

Integrals of complex variables

In this chapter we discuss several techniques for computing integrals on the complex plane.

1.1 Fourier Transform

One of the most frequent kind of complex integral is given by the *Fourier Transform* (FT). Let $f(x) \in L_2(\mathbb{R})$ be a square-integrable function. Then the Fourier transform maps $f(x)$ to another function $\tilde{f}(k)$ defined as follows:

Fourier transform

$$\mathcal{F}[f(x)](k) = \tilde{f}(k) \equiv \int_{\mathbb{R}} e^{-ikx} f(x) dx \quad f \in L_2(\mathbb{R}) \quad (1.1)$$

Similarly, it is possible to define the *inverse Fourier transform*, linking $\tilde{f}(k)$ back to $f(x)$:

Inverse Fourier transform

$$\mathcal{F}^{-1}[\tilde{f}(k)](x) = f(x) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{ikx} \tilde{f}(k) dk$$

The 2π factor is needed for normalization, so that:

$$\mathcal{F}^{-1}[\mathcal{F}[f(x)](k)](x) = f(x) \quad (1.2)$$

As long as (1.2) is satisfied, any different definition of the Fourier transforms is acceptable. For example, it is possible to *switch* the signs in the e^{ikx} , or split differently the normalization factor between \mathcal{F} and \mathcal{F}^{-1} .

Conventions

1.1.1 Refresher on functional analysis

The definition (1.1) is quite limited, as several interesting functions are not in $L_2(\mathbb{R})$ - for example $\sin(x)$, $\cos(x)$, $\theta(x)$. Fortunately, it is possible to extend the Fourier transform by considering *generalized functions* (**distributions**).

We start by defining a space $\mathcal{S}(\mathbb{R})$ (Schwartz space) containing all functions $\varphi \in$

Schwartz space

$C^\infty(\mathbb{R})$ that are *rapidly decreasing*, i.e. such that $\sup_{x \in \mathbb{R}} |x^\alpha \varphi^{(\beta)}(x)| < \infty \forall \alpha, \beta \in \mathbb{N}$. These are also called *test functions*.

Then a **tempered distribution** T is a **continuous linear** mapping $\mathcal{S}(\mathbb{R}) \rightarrow \mathbb{R}$. So it is possible to “apply” a distribution T to any test function $\varphi \in \mathcal{S}(\mathbb{R})$, resulting in a real number, denoted with $\langle T, \varphi \rangle$.

*Tempered
distributions*

The choice of \mathcal{S} is made expressly so that the Fourier transform is a linear and invertible operator on \mathcal{S} . However, other choices can be made for the space of test functions. For example, one can take the set \mathcal{D} of all functions with *compact support*, i.e. that vanish (along with all their derivatives) outside a compact region.

We can now see that distributions *generalize* the concept of function. We start by noting that any **locally integrable** function $f: \mathbb{R} \rightarrow \mathbb{R}$ can be used to define a distribution, by considering its inner product with a test function:

$$\langle T_f, \varphi \rangle \equiv \int_{\mathbb{R}} dx f(x) \varphi(x) \quad \forall \varphi \in \mathcal{S}(\mathbb{R}) \quad (1.3)$$

Distributions that can be defined like this are called **regular**.

In the **complex** case, where $f: \mathbb{R} \rightarrow \mathbb{C}$, we instead use the Hermitian inner product:

$$\langle T_f, \varphi \rangle = \int_{\mathbb{R}} dx f(x)^* \varphi(x)$$

where $f(x)^*$ is the complex conjugate of $f(x)$. The choice of the *position* of this conjugate (on the first or second entry) is a convention. Physicists tend to use the first position (due to Dirac notation), while mathematicians the second one.

Not all distributions are regular: in general, it is not possible to find a function $f(x)$ for a generic distribution T such that (1.3) is satisfied. The distributions for which this is not possible are called **singular**.

The simplest (and most important) singular distribution is the **Dirac Delta** $\delta(x)$, defined as follows:

$$\langle \delta, \varphi \rangle \equiv \varphi(0) \quad \varphi \in \mathcal{S}(\mathbb{R})$$

Dirac Delta

In other words, applying the δ to any test function φ returns the value of φ at 0. In practice, we often write *formally*:

$$\langle \delta, \varphi \rangle = \int_{\mathbb{R}} \delta(x) \varphi(x) dx$$

as if $\delta(x)$ were a function (but keep in mind that it isn't). This expression is often just a *shortcut* for quickly reaching useful results, as we will see in the following.

