Problem 1. Gaussian Integrals and moment generating functions

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.

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 to evaluating evaluating the integrals I_n known as the moment generating function. Instead of considering I_n, consider

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

with f a fixed real number. Why would one ever want to do this? Well, if you expand the exponent

$$e^{fx} = 1 + fx + \frac{1}{2!}f^2x^2 \ldots \tag{5}$$

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

$$I(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\frac{1}{2}x^2} \left(1 + fx + \frac{1}{2!}f^2x^2 + \ldots\right) \tag{6}$$

$$= 1 + \langle x \rangle f + \left\langle x^2 \right\rangle \frac{f^2}{2!} + \left\langle x^3 \right\rangle \frac{f^3}{3!} + \ldots \tag{7}$$

Thus knowing $I(f)$ amounts to knowing *all* $I_n = \langle x^n \rangle$. Once simply needs to Taylor expand $I(f)$ in f and read off the coefficients in frount of f^n – that coefficient is $I_n/n!$. $\left\langle e^{fx} \right\rangle$ is known as the moment generating function since it "generates" integrals the moments $\langle x^n \rangle$. Now we only need to find $I(f)$

(a) (Optional) Show that

$$\boxed{I_0 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\frac{1}{2}x^2} = 1} \tag{8}$$

(b) Show that

$$I(f) = e^{\frac{1}{2}f^2} \tag{9}$$

Hint: Complete the square

$$-\frac{1}{2}x^2 + fx = -\frac{1}{2}(x - f)^2 + \frac{1}{2}f^2 \tag{10}$$

and then do the integral by a change of variables.

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

$$\left\langle x^2 \right\rangle = 1 \qquad \left\langle x^4 \right\rangle = 3 \qquad \left\langle x^6 \right\rangle = 15 \tag{11}$$

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

$$I_{2n} = \frac{2n!}{n!2^n} \tag{12}$$

Hint: expand the result of (b) and compare with Eq. (7)

(d) For a distribution of the form

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \tag{13}$$

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 $u = x/\sigma$.

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

$$\boxed{\langle x^n \rangle = \sigma^n \frac{(2n)!}{n!2^n}} \tag{14}$$

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

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

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

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

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

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

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 $u = x/\sigma$

$$\begin{aligned}\langle x^n \rangle =& \int_{-\infty}^{\infty} \mathrm{d}x x^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}x^2/\sigma^2} && (28)\\ =&\sigma^n \int \frac{dx/\sigma}{\sqrt{2\pi}} \left(\frac{x}{\sigma}\right)^n e^{-\frac{1}{2}x^2/\sigma^2} && (29)\\ =&\sigma^n \int \frac{du}{\sqrt{2\pi}} u^n e^{-\frac{1}{2}u^2} && (30)\\ =&\sigma^2 I_n && (31)\end{aligned}$$

Thus

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

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

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

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

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

So proved below

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

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

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

- The explicit computation gives

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

- 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

$dv = e^{-u}$

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

$$= -e^{-u} u\Big|_0^\infty + \underbrace{\int_0^\infty e^{-u}\, du}_{\text{we did it above}}$$

$$= 0 + 1$$

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

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

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

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

Gamma Fcn

(a) According to the previous problem

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

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

(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)

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

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

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

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

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

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

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

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

Random Walk

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

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

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

So

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

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

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

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

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

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

Speed of Nitrogen Gas: N_2 diatomic nitrogen

$$PV = N k_B T$$

- So

$$k_B T = \frac{PV}{N} = \frac{(5 \times 10^5 N/m^2)(6 \times (0.1m)^3)}{2 \times 6 \times 10^{23}}$$

$$= 2.5 \times 10^{-21} \text{ J} \qquad k_B = \frac{1/44}{273} \frac{eV}{°K}$$

$$\simeq 0.016 \text{ eV} \qquad T = 180 °K$$

- So the molecule has five degrees of freedom

$$E = \frac{5}{2} k_B T \simeq 0.040 \text{ eV}$$

- The translational motion is 3-degrees of freedom

$$\langle \frac{1}{2} m v^2 \rangle = 3 \times \frac{1}{2} k_B T$$

So

$$\sqrt{\langle v^2 \rangle} = \sqrt{\frac{3 k_B T}{m}}$$

$$V_{rms} = \left(\frac{3 k_B N_A T}{m N_A} \right)^{1/2}$$

Now $\quad k_B N_A = 8.32 \frac{J}{°K} \qquad T = 180°K$

So $\quad \underline{m N_A = \text{molar mass} \simeq 28g = 2 \times 14g}$

$$V_{rms} = \left(\frac{3 \cdot 8.32 \frac{J}{K} \; 180°K}{28g} \right)^{1/2}$$

$$\simeq 400 m/s$$