Problem 1. Gaussian Integrals and moment generating functions

Motivation: Consider a harmonic oscillator with potential energy $U(x) = \frac{1}{2}kx^2$. If the harmonic oscillator is subjected to an additional constant force f in the x direction its potential energy is $U(x, f) = \frac{1}{2}kx^2 - fx$. As we will see shortly, the probability to find the harmonic oscillator coordinate between x and $x + dx$ is

$$P(x)\mathrm{d}x = Ce^{-U(x,f)/k_BT}\mathrm{d}x\,. \tag{1}$$

This motivated people to study integrals of the form

$$I(f) \equiv C\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\frac{1}{2}x^2+fx} \tag{2}$$

where f is a real number and C is a normalizing constant.

Method: Consider integrals of the following form

$$I_n = \langle x^n \rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\frac{1}{2}x^2} x^n \tag{3}$$

which come up a lot in this course. There is a neat trick for evaluating the integrals I_n, known as the moment generating (or characteristic) function.

Instead of considering I_n, consider the average of $\langle e^{ax} \rangle$.

$$I(a) \equiv \langle e^{ax} \rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} e^{ax} \tag{4}$$

with a a fixed real number. Why would one ever want to do this? Well, if you differentiate with respect to a (under the integral sign) and then set $a = 0$, you pull down an x:

$$\left.\frac{d}{da}e^{ax}\right|_{a=0} = \left.e^{ax}x\right|_{a=0} = x\,. \tag{5}$$

Thus, we may differentiate under the integral sign and find $\langle x \rangle$ from $I(a)$:

$$\left.\frac{d}{da}I(a)\right|_{a=0} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} x = \langle x \rangle \tag{6}$$

The trick can be repeated any number of times. For instance since

$$\left.\left(\frac{d}{da}\right)^4 e^{ax}\right|_{a=0} = \left.e^{ax}x^4\right|_{a=0} = x^4 \tag{7}$$

We have

$$\left.\left(\frac{d}{da}\right)^4 I(a)\right|_{a=0} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} x^4 = \langle x^4 \rangle \tag{8}$$

In summary, knowing $I(a)$ amounts to know all moments of the probability distribution

$$\langle x^n \rangle \tag{9}$$

by differentiation[1]. That is why $I(a)$ is called the moment generating function. This procedure works for any probability distribution and not just the Gaussian (or bell-curve). Now we only need to find $I(a)$

(a) (Optional) This was done in class. Look over the notes to find it. Show that

$$\boxed{I_0 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \, e^{-\frac{1}{2}x^2} = 1} \tag{13}$$

(b) Show that

$$I(a) = e^{\frac{1}{2}a^2} \tag{14}$$

Hint: Complete the square

$$-\frac{1}{2}x^2 + ax = -\frac{1}{2}(x-a)^2 + \frac{1}{2}a^2 \tag{15}$$

and then do the integral by a change of variables.

(c) Use the method of generating functions outlined above to prove that

$$\left\langle x^2 \right\rangle = 1 \qquad \left\langle x^4 \right\rangle = 3 \tag{16}$$

If you are interested, try to prove the general result for yourself

$$I_{2n} = \frac{(2n)!}{n! 2^n} \tag{17}$$

Hint: expand the result of (b) and compare with Eq. (12)

(d) For a distribution of the form

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \tag{18}$$

where σ and x have units of length, determine $\langle x^2 \rangle$ and $\langle x^4 \rangle$ using the results of part (c) and a change of variables to $u = x/\sigma$.

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[1] An entirely equivalent way of saying this is that the since the Taylor series of e^{ax} is

$$e^{ax} = 1 + ax + \frac{1}{2!}a^2x^2 \ldots \tag{10}$$

we can see that the Taylor series of $I(a)$ takes the form

$$I(a) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \, e^{-\frac{1}{2}x^2} \left(1 + ax + \frac{1}{2!}a^2x^2 + \ldots \right) \tag{11}$$

$$= 1 + \langle x \rangle a + \left\langle x^2 \right\rangle \frac{a^2}{2!} + \left\langle x^3 \right\rangle \frac{a^3}{3!} + \ldots \tag{12}$$

Thus knowing they Taylor series of $I(a)$ amounts to knowing *all* $I_n = \langle x^n \rangle$. Once simply needs to Taylor expand $I(a)$ in a and read off the coefficients in frount of a^n – that coefficient is $I_n/n!$.

