Gaussians for Physicists

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1 The Gaussian

This goal of this document is to give an overview of the Gaussian from the perspective of its use in physics. In the beginning things are built up in excruciating detail with the goal that 2nd year undergrads can follow it. The concepts in the following sections get increasingly complex and, while still worked out to a great deal of detail, are targeted at a Graduate level.

1.1 The Single Variable Gaussian

The Gaussian function in it's most basic form is

$$f(x) = e^{-ax^2} \tag{1}$$

for some real argument x. Most often we are interested in the integral of the Gaussian over the entire real line, that is

$$I_1 = \int_{-\infty}^{\infty} dx e^{-ax^2}. \tag{2}$$

The trick to solving this integral is rather unusual. We begin by considering instead the square of the integral.

$$I_1^2 = \int_{-\infty}^{\infty} dx e^{-ax^2} \int_{-\infty}^{\infty} dy e^{-ay^2} \tag{3}$$

and here we have used y as the variable in the second integral since the choice of the variable in a definite integral is arbitrary. Since these integrals have no cross-terms, we can rewrite the integral in the more compact form

$$I_1^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy e^{-a(x^2+y^2)} \tag{4}$$

and switch to polar coordinates:

$$I_1^2 = \int_0^{2\pi} \int_0^{\infty} dr d\theta r e^{-ar^2}. \tag{5}$$

We now have an integral that can be easily solved by making the substitution $u = ar^2$. We can implicitly differentiate u to give $du = 2ardr$ so we have $rdr = du/2a$ and hence

$$I_1^2 = \frac{1}{2a}\int_0^{2\pi}\int_0^{\infty} dud\theta e^{-u} = -\frac{\pi}{a}e^{-u}\Big|_0^{\infty} = -\frac{\pi}{a}(0-1) = \frac{\pi}{a}. \quad (6)$$

Now we need only take the square root to arrive at our desired result

$$I_1 = \int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}} \quad (7)$$

1.2 Getting more complicated

Notice that with eq. (7) we now have the ability to solve integrals of the form

$$I_2 = \int_{-\infty}^{\infty} dx e^{-a(x+\mu)^2+\alpha} \quad (8)$$

where α and μ are constants. We can see this by first making the substitution $u = x + \mu$

$$I_2 = \int_{-\infty}^{\infty} du e^{-au^2+\alpha} \quad (9)$$

and then we can use the fact that $e^{x+y} = e^x e^y$ to rewrite the integral as

$$I_2 = e^{\alpha}\int_{-\infty}^{\infty} du e^{-au^2} \quad (10)$$

where we have used the fact that e^{α} is just a constant prefactor that can be pulled outside the integral. Now, reading off the solution from eq. (7), we have

$$I_2 = e^{\alpha}\sqrt{\frac{\pi}{a}}. \quad (11)$$

But what about e raised to the power of some arbitrary 2nd order polynomial? Can we solve integrals of the form

$$I_3 = \int_{-\infty}^{\infty} dx e^{-(ax^2+bx+c)} \quad (12)$$

too? As a matter of fact, we can. The trick is to make the integral look like the one in eq. (8). This can be done by completing the square. We simply let d, e and f be variables such that

$$d(x+e)^2 + f = ax^2 + bx + c. \quad (13)$$

We can expand the left hand side and then equate coefficients of like powers

$$dx^2 + 2dex + de^2 + f = ax^2 + bx + c \quad (14)$$

This gives us a system of equations

$$d = a \tag{15}$$
$$2de = b \tag{16}$$
$$de^2 + f = c \tag{17}$$

which can be solved to yield

$$d = a \tag{18}$$
$$e = b/2a \tag{19}$$
$$f = c - a(b/2a)^2 = c - b^2/4a \tag{20}$$

thus

$$ax^2 + bx + c = a(x + b/2a)^2 + c - b^2/4a \tag{21}$$

and setting $\mu = b/2a$ and $-\alpha = c - b^2/4a$ we have

$$\begin{aligned}\int_{-\infty}^{\infty} dx e^{-(ax^2+bx+c)} &= \int_{-\infty}^{\infty} dx e^{-(a(x+b/2a)^2+c-b^2/4a)} \\ &= \int_{-\infty}^{\infty} dx e^{-a(x+\mu)^2+\alpha} = e^{\alpha}\sqrt{\frac{\pi}{a}}\end{aligned} \tag{22}$$

where we have used the solution from eq.(11) to arrive at the final equality. Replacing back the variables a, b, and c we arrive at

$$I_3 = \int_{-\infty}^{\infty} dx e^{-(ax^2+bx+c)} = e^{b^2/4a-c}\sqrt{\frac{\pi}{a}}. \tag{23}$$

This is the most general solution to a Gaussian of one variable.

