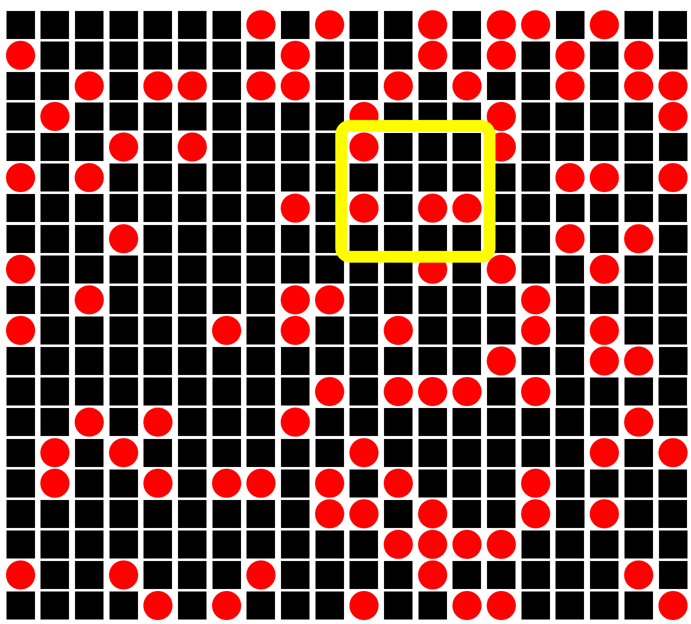
(a) Determine the temperature at which the number of excited atoms reaches $N/4$. You should find $kT = \Delta/\ln 3$.

(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:

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

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

(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?



Solution

(a) The probability of being excited is (see lecture):

$$P_1 = \frac{e^{-\beta\Delta}}{Z} = \frac{e^{-\beta\Delta}}{1+e^{-\beta\Delta}} = \frac{1}{e^{\beta\Delta}+1}.$$

We want to find T (or $\beta = 1/kT$) when $P_1 = \frac{1}{4}$. Simple algebra yields:

$$e^{\beta\Delta} + 1 = 4 \quad \Rightarrow \quad kT = \frac{\Delta}{\ln(3)}.$$

(b) The mean energy is:

$$\langle \epsilon \rangle = P_0 \cdot 0 + P_1 \cdot \Delta = P_1 \Delta = \frac{\Delta}{e^{\beta\Delta}+1}.$$

The mean energy squared is:

$$\left\langle \epsilon^2 \right\rangle = P_0 \cdot 0^2 + P_1 \cdot \Delta^2 = P_1 \Delta^2 = \frac{\Delta^2}{e^{\beta\Delta}+1}.$$

Thus, the variance is given by:

$$\begin{aligned} \left\langle (\delta\epsilon)^2 \right\rangle &= \left\langle \epsilon^2 \right\rangle - \langle \epsilon \rangle^2 && (34) \\ &= \frac{\Delta^2}{e^{\beta\Delta}+1}\left(1 - \frac{1}{(e^{\beta\Delta}+1)^2}\right) && (35) \\ &= \frac{\Delta^2 e^{\beta\Delta}}{(e^{\beta\Delta}+1)^2}, && (36) \end{aligned}$$

which matches the problem statement after simplification.

(c) The energy is a sum:

$$E = \epsilon_1 + \ldots \epsilon_{16}.$$

The total energy behaves like a random walk, with each atom having $\epsilon = 0$ or $\epsilon = \Delta$. Since the atoms are identical:

$$\langle E \rangle = 16 \langle \epsilon \rangle.$$

Similarly, for a sum of statistically independent terms. The variance of a sum is the sum of the variances:

$$\left\langle (\delta E)^2 \right\rangle = 16 \left\langle (\delta\epsilon)^2 \right\rangle.$$

Utilizing the identical nature of the atoms, we find:

$$\begin{aligned} \left\langle E^2 \right\rangle &= \langle E \rangle^2 + \left\langle (\delta E)^2 \right\rangle && (37) \\ &= 16^2 \langle \epsilon \rangle^2 \left(1 + \frac{1}{16}\frac{\left\langle (\delta\epsilon)^2 \right\rangle}{\langle \epsilon \rangle^2}\right), && (38) \\ &= 16^2 \langle \epsilon \rangle^2 \left(1 + \frac{e^{\beta\Delta}}{16}\right). && (39) \end{aligned}$$

In the limit that 16 is very large the second term can often be neglected.

Since E is a *sum* of many (i.e. 16) *independent and identical* objects, we have that its probability distribution will tend to a Gaussian. This is the Central Limit Theorem. The probability of having energy between E and $E + \mathrm{d}E$ is

$$\mathrm{d}\mathscr{P} = \frac{1}{\sqrt{2\pi \left\langle \delta E^2 \right\rangle}} e^{-(E - \langle E \rangle)^2 / 2 \left\langle \delta E^2 \right\rangle} \mathrm{d}E \tag{40}$$

where $\langle \delta E^2 \rangle$ and $\langle E \rangle$ were given above. In the notation we have adopted, the probability density is

$$\frac{\mathrm{d}\mathscr{P}}{\mathrm{d}E} = P(E) = \frac{1}{\sqrt{2\pi \left\langle \delta E^2 \right\rangle}} e^{-(E - \langle E \rangle)^2 / 2 \left\langle \delta E^2 \right\rangle} \tag{41}$$