The results of this problem show that for a Gaussian probability distribution as presented

$$\boxed{\langle x^n \rangle = \sigma^n \frac{(2n)!}{n! 2^n}} \tag{19}$$

Solution:

(a) See book

(b) Completing the square we have

$$I(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}(x-f)^2 + \frac{1}{2}f^2} \tag{15}$$

Pulling out the $e^{\frac{1}{2}f^2}$, and changing variables to $u = (x - f)$ we find

$$\begin{aligned} I(f) &= e^{\frac{1}{2}f^2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} du e^{-\frac{1}{2}u^2} \qquad (16) \\ &= e^{\frac{1}{2}f^2} \qquad (17) \end{aligned}$$

(c) We expand $e^{\frac{1}{2}f^2}$ and compare with

$$\left\langle e^{fx} \right\rangle = I_0 + I_1 f + I_2 \frac{f^2}{2!} + I_3 \frac{f^3}{3!} + \ldots \tag{18}$$

We have

$$e^{\frac{1}{2}f^2} = 1 + \frac{f^2}{2} + \frac{1}{2!}\left(\frac{f^2}{2}\right)^2 + \frac{1}{3!}\left(\frac{f^2}{2}\right)^3 \tag{19}$$

Comparing the terms of f^n

$$\begin{aligned} I_0 &= 1 \qquad (20) \\ I_1 &= 0 \qquad (21) \\ \frac{I_2}{2!} &= \frac{1}{2} \qquad (22) \\ \frac{I_3}{3!} &= 0 \qquad (23) \\ \frac{I_4}{4!} &= \frac{1}{2!}\frac{1}{2^2} \qquad (24) \\ \frac{I_6}{6!} &= \frac{1}{3!}\frac{1}{2^3} \qquad (25) \end{aligned}$$

So

$$I_2 = 1 \qquad I_4 = 3 \qquad I_6 = 15 \tag{26}$$

More generally we wee that

$$I_{2n} = \frac{2n!}{2^n n!} \tag{27}$$

(d) This is just a change of variables to $u = x/\sigma$

$$\langle x^n \rangle = \int_{-\infty}^{\infty} \mathrm{d}x x^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}x^2/\sigma^2} \tag{28}$$

$$= \sigma^n \int \frac{dx/\sigma}{\sqrt{2\pi}} \left(\frac{x}{\sigma}\right)^n e^{-\frac{1}{2}x^2/\sigma^2} \tag{29}$$

$$= \sigma^n \int \frac{du}{\sqrt{2\pi}} u^n e^{-\frac{1}{2}u^2} \tag{30}$$

$$= \sigma^2 I_n \tag{31}$$

Thus

$$\left\langle x^2 \right\rangle = \sigma^2 \qquad \left\langle x^4 \right\rangle = 3\sigma^4 \tag{32}$$

Problem 2. Exponential distribution

A particle is created at time $t = 0$ and flies a distance x (greater than zero) before being destroyed. The probability of surviving up to a given distance between x and $x + \mathrm{d}x$ is

$$P(x)\mathrm{d}x = Ae^{-x/\ell}\mathrm{d}x \tag{20}$$

with $x > 0$. For parts (a), (b), you should do the integrals yourself (showing your work explicitly) and dont use Mathematica. For pracitce switch to some dimensionless variables i.e. $u = x/\ell$ before trying to do the integrals. In part (d) you will prove the boxed integral.

(a) Find the value of A that makes $P(x)$ a well defined normalized probability distribution with $\int_0^\infty \mathrm{d}x\, P(x) = 1$. What are the units of A?

(b) Show that the mean survival length is ℓ, i.e. show that $\langle x \rangle = \int_0^\infty \mathrm{d}x\, xP(x) = \ell$.