1.3 The multivariate Gaussian

With the solution provided by eq. (23), we can now immediately solve integrals of the form

$$I_4 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy e^{ax^2+bx+c+dy^2+ey^2+f} \tag{24}$$

by splitting up the exponent into an x and y part and then factorizing the integral:

$$I_4 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy e^{ax^2+bx+c} e^{dy^2+ey^2+f} = \int_{-\infty}^{\infty} dx e^{ax^2+bx+c} \int_{-\infty}^{\infty} dy e^{dy^2+ey^2+f} \tag{25}$$

and now the integral has been reduced to two integrals of the form (12) whose solution is known viz.

$$I_4 = e^{b^2/4a-c} e^{e^2/4d-f}\sqrt{\frac{\pi^2}{ad}} = \frac{\pi}{\sqrt{ad}} e^{b^2/4a-c+e^2/4d-f}. \tag{26}$$

But what if now though we also had the cross term xy? Adding this cross term gives the most general possible quadratic for 2 variables:

$$Q = ax^2 + bx + c + dy^2 + ey + f + gxy + hyx$$

If x and y commute then the final term is redundant, but if x and y represent operators as is often the case when physicsts are using Gaussians, then the last term must also be included. At this point our expressions are getting very long, so it is convenient to introduce matrix notation to simplify things. First we complete the squares for x and y so that Q may be written as

$$Q = a'(x-\mu_x)^2 + b'(y-\mu_y)^2 + g'(x-\mu_x)(y-\mu_y) + h'(y-\mu_y)(x-\mu_x) + c'$$

We can always expand this expression and enforce the requirement that the coefficients of like powers must match to solve for the primed variables and the μ_i's. However, at present the exact relation is not relevant. With the quadratic in this form we can introduces matrices to notationally simplify Q further:

$$\mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}$$

$$\boldsymbol{\Sigma}^{-1} = \begin{bmatrix} a' & g' \\ h' & b' \end{bmatrix}$$

The choice for calling the 2x2 matrix $\boldsymbol{\Sigma}^{-1}$ rather than just $\boldsymbol{\Sigma}$ is chosen for notational consistency for later. Now we may write Q as

$$Q = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) + c'$$

Which the reader can verify by expanding the following expression:

$$(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) = \begin{bmatrix} x-\mu_x & y-\mu_y \end{bmatrix} \begin{bmatrix} a' & g' \\ h' & b' \end{bmatrix} \begin{bmatrix} x-\mu_x \\ y-\mu_y \end{bmatrix}$$

There are two benefits from using matrix algebra here. The first is that the expression can easily be generalized to higher dimensions. The second is that it makes determining the integral of multidimensional Gaussians much easier. This is because there always exists a transformation that can be made to diagonalize $\boldsymbol{\Sigma}^{-1}$ provided that $\det(\boldsymbol{\Sigma}^{-1}) \neq 0$. Diagonalization of $\boldsymbol{\Sigma}^{-1}$ allows e^Q to be written in a form whose integrals factorize and thus can be solved by the methods discussed previously. Note that if x and y commute, $\boldsymbol{\Sigma}^{-1}$ is a normal matrix (it commutes with its conjugate transpose). The diagonalization then is a unitary transformation, so the Jacobian of the transformation will simply be unity. With this in hand we can reason our way to what $\int_{-\infty}^{\infty} dx e^Q$ must be based on comparison with eq. (26). As is well known from linear algebra, a diagonal matrix has its eigenvalues for its diagonal. Labeling the variables as x_i and their corresponding eigenvalue as λ_i we have for a Gaussian of arbitrary dimension

$$\begin{aligned} I &= \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} dx_1...dx_N \exp[(\mathbf{x}-\mu)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)] \\ &= \sqrt{\frac{(2\pi)^N}{\Pi_1^N \lambda_i}} = \sqrt{\frac{(2\pi)^N}{\det \mathbf{\Sigma^{-1}}}} = \sqrt{(2\pi)^N \det \mathbf{\Sigma}} \end{aligned} \tag{27}$$

where we have used the fact that the determinant is an invariant of the matrix equal to the product of its eigenvalues and that for any matrix A, $\det A^-1 = 1/\det A$ provided $\det A \neq 0$.

