Gaussian integrals

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1 The basic Gaussian and its normalization

The Gaussian function or the normal distribution,
\[ \exp\left(-\alpha x^2\right), \] (1)
is a widely used function in physics and mathematical physics, including in quantum mechanics. It is therefore useful to know how to integrate it. In this and in future notes I will discuss the basic integrals you should memorize and how to derive other related integrals.

An example Gaussian is shown in Fig. 1.

As always, it can be useful to draw pictures to help you think about integrals. The fundamental integral is
\[ \int_{-\infty}^{+\infty} \exp\left(-\lambda x^2\right) dx = \sqrt{\frac{\pi}{\lambda}} \] (2)
You should memorize either this or the related integral (I prefer the first one)
\[
\int_{0}^{+\infty} \exp (-\lambda x^2) \, dx = \frac{1}{2} \sqrt{\frac{\pi}{\lambda}}
\]  \hspace{1cm} (3)

The only difference between these two is the limits of integration. Always pay attention to the limits of integration. Always. Not paying attention to the limits of integration is a common source of mistakes.

We can see this by drawing the second function and because integrals are

![Figure 2: areas under a curve](image)

areas under a curve it becomes obvious that Eq. 3 is half of Eq. 2.

(As an aside, although you do not need to learn this derivation, this is how one can derive the basic Gaussian integral. Suppose we want
\[
I = \int_{-\infty}^{+\infty} \exp (-\lambda x^2) \, dx.
\]

Then we square this:
\[
I^2 = \int_{-\infty}^{+\infty} \exp (-\lambda x^2) \, dx \int_{-\infty}^{+\infty} \exp (-\lambda y^2) \, dy
\]  \hspace{1cm} (4)

which we rewrite as
\[
I^2 = \int \int \exp (-\lambda (x^2 + y^2)) \, dx \, dy.
\]  \hspace{1cm} (5)

Now we go from Cartesian coordinates \((x, y)\) to polar coordinates \((r, \theta)\):
\[
I^2 = \int \int \exp (-\lambda r^2) \, rdr \, d\theta.
\]  \hspace{1cm} (6)
The integral over $\theta$ is easy, leaving

$$I^2 = 2\pi \int_0^\infty \exp(-\lambda r^2) rd\tau. \quad (7)$$

Now we make a substitution: $u = r^2$, with $du = 2rd\tau$ or

$$I^2 = 2\pi \int_0^\infty \exp(-\lambda u) \frac{1}{2} du. \quad (8)$$

But this is the simple integral of an exponential (you have to start with some sort of integral) and

$$I^2 = \pi \times \frac{1}{-\lambda} \exp(-\lambda u) \bigg|_0^\infty = \frac{\pi}{\lambda}. \quad (9)$$

From this we immediately get $I$ is Eq. 2.)

What about the integral of a shifted Gaussian

$$\int_{-\infty}^{+\infty} \exp\left(-\lambda(x-a)^2\right) dx \quad (10)$$

where $x_0$ is some constant? Well, again it helps to draw the Gaussian: It should look clear that the area in Fig. 3 is the same as in 1. We can prove this formally, however, by doing a substition:

$$u = x - a$$

Figure 3:
with \( dx = du \) and then we get
\[
\int_{-\infty}^{+\infty} \exp\left(-\lambda(x-a)^2\right) \, dx = \int_{-\infty}^{+\infty} \exp\left(-\lambda u^2\right) \, du = \sqrt{\frac{\pi}{\lambda}}
\]  
(11)
as we expect.

However, we have to be careful about limits of integration. If we integrate only from zero to infinity, that is
\[
\int_{0}^{+\infty} \exp\left(-\lambda(x-a)^2\right) \, dx
\]
we can draw this as and it is no longer obvious the area under the curve is half that of Eq. 3—in fact it won’t be, in general. One has to resort to using the error function to express the integral. It’s useful to know about the error function, but we won’t be using it in this course.

2 Expectation values with Gaussians

Now suppose we want to compute expectation values with Gaussian. It is vital to use normalized distributions when computing an expectation value. So we now use the normalized Gaussian,
\[
\rho(x) = \sqrt{\frac{\lambda}{\pi}} \exp\left(-\lambda x^2\right).
\]
The expectation value of \( x \) is then
\[
\int_{-\infty}^{+\infty} x \rho(x) \, dx = \int_{-\infty}^{+\infty} x \sqrt{\frac{\lambda}{\pi}} \exp\left(-\lambda x^2\right) \, dx.
\]  
(12)
Now, if you look at Fig. 1 you might guess the expectation value (average) to be zero, and you would be correct. We can reinforced this a bit more by drawing the integrand. (You should practice sketching function; if you aren’t certain, it’s okay to write a little computer code to generate a function, or use a program such as MatLab or Mathematica. Just be sure use of computers add to your intuition and aren’t used to replace intuition.)

Figure 5:

If you have trouble arriving at this figure—nd it takes practice to develop this skill—look at the integrand: \( x \exp(-\lambda x^2) \) (ignoring constants). At \( x = 0 \), the integrand is zero. For small \( x \) near zero, we use a Taylor expansion. In general \( \exp(x) = 1 + x + \ldots \) so \( \exp(-\lambda x^2) = 1 - \lambda x^2 + \ldots \) and so \( \exp(-\lambda x^2) = x + \ldots \), that is, in the vicinity of \( x = 0 \) the function is approximately \( x \). And you can see in Fig. 5 this is true. Eventually the exponential wins out and the function curves back over.