(c) Show that variance and std. deviation of the survival length are ℓ^2 and ℓ respectively. For any dimensionfull integrals that come up you *must* do the following:

   (i) First switch to a dimensionless variable $u = x/\ell$ (x in units of ℓ), to express the dimensionfull result as ℓ to some power (so that the units are correct), times a dimensionless integral. In this case the dimensionless integrals can be done analytically using the results of the next item, which you may just quote

(d) For simplicity set $\ell = 1$ in what follows. This is the equivalent to saying we will measure x in units of ℓ. Use the generating function method of a previous problem, and calculate $\langle \exp(ax) \rangle$. Use the result to prove that

$$\langle x^n \rangle = n!$$

The taylor series can be helpful but not essential:

$$\frac{1}{1-a} = 1 + a + a^2 + a^2 + \dots \tag{21}$$

This problem establishes that

$$\boxed{n! = \int_0^\infty e^{-x} x^n \, \mathrm{d}x} \tag{22}$$

Exponential Distribution

a) $$\int_0^\infty dx\, A\, e^{-x/\ell} = 1$$

Changing variables $u = x/\ell$

$$A\ell \int_0^\infty \frac{dx}{\ell}\, e^{-x/\ell} = 1$$

$$A\ell \underbrace{\int_0^\infty du\, e^{-u}}_{1 \text{ proved below}} = 1$$

$$\boxed{A = 1/\ell}$$

b) Then

$$\langle x \rangle = \int_0^\infty \frac{dx}{\ell}\, x\, e^{-x/\ell}$$

$$= \ell \int_0^\infty \frac{dx}{\ell}\, \frac{x}{\ell}\, e^{-x/\ell}$$

$$= \ell \underbrace{\int_0^\infty du\, u\, e^{-u}}_{1 \text{ proved below}} = \ell$$

c)

c) We have

$$\langle x^2 \rangle = \int_0^\infty dx \; x^2 \; \frac{e^{-x/\ell}}{\ell}$$

$$\langle x^2 \rangle = \ell^2 \int_0^\infty \frac{dx}{\ell} \left(\frac{x}{\ell}\right)^2 e^{-x/\ell}$$

$$\langle x^2 \rangle = \ell^2 \underbrace{\int_0^\infty du \; u^2 e^{-u}}_{2! \text{ proved below}} = \ell^2 \, 2!$$

So

$$\langle \delta x^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = 2\ell^2 - \ell^2 = \ell^2 = \langle \delta x^2 \rangle$$

So

$$\boxed{\sigma_x = \sqrt{\langle \delta x^2 \rangle} = \ell}$$

d) We have

$$\langle e^{fx} \rangle = \int_0^\infty dx \; e^{fx} \; e^{-x}$$

$$= \int_0^\infty dx \; e^{-(1-f)x}$$

$$= \frac{1}{1-f}$$

- Now according to the generating fcn method

$$\langle e^{fx}\rangle = 1 + \langle x\rangle f + \frac{\langle x^2\rangle f^2}{2!} + \frac{\langle x^3\rangle f^3}{3!} + \cdots$$

- The explicit computation gives

$$\langle e^{fx}\rangle = \frac{1}{1-f} = 1 + f + f^2 + f^3 + \cdots$$

- So, for instance, comparing the coefficient of f^3 we conclude

$$\frac{\langle x^3\rangle f^3}{3!} = f^3 \quad \text{or} \quad \langle x^3\rangle = 3!$$

- More generally

$$\frac{\langle x^n\rangle f^n}{n!} = f^n \quad \text{or} \quad \boxed{\langle x^n\rangle = n!}$$