1.4 Standard Statistical Notation

If the Gaussian is used as a probability distribution function (pdf) then it's integral over all x must be unity. That is, the probability of x being *something* must be 100 percent. But the Gaussians we've looked at so far don't integrate to one. The remedy is to put a normalizing factor out front:

$$\rho(x) = Ae^{-a(x-\mu)^2} \tag{28}$$

We can then carry out the integral of this pdf quite easily to arrive at

$$\int_{-\infty}^{\infty} \rho(x) = A\int_{-\infty}^{\infty} e^{-a(x-\mu)^2} = A\sqrt{\frac{\pi}{a}} \tag{29}$$

This integral must be 1 so

$$A\sqrt{\frac{\pi}{a}} = 1 \rightarrow A = \sqrt{\frac{a}{\pi}}.$$

Finally for reasons that are beyond the scope of the discussion, we define a new variable σ such that $a = 1/2\sigma^2$ and we arrive at the "standard normal distribution"

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \tag{30}$$

μ and σ^2 are called the mean and variance. The mean is a measure of where the probability distribution is centered, and the variance is a measure of how spread out the pdf is.

For a multivariate distribution, $\mathbf{\Sigma}$ is called the variance-covariance matrix. The diagonal elements contain the variances of the random variables, and the off diagonal elements contain the covariances.

The mean and variance are the first and second cumulants of the Gaussian pdf respectively. This can most easily be shown using the cumulant generating function, but this requires the Fourier transform. Therefore, the next section introduces the Fourier transform of a Gaussian followed by a discussion on generating functions and cumluants.

2 The Fourier Transform of the Gaussian

This next bit of machinery is especially important in quantum mechanics, although as we shall see it has its uses in statistics as well. The Fourier transform of a function $f(x)$ is given by

$$F(k) = \int_{-\infty}^{\infty} dx\, f(x) e^{-ikx} \tag{31}$$

Sometimes there is also a factor of $1/2\pi$ or $1/\sqrt{2\pi}$ in front of the integral. This choice depends on the application. For quantum mechanics we shall use the fully symmetric definition which includes the factor $1/\sqrt{2\pi}$. In statistics the above definition is often more appropriate.

I'm assuming the reader has some familiarity with the Fourier transform, but I will mention some pitfalls that confused me about the transform when first using it.

- What is k? We can tease out something about k by dimensional analysis. e cannot be raised to the power of something with physical units. Therefore, k must have the inverse of x's units. If x has units of time, then k must have units of 1/time or Hz. Thus k is a frequency. If x is a length, k has units of 1/length e.g. wavelengths. In quantum mechanics k is also divided by $\hbar$ while x is a position so k will have units of $\mathrm{J \cdot s/m} = \mathrm{kg \cdot m/s}$ so k is a momentum.

- Is k a variable or a constant? k *is* a variable, but the integral is over x *not* k. So when evaluating the integral k can be treated as a constant, but don't let this trick you into thinking k is always a constant.

- How do you deal with the fact that the numbers are now complex rather than strictly real? It is important to emphasize that x remains a real number. Now however we are dealing with an integral in the complex plane, and so the path of integration must be specified. Since x is a real number, the bounds in eq. (31) tell us that this path is simply across the entire real number line.

Now let's look at the case that our function to be transformed, $f(x)$, is a single variable Gaussian.

$$F(k) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 - ikx} \tag{32}$$

This can be found by completing the square. We have

$$-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 - ikx = -\frac{1}{2\sigma^2}(x^2 + 2(2ik\sigma^2 - \mu)x + \mu^2).$$