Another important way to think about this curve is its parity. The original Gaussian function in Eq. 1 is an even function, that is,

\[ f(-x) = +f(x) \]

which means it symmetric with respect to \( x = 0 \). On the other hand, the integrand of Eq. 12 is an odd function, that is,

\[ f(-x) = -f(x). \]

The integral of an odd function, when the limits of integration are the entire real axis, is zero. We can formally show this by splitting up the integral:

\[
\int_{-\infty}^{+\infty} f(x)dx = \int_{-\infty}^{0} f(x)dx + \int_{0}^{+\infty} f(x)dx. \quad (13)
\]
In the first integral, make the substitution $u = -x$:

$$\int_{-\infty}^{0} f(x) dx = \int_{0}^{\infty} f(-u)(-du) = - \int_{0}^{\infty} f(-u)(-du) \int_{0}^{\infty} f(-u) du \quad (14)$$

(note we pick up a minus sign from switching the order of the limits). Now if $f$ is an odd function, this is now

$$\int_{0}^{\infty} f(-u) du = - \int_{0}^{\infty} f(u) du$$

which then cancels the other half of the integral.

You can see this in Fig. 6, where the contributions from the left hand side cancel those from the right hand side:

![Figure 6](image)

It is very important to keep in this mind this only works when the limits of integration are from $-\infty$ to $+\infty$. What about half that, that is,

$$\int_{0}^{+\infty} x \exp(-\lambda x^2) dx? \quad (15)$$

Again, let’s draw this in Fig. 7:

To evaluate Eq. 15 I recommend making the substitution $u = x^2$. You’ll find this does it. However, once again, this only works for the limits of integration from 0 to $\infty$.

You try (1) : Evaluate Eq. 15. Note this is not a normalized distribution. (Solution at end.)
What about the expectation value of $x$ for a shifted Gaussian, that is,

$$\int_{-\infty}^{+\infty} x \exp(-\lambda(x-a)^2)dx$$

Don’t try drawing this; instead, look at the shifted Gaussian $\exp(-\lambda(x-a)^2)$ drawn in Fig. 3. It looks like $\langle x \rangle = a$, right? You would be correct.

We can show this formally by, again, the substitution $u = x - a$. Don’t forget to use the normalized Gaussian!

$$\int_{-\infty}^{+\infty} x \sqrt{\frac{\lambda}{\pi}} \exp(-\lambda(x-a)^2)dx = \int_{-\infty}^{+\infty} (u+a) \sqrt{\frac{\lambda}{\pi}} \exp(-\lambda u^2)du$$

$$= \int_{-\infty}^{+\infty} u \sqrt{\frac{\lambda}{\pi}} \exp(-\lambda u^2)du + \int_{-\infty}^{+\infty} a \sqrt{\frac{\lambda}{\pi}} \exp(-\lambda u^2)du = 0 + a$$

because the first integral vanishes as we showed before, and as $a$ is a constant, we can pull it outside the integral; the remainder is normalized to 1.

### 3 Completing the square

Sometimes we need to evaluate an integral like

$$\int_{-\infty}^{+\infty} \exp(-ax^2 + bx)$$

We can solve this by completing the square. Note we can always evaluate

$$\int_{-\infty}^{+\infty} \exp(-a(x-x_0)^2)$$
by the substitution $y = x - x_0$. This motivates us to rewrite the argument of the exponent in (17) as

$$ax^2 - bx = a(x^2 - \frac{b}{a}x) = a\left(x^2 - \frac{b}{a}x + \frac{b^2}{4a^2} - \frac{b^2}{4a^2}\right)$$

where I’ve merely added and subtracted the same quantity inside the parentheses. But now we can rewrite this as a quantity squared

$$= a\left(x - \frac{b}{2a}\right)^2 - \frac{b^2}{4a}$$

and the original integral (17) becomes

$$\int_{-\infty}^{+\infty} \exp(-ax^2 + bx) = e^{b^2/4a} \int_{-\infty}^{+\infty} \exp(-a(x - b/2a)^2) = e^{b^2/4a} \sqrt{\pi/a} \tag{19}$$

where I’ve left off the final substitution $y = x - b/2a$. Completing the square is a very useful technique.

4 Shifting the axis of integration into the complex plane

What happens if, when we complete the square as in the previous section, the shift is complex valued? That is, suppose we have the integral

$$\int_{-\infty+ic}^{+\infty+ic} \exp(-ax^2) \tag{20}$$

where $c$ is some (real) constant. Can we evaluate it?

We can, the reason is due to Cauchy’s theorem, which you learned about (and may have subsequently forgotten) in your mathematical methods course. I won’t go into the details, but the summary is thus: Cauchy’s theorem says that an integral along a closed loop in the complex plane is proportional to the residue of any simple poles, a pole $z_0$ being some complex value where a function $f(z) \approx r/(z - z_0)$ (where $r$ is the residue). The relevant point here is that the Gaussian function has no poles in the complex plane, and hence any loop integral must be zero. From this one can show that the integral (20) has the same value independent of $c$.

A final note: pay attention to limits of integration! And draw a picture!

5 Answers to selected problems

(1) $\int_{0}^{+\infty} x \exp(-\lambda x^2)dx = 1/(2\lambda)$. 