☆ Above we used the following integrals

- $I_0 = \int_0^\infty e^{-u}\, du = -e^{-u}\Big|_0^\infty = 1$

- $I_1 = \int_0^\infty e^{-u}\, u\, du$ We do this by parts

$dv = e^{-u}$

$$= \int_0^\infty -d(e^{-u})\, u\, du$$

$$= -e^{-u} u\Big|_0^\infty + \underbrace{\int_0^\infty e^{-u}\, du}_{1}$$

we did it above

$$= 0 + 1$$

- $I_2 = \int_0^\infty e^{-u}\, u^2\, du$ We do this by parts twice, $dv = e^{-u} = d(-e^{-u})$

$$= \int_0^\infty (-d e^{-u})\, u^2\, du$$

$$= -e^{-u} u^2\Big|_0^\infty + \int_0^\infty e^{-u}\, 2u\, du$$

$$= 0 + 2 \cdot \underbrace{\int_0^\infty e^{-u}\, u\, du}_{1} = 2$$

Problem 3. The Gamma function

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

$$\boxed{\Gamma(x) = \int_0^\infty \mathrm{d}u e^{-u} u^{x-1}} \tag{23}$$

A plot of $\Gamma(x)$ is shown below. $\Gamma(n)$ provides a generalization of $(n-1)!$ when 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.

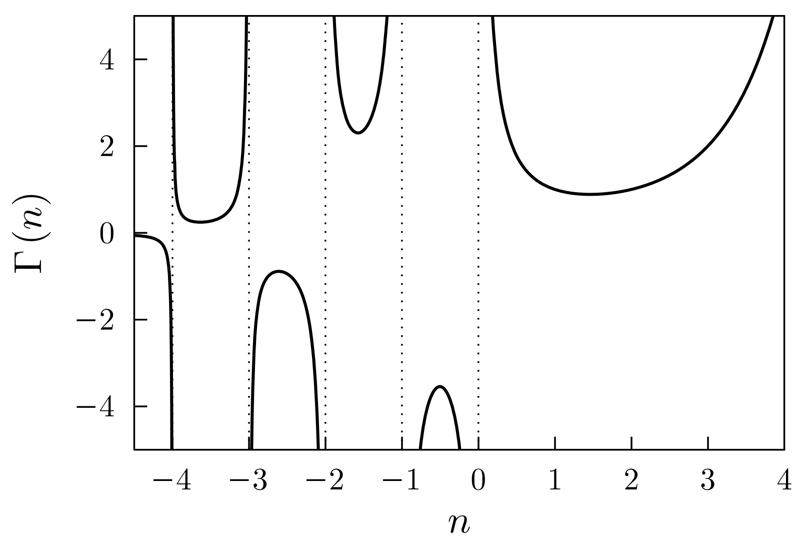


Fig. C.1 The gamma function $\Gamma(n)$ showing the singularities for integer values of $n \leq 0$. For positive, integer n, $\Gamma(n) = (n-1)!$.

Figure 1: 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.

$$\boxed{\Gamma(x+1) = x\Gamma(x)\,,} \tag{24}$$

or

$$x! = x \cdot (x-1)!\,, \tag{25}$$

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. (24).

[2] I 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 $u \to u' = \lambda u$ 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)

$$A_d(r) = \frac{2\pi^{d/2}}{(\frac{d}{2}-1)!} r^{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1} \tag{26}$$

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 $y = \sqrt{x}$, $dy = \frac{1}{2} \frac{dx}{\sqrt{x}}$, 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) $$A_2 = \frac{2\pi^{2/2}}{\Gamma(1)} r = 2\pi r$$

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

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

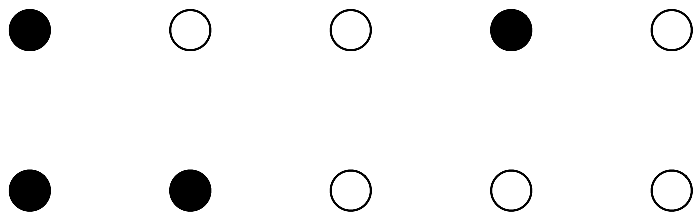
$$A_3 = 4\pi r^2$$

Problem 4. Combinatorics and The Stirling Approximation

Consider a chain of 6×10^{23} atoms, laid out in a row. The atoms can be in two states, a ground state, and an excited state. 1/3 of them are in the excited states. Using the Stirling approximation, show that the number of configurations with this number of excited states is approximately

$$10^{1.67\times10^{23}} \tag{27}$$

For instance, if the number of atoms is five, and the number of excited atoms (shown by the black circles) is 2, then two possible configurations are shown below.