By using the system of equations (18) and recognizing $a = 1$, $b = 2(ik\sigma^2 - \mu)$ and $c = \mu$, we have

$$-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 - ikx = -\frac{1}{2\sigma^2}(x^2 + 2(2ik\sigma^2 - \mu)x + \mu^2) \tag{33}$$

$$= -\frac{1}{2\sigma^2}\left[(x - \mu + ik\sigma^2)^2 + \mu^2 - \mu^2 + 2ik\mu\sigma^2 + \sigma^4 k^2\right] \tag{34}$$

$$= -\frac{1}{2\sigma^2}(x-\lambda)^2 - ik\mu - \frac{\sigma^2 k^2}{2} \tag{35}$$

where $\lambda = \mu - ik\sigma^2$. Returning to the Fourier transform,

$$\begin{aligned} F(k) &= \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 - ikx} \\ &= \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} dx \exp\left(-\frac{1}{2\sigma^2}(x-\lambda)^2 - ik\mu - \frac{\sigma^2k^2}{2}\right) \\ &= \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-ik\mu - \frac{\sigma^2k^2}{2}\right)\int_{-\infty}^{\infty} dx \exp\left(-\frac{1}{2\sigma^2}(x-\lambda)^2\right) \\ &= \exp\left(-ik\mu - \frac{k^2\sigma^2}{2}\right) \end{aligned} . \tag{36}$$

So the Fourier transform of a Gaussian is also a Gaussian.

3 Gaussians in the wild

In this section I would like to focus on two main topics. The first is the statistical under pinnings of the Gaussian which we shall explore from the perspective of cumulants and how they relate to statistical mechanics. The second topic is on how Gaussians arise in quantum mechanics from the perspective of Gaussian wave packets.

3.1 The statistical features of a Gaussian

Recall that the nth moment of a function x is defined as

$$\langle x^n \rangle = \int dx x^n f(x).$$

There is a nice way to easily find these moments for a Gaussian. We simply need to use the moment generating functions. In statistics, the moment generation function of a pdf is by definition the Fourier transform of the pdf which for a Gaussian is given by eq. (36). But why is the Fourier transform of a pdf its moment generating function? The answer lies in the Taylor expansion of e^z which is

$$e^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + ... = \sum_{n=0}^{\infty} \frac{z^n}{n!}$$

We can expand the e^{-ikx} term in the Fourier transform to produce

$$\begin{aligned} F(k) &= \int dx f(x) \left(1 - ikx - \frac{k^2x^2}{2} + \frac{(-ik)^3x^3}{3!} + ...\right) \\ &= \int dx f(x) - ik \int dx x f(x) - \frac{k^2}{2} \int dx x^2 f(x) + ... \\ &= 1 + (-ik)\langle x \rangle + \frac{(-ik)^2}{2}\langle x^2 \rangle + ... = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!}\langle x^n \rangle \end{aligned} \tag{37}$$

which is a sum over all moments with each moment multiplied by (ik) raised to the appropriate power. To extract the nth moment from this function, we simply take n derivatives with respect to k, divide by $(-i)^n$, and evaluate at k = 0:

$$\langle x^n \rangle = i^n \frac{d^n}{dk^n} (F(k)) \Bigg|_{k=0} \tag{38}$$

The reason for this is because taking n derivatives with respect to k causes the term containing the n^{th} moment to the leading order term. It will also be a constant so evaluating at $k = 0$ causes all the higher order terms to vanish. Finally there is still a factor of $(-i)^n$ out front that needs to be rid of so we divide by $(-i)^n$.

We can apply this to our Fourier transformed Gaussian, eq. (36), to find its moments. The first two moments are:

$$\langle x \rangle = \mu \tag{39}$$

$$\langle x^2 \rangle = \mu^2 + \sigma^2 \tag{40}$$

which the reader is encouraged to verify. The details of deriving the previous two equations have been skipped because there is in fact a faster method to deriving moments using cumulants.

Cumulants are defined in a rather peculiar fashion. We begin by taking the log of the moment generating function viz. $\ln F(k)$. Since this is a function of the variable k, we can represent it as a power series so long as $F(k)$ is analytic in the region of interest:

$$\ln F(k) = \sum_{n=0}^{\infty} A_n k^n. \tag{41}$$

The problem is, we don't know what the A_n coefficients are. To help us determine this, and since I already know the final answer, we define a new set of coefficients, C_n, related to A_n in the following way

$$A_n = \frac{(-i)^n}{n!} C_n \tag{42}$$

leading to

$$\ln F(k) = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} C_n \tag{43}$$

which makes our cumulant generating function look extremely similar in form to the moment generating function, eq. (37). In fact, this is taken as the definition of the cumulants; the cumulants are the C_n coefficients.

