A Gaussian integral with a purely imaginary argument

The Gaussian integral,

$$\int_0^\infty e^{-ax^2}\,dx = \sqrt{\frac{\pi}{4a}}\,, \quad \text{Where } \operatorname{Re} a > 0\,, \tag{1}$$

is a well known result. Students first learn how to evaluate this integral in the case where a is a real, positive constant. It is not difficult to show that eq. (1) is valid for complex values of a in the case of $\operatorname{Re} a > 0$. Writing $a = a_R + ia_I$, where $a_R > 0$, it follows that

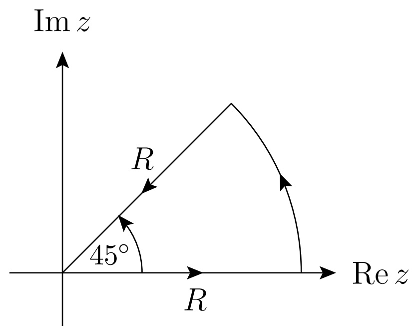
$$e^{-ax^2} = e^{-a_R x^2} e^{-ia_I x^2}\,.$$

The presence of the $e^{-a_R x^2}$ term guarantees that the integral given in eq. (1) converges, due to the exponential suppression of the integrand as $|x| \to \infty$.

In this note, I wish to evaluate the integral in eq. (1) in the case of an exponential function with a purely imaginary argument; i.e., $a_R = 0$. To treat this case, we shall first consider the following integral that is integrated over a closed contour C in the complex plane,

$$\oint_C e^{iaz^2}\,dz\,, \quad \text{where } a > 0 \text{ is a real constant}\,, \tag{2}$$

and the closed contour C is exhibited below.



Since there are no singularities in the region of the complex plane enclosed by C (and no singularities on the contour itself), we can use Cauchy's theorem to conclude that

$$\oint_C e^{iaz^2}\,dz = 0\,.$$

We can evaluate this integral in another way by considering three separate contributions,

$$\oint_C e^{iaz^2}\,dz = \int_0^R e^{iax^2}\,dx + \int_S e^{iaz^2}\,dz + \int_D e^{iaz^2}\,dz = 0\,, \tag{3}$$

where $z = x + iy$, S indicates the integral over the arc portion of the contour and D indicates the integral over the diagonal portion of the contour (in the direction indicated by the arrows).

Along D, we have $x = y$, where $x = r\cos(\pi/4)$ and $y = r\sin(\pi/4)$. That is, $z = re^{i\pi/4}$ and $dz = e^{i\pi/4}dr$. Hence,

$$\int_D e^{iaz^2}\,dz = e^{i\pi/4}\int_R^0 e^{ia(re^{i\pi/4})^2}\,dr = e^{i\pi/4}\int_R^0 e^{-ar^2}\,dr\,, \tag{4}$$

after using $e^{i\pi/2} = i$ in the argument of the exponent. Along S, $z = Re^{i\theta}$, with $0 \leq \theta \leq \pi/4$. Then $dz = iRe^{i\theta}\,d\theta$ and

$$\int_S e^{iaz^2}\,dz = \int_0^{\pi/4} e^{iaR^2(\cos 2\theta + i\sin 2\theta)}iRe^{i\theta}\,d\theta\,. \tag{5}$$

We shall now demonstrate that

$$\lim_{R\to\infty}\int_S e^{iaz^2}\,dz = 0\,. \tag{6}$$

First, we employ the generalization of the triangle inequality, $|a+b| \leq |a| + |b|$, to integrals,

$$\left|\int_a^b f(x)\,dx\right| \leq \int_a^b |f(x)|\,dx\,.$$

Applying this inequality to eq. (5), it follows that

$$\left|\int_S e^{iaz^2}\,dz\right| \leq R\int_0^{\pi/4} e^{-aR^2\sin 2\theta}\,d\theta\,.$$

Changing variables to $\alpha = 2\theta$, it follows that

$$\left|\int_S e^{iaz^2}\,dz\right| \leq \frac{R}{2}\int_0^{\pi/2} e^{-aR^2\sin\alpha}\,d\alpha\,. \tag{7}$$

To make further progress, we employ the following result, known as Jordan's inequality, which is established in Appendix A,

$$\frac{2\alpha}{\pi} \leq \sin\alpha \leq \alpha\,, \quad \text{for } 0 \leq \alpha \leq \tfrac{1}{2}\pi\,. \tag{8}$$

Using this result, eq. (7) yields

$$\left|\int_S e^{iaz^2}\,dz\right| \leq \frac{R}{2}\int_0^{\pi/2} e^{-aR^2\sin\alpha}\,d\alpha \leq \frac{R}{2}\int_0^{\pi/2} e^{-2aR^2\alpha/\pi}\,d\alpha \leq \frac{\pi}{4aR}\big(1 - e^{-aR^2}\big)\,.$$

Taking the $R \to \infty$ limit and recalling that $a > 0$, we end up with the result quoted in eq. (6).