Combinatorics and Stirling

- The number of selections is

$$^{N_A}C_r = \frac{N_A!}{\left(\frac{1}{3}N_A\right)!\left(\frac{2}{3}N_A\right)!} \qquad \text{with } r \equiv \frac{1}{3}N_A$$

- Taking the log

$$\log {}^{N_A}C_r = \log N_A! - \log\left(\left(\tfrac{1}{3}N_A\right)!\right) - \log\left(\left(\tfrac{2}{3}N_A\right)!\right)$$

$$= N_A \log N_A - N_A - \left(\frac{1}{3}N_A \log\left(\frac{1}{3}N_A\right) - \frac{1}{3}N_A\right)$$

$$- \left(\frac{2}{3}N_A \log\left(\frac{2}{3}N_A\right) - \frac{2}{3}N_A\right)$$

$$= \frac{1}{3}N_A \log(3) + \frac{2}{3}N_A \log\left(\frac{3}{2}\right)$$

$$= \frac{N_A}{3}\log\left(\frac{27}{4}\right) = 0.64\, N_A$$

- So

$$^{N_A}C_r = e^{0.64 N_A} = \left(e^{\log 10}\right)^{0.64 N_A/\log 10}$$

$$= 10^{0.64 N_A/\log 10} \simeq 10^{1.66\times 10^{23}}$$

Problem 5. 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) What is the mean and variance variance in his position X after one step, and after two steps.

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

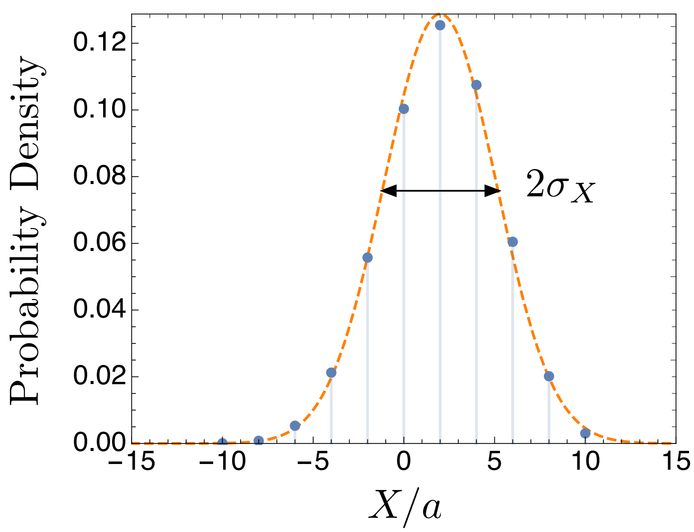


Figure 2: Probability of our drunkard having position X after $n = 10$ steps (the blue points). Of course after 10 steps the drunkard will be between $-10 \ldots 10$, and it is easy to show that he will be only at the even sites, i.e. $-10, -8, -6, \ldots 10$. For $p = 0.6$, I find $\langle X \rangle = 2.0$. 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.

(c) (Optional. Don't turn in) If p is very nearly $\frac{1}{2}$, say $p = 0.5001$, determine how many steps it will take before the mean value $\langle X \rangle$ is definitely different from zero. By "definitely" I mean that $\langle X \rangle$ is "more than two sigma" away from zero, $\langle X \rangle > 2\sigma_X$. If $p = \frac{1}{2} + \epsilon$ (with ϵ tiny), you should find (approximately) that

$$N_{\mathrm{steps}} \simeq \frac{1}{\epsilon^2} \tag{28}$$

up to corrections of order ϵ. Here $p = \frac{1}{2} + \epsilon$ with $\epsilon = 0.0001$, how does the result scale with ϵ, e.g. if I where two half ϵ how would the number of required steps change?

Random Walk

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

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

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

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: $4\sqrt{\frac{1}{2}\frac{1}{2}} \simeq 2$

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

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

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

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