The cumulants thus arise from a series expansion of the *logarithm*. But we could also take the series expansion of $F(k)$, eq. (37), and insert this directly into the logarithm.

$$\ln\left(\sum_{n=0}^{\infty}\frac{(-ik)^n}{n!}\langle x^n\rangle\right) = \ln\left(1+\sum_{n=1}^{\infty}\frac{(-ik)^n}{n!}\langle x^n\rangle\right) \tag{44}$$

we can then use the following Taylor expansion

$$ln(1+\epsilon) = \sum_{n=1}^{\infty}(-1)^{n+1}\frac{\epsilon^n}{n} = \epsilon - \frac{\epsilon^2}{2} + \frac{\epsilon^3}{3} - ... \tag{45}$$

to find an expansion of $\ln F(k)$ in terms of moments. For clarity, here we are defining ϵ as

$$\epsilon = \sum_{n=1}^{\infty}\frac{(-ik)^n}{n!}\langle x^n\rangle.$$

We now have two different expansions of $\ln F(k)$: one in terms of the moments (45), the others in terms of the C_n coefficients (43). A subtlety to notice here is that since ϵ is a sum over k beginning at first order, by looking at equation (45) we see there cannot be any terms of zeroth order in $\ln F(k)$. This means we can change the index in eq. (43) to start at $n = 1$. We can now equate the two sums and use the old trick that coefficients of like powers must be the same to find a relation between the C_n coefficients and the moments. As mentioned earlier, the C_n coefficients are the cumulants, which we will now label as $C_n = \langle x^n\rangle_c$ for symmetry with the notation for moments.

The expansion in terms of moments can be rather tricky to carry out in practice, but it is instructive to show how this can be done to obtain the first few cumulants.

We'll start with the first cumulant $\langle x\rangle_c$. We can see from equation (43) that $\langle x\rangle_c$ is the coefficient of k. Therefore we need to find all the terms in the moment expansion that are first order in k. Clearly there is only one term since the ϵ^2 and higher terms will all begin with at least 2nd order. Thus we have that

$$-ik\langle x\rangle_c = -ik\langle x\rangle \rightarrow \langle x\rangle_c = \langle x\rangle \tag{46}$$

Similarly, for the second cumulant, we need only the terms that are second order in k and thus need only to consider the first two terms in eq. (45). From ϵ we have the term

$$-\frac{k^2}{2}\langle x^2\rangle.$$

From ϵ^2 we have,

$$-\frac{\epsilon^2}{2} = -\frac{1}{2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} -\frac{1}{2}\frac{(-ik)^n(-ik)^m}{n!m!}\langle x^n\rangle\langle x^m\rangle \tag{47}$$

and since the sums begin at one, the only second order term is

$$(-ik)(-ik)\langle x\rangle\langle x\rangle = \frac{k^2}{2}\langle x\rangle^2.$$

Putting this all together we arrive at

$$\frac{-k^2}{2}\langle x^2\rangle_c = \frac{-k^2}{2}\langle x^2\rangle + \frac{k^2}{2}\langle x\rangle^2$$

hence

$$\langle x^2\rangle_c = \langle x^2\rangle - \langle x\rangle^2. \tag{48}$$

We can also find the moments in terms of cumulants. Inserting eq. (46) into eq. (48) we can solve for the 2nd moment as

$$\langle x^2\rangle = \langle x^2\rangle_c + \langle x\rangle_c \tag{49}$$

The application to the Gaussian is particularly elegant for we have

$$\ln F(k) = -ik\mu - \frac{\sigma^2 k^2}{2} \tag{50}$$

which is conveniently already a series expansion in k, so we can immediately read off the cumulants:

$$\langle x\rangle_c = \mu \tag{51}$$

$$\langle x^2\rangle_c = \sigma^2 \tag{52}$$

and all higher cumulants vanish. And from this we can quickly obtain the first two moments using eqs. (46) and (49), which can easily be verified to agree with the moments derived previously.