In light of eq. (6), eqs. (3) and (4) yields

$$\int_0^\infty e^{iax^2}\,dx = -\lim_{R\to\infty}\int_D e^{iaz^2}\,dz = e^{i\pi/4}\int_0^\infty e^{-ar^2}\,dr = e^{i\pi/4}\sqrt{\frac{\pi}{4a}}\,, \tag{9}$$

where we have employed eq. (1) in the final step above.

It is amusing to note that if we interpret $i^{1/2} = e^{i\pi/4}$ (which implies that we are defining the complex square root function as its principal value on the first Riemann sheet), then, one can rewrite eq. (9) as

$$\int_0^\infty e^{iax^2}\,dx = \sqrt{\frac{i\pi}{4a}}\,. \tag{10}$$

Note that eq. (10) coincides with eq. (1) if a is replaced by $-ia$. That is, it appears that eq. (1) is valid even when $\operatorname{Re} a = 0$.[1]

Thus, we have established the formula,

$$\int_0^\infty e^{iax^2}\,dx = e^{i\pi/4}\sqrt{\frac{\pi}{4a}}\,, \quad \text{for } a > 0. \tag{11}$$

The corresponding result for $a < 0$ can be obtained simply by complex conjugating the above result,[2]

$$\int_0^\infty e^{-iax^2}\,dx = e^{-i\pi/4}\sqrt{\frac{\pi}{4a}}\,, \quad \text{for } a > 0. \tag{12}$$

Eqs. (11) and (12) can be combined into one formula,

$$\boxed{\int_0^\infty e^{iax^2}\,dx = e^{i\pi\,\mathrm{sgn}(a)/4}\sqrt{\frac{\pi}{4|a|}}\,, \quad \text{where } a \neq 0 \text{ is a real constant,}} \tag{13}$$

and the sign function is defined as $\mathrm{sgn}(a) = a/|a|$ for real $a \neq 0$. Taking the real and imaginary parts of eq. (13) yields the Fresnel integrals,

$$\int_0^\infty \sin(ax^2)\,dx = \mathrm{sgn}(a)\sqrt{\frac{\pi}{8|a|}}\,, \qquad \int_0^\infty \cos(ax^2)\,dx = \sqrt{\frac{\pi}{8|a|}}\,.$$

It is instructive to employ eq. (12) in evaluating the Fourier transform of e^{-iax^2},

$$F(k) = \int_{-\infty}^\infty e^{-iax^2} e^{-ikx}\,dx\,,$$

assuming that $a > 0$. By "completing the square," one can write

$$-i(ax^2 + kx) = -ia\left(x + \frac{k}{2a}\right)^2 + \frac{ik^2}{4a}\,.$$

Hence,

$$\int_{-\infty}^\infty e^{-iax^2} e^{-ikx}\,dx = e^{ik^2/(4a)}\int_{-\infty}^\infty \exp\left\{-ia\left(x + \frac{k}{2a}\right)^2\right\}dx\,.$$

Changing integration variables by defining $x' = x + k/(2a)$, it follows that

$$\int_{-\infty}^\infty e^{-iax^2} e^{-ikx}\,dx = e^{ik^2/(4a)}\int_{-\infty}^\infty e^{-iax'^2}\,dx' = 2e^{ik^2/(4a)}\int_0^\infty e^{-iax'^2}\,dx'\,,$$

[1] This conclusion is correct as long as one remembers to interpret $i^{1/2} = e^{i\pi/4}$ in eq. (10).

[2] One can also obtain eq. (12) by repeating the calculation of eq. (3), where the closed contour C is now located in the fourth quadrant of the complex plane with an arc that makes an angle of $-45°$.

where the final step makes use of the fact that the integrand is an even function of x. Using eq. (12), we arrive at the desired result,

$$F(k) = \int_{-\infty}^{\infty} e^{-iax^2} e^{-ikx}\, dx = \sqrt{\frac{\pi}{a}}\, e^{-i\pi/4}\, e^{ik^2/(4a)}\,, \quad \text{for real } a > 0. \tag{14}$$

Additional results can be obtained by differentiating eq. (14). For example,

$$i\frac{\partial F}{\partial k} = \int_{-\infty}^{\infty} x\, e^{-iax^2} e^{-ikx}\, dx\,. \tag{15}$$

It then follows that

$$\int_{-\infty}^{\infty} x\, e^{-iax^2} e^{-ikx}\, dx = -\frac{1}{2}\sqrt{\frac{\pi}{a^3}}\, e^{-i\pi/4}\, e^{ik^2/(4a)}\,, \quad \text{for real } a > 0. \tag{16}$$

Eq. (16) was employed in class in evaluating the free particle propagator in three dimensions.

