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

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

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

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

(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 $u = x/\sigma$

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

Thus

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