3.2 Gaussians in Statistical Mechanics

The Gaussian comes up in statistical physics quite often. This is because distributions in statistical physics are often of the form $e^{\beta H}$ where H is the system's Hamiltonian and β is a proportionality constant with units of inverse energy. For a system of particles in no potential, the Hamiltonian takes the simple form $H = \sum_i p_i^2/2m$ and so the distribution becomes

$$p(p_i) = e^{\beta \sum_i p_i^2/2m}$$

which we can identify as a multivariate Gaussian over the variables p_i. Similarly, if the particles are in a harmonic oscillator potential, $U = \sum_i m\omega^2 x_i^2/2$, then we still have a Gaussian

$$p(p_i, x_i) = e^{\beta \sum_i p_i^2/2m + \beta \sum_i m\omega^2 x_i^2/2}$$

specifically, a multivariate Gaussian over the p_i's and x_i's. I am of course glossing over much of the details that go into deriving a distribution (such as the partition function), but the point is that harmonic oscillator potentials are very useful in statistical mechanics because it results in a Gaussian, which is to say, something that's tractable.

3.3 Gaussians in Quantum Mechanics

In quantum mechanics, quite often the time evolution operator takes the form

$$\hat{T}(t) = exp\,(i\beta Ht) \tag{53}$$

where t represents time, $\hat{H}$ is the Hamiltonian again, and now β has units of inverse energy multiplied by inverse time (e.g. $1/J \cdot s$). Here though $\hat{H}$ is an operator. Despite being an operator however, the Hamiltonian of a free particle is still quadratic in momentum. It takes the same form as in the statistical mechanics case described above, with p simply raised to the roll of an operator $\hat{p}$: $\hat{H} = \hat{p}^2/2m$ (note there is no subscript i because here we are talking about only 1 particle rather than many). So we see that for a free particle the time evolution operator is again a Gaussian. Similarly, raising x to the roll of an operator we can see also that in quantum mechanics a harmonic oscillator potential will produce a Gaussian.

The machinery built up for analyzing Gaussians also plays an excellent roll in wave packets. Suppose we have a wave function in a Gaussian state at some initial time t_0

$$\langle x|\psi\rangle = \psi(x, t_0) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-x^2/4\sigma_x^2} \tag{54}$$

This is actually the square root of the typical Gaussian form (30) since it is the square of the wave function that is a probability distribution. To see this we can check that this wave function is properly normalized:

$$\int dx|\psi|^2 = \int dx \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-x^2/2\sigma_x^2} = \frac{1}{\sqrt{2\pi\sigma_x^2}} \cdot \sqrt{\frac{\pi}{1/(2\sigma_x^2)}} = 1. \tag{55}$$

The wave packet's momentum representation, $\langle p|\psi\rangle$, can be found by inserting a complete set of position-space eigenstates:

$$\langle p|\psi\rangle = \tilde{\psi}(p) = \langle p| \left(\int dx|x\rangle\langle x| \right) |\psi\rangle = (2\pi\hbar)^{-1/2} \int dx e^{-ipx/\hbar} \langle x|\psi\rangle \tag{56}$$

where we have used the relation $\langle p|x\rangle = (2\pi\hbar)^{-1/2} e^{-ipx/\hbar}$. Notice that the momentum-space representation is a Fourier transform of the position-space representation! We know how to evaluate these using our old trick of completing the square:

$$\begin{aligned} \tilde{\psi}(p) &= (2\pi\hbar)^{-1/2} \int dx e^{-ipx/\hbar} \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-x^2/4\sigma_x^2} \\ &= \frac{(2\pi\hbar)^{-1/2}}{(2\pi\sigma_x^2)^{1/4}} \int dx \exp\left[\frac{-x^2}{4\sigma_x^2} - \frac{ip}{\hbar} x \right] \end{aligned} \tag{57}$$