It should be noted that strictly speaking, eq. (15) is false, which then casts doubt on the validity of eq. (16). One is permitted to compute $\partial F/\partial k$ by differentiating under the integral sign only if certain conditions are satisfied.[3] Unfortunately, eq. (15) does not satisfy the necessary conditions. Nevertheless, if we regard $e^{-iax^2}e^{ikx}$ as a generalized function (also called a distribution), then one can justify eq. (15) *in the sense of distributions*. An alternative (and ultimately equivalent) approach is to insert a convergence factor, $e^{-\varepsilon x^2}$, into the integrand of $F(k)$, where ε is a real positive infinitesimal quantity. In this case, one simply modifies eqs. (14)–(16) by replacing $a \to a - i\varepsilon$. Eq. (15) is then valid as long as $\varepsilon \neq 0$. At the end of the calculation, one takes $\varepsilon \to 0$ to recover eq. (16).

APPENDIX A: Proof of Jordan's inequality

In this appendix, we shall prove Jordan's inequality,

$$\frac{2x}{\pi} \leq \sin x \leq x\,, \quad \text{for } 0 \leq x \leq \tfrac{1}{2}\pi\,. \tag{17}$$

The simplest proof is a graphical one. Plot the following three functions in the x-y plane: (i) $y = x$; (ii) $y = \sin x$; and (iii) $y = 2x/\pi$ for values of $0 \leq x \leq \frac{1}{2}\pi$. It is easy to see that the the graph of $y = \sin x$ lies below the graph of $y = x$ over the entire range of $0 \leq x \leq \frac{1}{2}\pi$. Likewise, it is easy to see that the graph of $y = \sin x$ lies above the graph of $y = 2x/\pi$ over the same range. All three functions meet at $x = 0$ and the graphs of $y = \sin x$ and $y = 2x/\pi$ intersect again at $x = \frac{1}{2}\pi$. (I leave the explicit graphing of these three functions to the reader). Thus, eq. (17) is verified.[4]

[3] For a discussion of the precise conditions, see, e.g., p. 272 of T.W. Körner, *A Companion to Analysis* (American Mathematical Society, Providence, RI, 2004).

[4] More details on the graphical proof of eq. (17) can be found on pp. 43–45 of Debabrata Basu, *Introduction to Classical and Modern Analysis and their Application to Group Representation Theory* (World Scientific, Singapore, 2011).

For the more analytically minded student, here is another proof. First, we define a function,

$$f(x) = x - \sin x\,, \quad \text{for } 0 \leq x \leq \tfrac{1}{2}\pi\,.$$

Then, $f'(x) \equiv (df/dx) = 1 - \cos x \geq 0$. In particular, one achieves $f'(x) = 0$ at $x = 0$ in the x range of interest. Since $f(0) = 0$ and the slope of $f(x)$ is positive for $0 < x \leq \frac{1}{2}\pi$, it follows that $f(x) > 0$ for $0 < x \leq \frac{1}{2}\pi$. It then follows that $\sin x < x$ for $0 < x \leq \frac{1}{2}\pi$, with equality achieved only at $x = 0$.

Next, we consider a different function,

$$g(x) = \pi \sin x - 2x\,.$$

Computing the first and second derivatives,

$$g'(x) = \pi \cos x - 2\,, \qquad g''(x) = -\pi \sin x < 0\,, \text{ for } 0 < x \leq \tfrac{1}{2}\pi.$$

In particular, $g'(x)$ is decreasing as x increases from 0 to $\frac{1}{2}\pi$. Since $g'(0) = \pi - 2 > 0$ and $g'(\frac{1}{2}\pi) = -2$, there must exist some value of x (call it x_0) in the range $0 < x_0 < \frac{1}{2}\pi$ such that $g'(x_0) = 0$. It follows that $g(x)$ is an monotonically increasing function in the range $0 < x < x_0$ and $g(x)$ is a monotonically decreasing function for $x_0 < x < \frac{1}{2}\pi$. Since $g(0) = g(\frac{1}{2}\pi) = 0$, we can conclude that $g(x) > 0$ for $0 < x < \frac{1}{2}\pi$. That is,

$$g(x) = \pi \sin x - 2x > 0\,, \text{ for } 0 < x < \tfrac{1}{2}\pi,$$

with equality achieved only at the two endpoints $x = 0$ and $x = \frac{1}{2}\pi$. It therefore follows that $\sin x \geq 2x/\pi$ for $0 < x \leq \frac{1}{2}\pi$. The proof of eq. (17) is now complete.