So here $a = -1/4\sigma_x^2$ and $b = -ip/\hbar$ hence

$$\begin{aligned}
\tilde{\psi}(p) &= \frac{1}{(2^3\pi^3\hbar^2\sigma_x^2)^{1/4}} \int dx \exp\left[-\left(x + 2\sigma^2 ip/\hbar\right)^2 /4\sigma_x^2 - \sigma_x^2 p^2/\hbar^2\right] \\
&= \frac{1}{(2^3\pi^3\hbar^2\sigma_x^2)^{1/4}} e^{-\sigma_x^2 p^2/\hbar^2} \int dx' e^{-x'^2/4\sigma_x^2} \\
&= \frac{1}{(2^3\pi^3\hbar^2\sigma_x^2)^{1/4}} e^{-\sigma_x^2 p^2/\hbar^2} \sqrt{\frac{\pi}{1/(4\sigma_x^2)}} \\
&= \frac{\sqrt{4\pi\sigma_x^2}}{(2^3\pi^3\hbar^2\sigma_x^2)^{1/4}} e^{-\sigma_x^2 p^2/\hbar^2} = \left(\frac{2^4\pi^2\sigma_x^4}{2^3\pi^3\hbar^2\sigma_x^2}\right)^{1/4} e^{-\sigma_x^2 p^2/\hbar^2} \\
&= \left(\frac{2\sigma_x^2}{\pi\hbar^2}\right)^{1/4} e^{-\sigma_x^2 p^2/\hbar^2}
\end{aligned} \tag{58}$$

and by looking at the exponent, we can define a momentum-space variance such that $\sigma_x^2/\hbar^2 = 1/4\sigma_p^2$ which leads to $\sigma_p^2 = \hbar^2/4\sigma_x^2$ which let's us simplify our representation even further to

$$\langle p|\psi\rangle = \tilde{\psi}(p) = \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-p^2/4\sigma_p^2} \tag{59}$$

which is also a Gaussian as we would expect. Notice that the position and momentum uncertainties saturate the uncertainty relation

$$\sigma_x\sigma_p = \sigma_x\left(\frac{\hbar}{2\sigma_x}\right) = \frac{\hbar}{2}$$

which means a Gaussian wave packet is a minimum uncertainty state.

Our position-space wave packet (54) is centered at $x = 0$. What if we want a wave packet centered at some arbitrary position x_0? Then we simply apply the translation operator

$$T(x_0) = e^{-i\hat{p}x_0/\hbar} \tag{60}$$

If we applied this to the position-space wave function, T will be $\exp\left[-ix_0\hbar\frac{\partial}{\partial x}\right]$ which looks like a terrible time. In momentum-space however we have

$$\begin{aligned}
\langle p|\psi_{x=x_0}\rangle &= \langle p|T(x_0)|\psi_{x=0}\rangle \\
&= \langle p|e^{-i\hat{p}x_0/\hbar}\left(\int dp'|p'\rangle\langle p'|\right)|\psi_{x=0}\rangle \\
&= \int dp\, e^{-ip'x_0/\hbar}\langle p|p'\rangle\langle p'|\psi_{x=0}\rangle \\
&= \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-p^2/4\sigma_p^2 - ipx_0/\hbar}
\end{aligned} \tag{61}$$

and now we need only to Fourier transform this back into position space!

$$\begin{aligned}
\langle x|\psi_{x=x_0}\rangle &= \langle x|\left(\int dp\,|p\rangle\langle p|\right)|\psi_{x=x_0}\rangle \\
&= \frac{(2\pi\hbar)^{-1/2}}{(2\pi\sigma_p^2)^{1/4}}\int dp\, e^{ipx/\hbar}e^{-p^2/4\sigma_p^2-ipx_0/\hbar} \\
&= \frac{1}{(2^3\pi^3\hbar^2\sigma_p^2)^{1/4}}\int dp\, e^{-p^2/4\sigma_p^2+ip(x-x_0)/\hbar}
\end{aligned} \tag{62}$$

and now we complete the square with $a=-1/4\sigma_p^2$ and $b=i(x-x_0)/\hbar$ so

$$\begin{aligned}
\langle x|\psi_{x=x_0}\rangle &= \frac{1}{(2^3\pi^3\hbar^2\sigma_p^2)^{1/4}}\int dp\, e^{-(p-2i\sigma_p^2(x-x_0)/\hbar)/4\sigma_p^2-\sigma_p^2(x-x_0)^2/\hbar^2} \\
&= \frac{1}{(2^3\pi^3\hbar^2\sigma_p^2)^{1/4}}\int dp'\, e^{-p'^2/4\sigma_p^2-\sigma_p^2(x-x_0)^2/\hbar^2} \\
&= \frac{\sqrt{4\pi\sigma_p^2}}{(2^3\pi^3\hbar^2\sigma_p^2)^{1/4}}e^{-\sigma_p^2(x-x_0)^2/\hbar^2} = \left(\frac{2^4\pi^2\sigma_p^4}{2^3\pi^3\hbar^2\sigma_p^2}\right)^{1/4} e^{-\sigma_p^2(x-x_0)^2/\hbar^2} \\
&= \left(\frac{2\sigma_p^2}{\pi\hbar^2}\right)^{1/4} e^{-\sigma_p^2(x-x_0)^2/\hbar^2} \\
&= \frac{1}{(2\pi\sigma_x^2)^{1/4}}e^{-(x-x_0)^2/4\sigma_x^2}
\end{aligned} \tag{63}$$

And now we have a wave packet that has been shifted to x_0 in position space. The reader is encouraged to Fourier transform this wave packet to momentum space where it can be seen that this packet is still centered at[1] $p=0$. We must go through the same procedures again using now the momentum translation operator:

$$T_p(p_0) = e^{-ip_0\hat{x}/\hbar} \tag{64}$$

And fortuitously, this is most easily applied in the position space representation:

$$\begin{aligned}
\langle x|\psi_{x=x_0,p=p_0}\rangle &= \langle x|T_p(p_0)|\psi_{x=x_0}\rangle = \langle x|e^{-ip_0\hat{x}}\left(\int dx'\,|x'\rangle\langle x'|\right)|\psi_{x=x_0}\rangle \\
&= e^{-ip_0x}\langle x|\psi_{x=x_0}\rangle \\
&= \frac{1}{(2\pi\sigma_x^2)^{1/4}}e^{-(x-x_0)^2/4\sigma_x^2-ip_0x/\hbar}
\end{aligned} \tag{65}$$

We can now take the Fourier transform of this function to get the momentum representation! But let's not; for I fear the reader is at least equally as tired of

[1] The easy way to do this is to make the substitution $x'=x-x_0$ and then we can see this is the same as the wave packet before it was space translated. Hence, the Fourier transform after space translation is the same as the Fourier transform before space translation, and the latter we've already seen is a momentum wave packet centered at $p=0$.

doing so as the author is. We could just have easily gone through the preceding procedure starting instead with the momentum wave packet, first boosting to p_0 then x_0. Thanks to the symmetry between position and momentum, the result is simply the same as equation (65) but with x and p swapped. Thus we have the position and momentum representation of a Gaussian wave packet at arbitrary position and momentum as

$$\psi_{x_0,p_0}(x,t_0) = \frac{1}{(2\pi\sigma_x^2)^{1/4}} e^{-(x-x_0)^2/4\sigma_x^2 - ip_0 x/\hbar} \tag{66}$$

$$\psi_{x_0,p_0}(p,t_0) = \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-(p-p_0)^2/4\sigma_p^2 - ix_0 p/\hbar}. \tag{67}$$

Now we have the general form of a Gaussian wave packet at some intial time t_0, but we would like to understand how these packets evolve over time for a free particle. To this end we may apply the Schrödinger equation

$$H|\psi\rangle = \frac{\hat{p}^2}{2m}|\psi\rangle = -i\hbar\frac{\partial}{\partial t}|\psi\rangle \tag{68}$$

in either the momentum or position basis. Explicity the options look like:

$$= \int dx \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\psi(x,t)|x\rangle\right) = \int dx \left(i\hbar\frac{\partial}{\partial t}\psi(x,t)|x\rangle\right) \tag{69}$$

$$= \int dp \left(\frac{p^2}{2m}\tilde{\psi}(p,t)|p\rangle\right) = \int dp \left(i\hbar\frac{\partial}{\partial t}\tilde{\psi}(p,t)|p\rangle\right) \tag{70}$$

In both cases we can just project onto a particular position or momentum to get the equations of motion for the wave functions:

$$-\hbar^2\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \qquad \frac{p^2}{2m}\tilde{\psi}(p,t) = i\hbar\frac{\partial}{\partial t}\tilde{\psi}(p,t). \tag{71}$$

For a free particle, the second one is easier to solve. It has the solution:

$$\tilde{\psi}(p,t) = e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}\tilde{\psi}(p,t). \tag{72}$$

So time-evolving the general Gaussian wave packet gives us:

$$\tilde{\psi}_{x_0,p_0}(p,t) = \frac{1}{(2\pi\sigma_p^2)^{1/4}} e^{-(p-p_0)^2/4\sigma_p^2 - ipx_0/\hbar - \frac{i}{\hbar}\frac{p^2}{2m}t} \tag{73}$$