The point of defining *distributions* is that they provide a way to extend rigorously many operations that cannot be done on normal functions. One such example is

differentiation. Given a distribution T , its **distributional derivative** is defined as:

$$\langle T', \varphi \rangle \equiv -\langle T, \varphi' \rangle \quad \forall \varphi \in S(\mathbb{R}) \quad (1.4) \quad \text{Distributional derivative}$$

This is done so that, for a *regular* distribution T_f , that result comes from integration by parts:

$$\langle T'_f, \varphi \rangle = \int_{\mathbb{R}} f'(x) \varphi(x) dx = \left. \underline{f(x)\varphi(x)} \right|_{-\infty}^{+\infty} - \int_{\mathbb{R}} f(x) \varphi'(x) dx = -\langle T_f, \varphi' \rangle \quad (1.5)$$

For a singular distribution we use directly the definition (1.4), as the construction in (1.5) has no meaning (but still, sometimes we will write it nonetheless, as a merely *formal* expression).

In the distributional sense, it is possible to differentiate the **Heaviside function** $\theta(x)$:

$$\theta(x) \equiv \begin{cases} 1 & x > 0 \\ \frac{1}{2} & x = 0 \\ 0 & x < 0 \end{cases} \quad (1.6) \quad \text{Heaviside step function}$$

As $\theta(x)$ is locally integrable, we can define a corresponding distribution - that we denote with the same symbol θ . Then:

$$\begin{aligned} \langle \theta', \varphi \rangle &= -\langle \theta, \varphi' \rangle = -\int_{\mathbb{R}} \theta(x) \varphi'(x) dx = -\int_0^{+\infty} \varphi'(x) dx = -[\varphi(+\infty) - \varphi(0)] = \\ &= \varphi(0) = \langle \delta, \varphi \rangle \end{aligned} \quad (1.7)$$

So $\theta' = \delta$ in the *distributional sense* - i.e. applying θ' or δ to any test function φ leads to the same result.

1.1.2 Fourier transform of distributions

We are finally ready to extend the **Fourier Transform** to tempered distributions. In fact, $S(\mathbb{R})$ has been chosen¹ such that any $\varphi(x) \in S(\mathbb{R})$ has a well-defined transform $\tilde{\varphi}(k)$. Then we define the Fourier transform of a distribution as follows:

$$\langle \mathcal{F}[T], \varphi \rangle \equiv 2\pi \langle T, \mathcal{F}^{-1}[\varphi] \rangle \quad \text{Fourier Transform of distributions}$$

Again, this comes from the expression for regular distributions:

$$\begin{aligned} \langle \mathcal{F}[T_f], \varphi \rangle &= \int_{\mathbb{R}} dk \{ \mathcal{F}[f(x)](k) \}^* \varphi(k) = \int_{\mathbb{R}} dk \int_{\mathbb{R}} dx [e^{-ikx} f(x)]^* \varphi(k) = \\ &= \int_{\mathbb{R}} dx f(x) \int_{\mathbb{R}} dk e^{ikx} \varphi(k) = \int_{\mathbb{R}} 2\pi f(x) \mathcal{F}^{-1}[\varphi(k)](x) dx = 2\pi \langle T, \mathcal{F}^{-1}[\varphi] \rangle \end{aligned}$$

Note that:

$$\langle \mathcal{F}[T], \mathcal{F}[\varphi] \rangle = 2\pi \langle T, \mathcal{F}^{-1} \mathcal{F}[\varphi] \rangle = 2\pi \langle T, \varphi \rangle \quad (1.8)$$

¹More precisely, the Fourier transform is an *automorphism* of \mathcal{S} , i.e. it is linear and invertible

Delta transform

Finally, we can use all this machinery to compute Fourier transforms of some *generalized functions*. We start with the δ :

$$\langle \mathcal{F}[\delta], \varphi \rangle = 2\pi \langle \delta, \mathcal{F}^{-1}[\varphi] \rangle = 2\pi \mathcal{F}^{-1}[\varphi(x)](0)$$

where:

$$\mathcal{F}^{-1}[\varphi(x)](k) = \frac{1}{2\pi} \int_{\mathbb{R}} dx e^{ikx} \varphi(x) \Rightarrow 2\pi \mathcal{F}^{-1}[\varphi(x)](0) = \int_{\mathbb{R}} dx \varphi(x) = \langle 1, \varphi \rangle$$

And so $\mathcal{F}[\delta] = 1$.

Note that the same result could be obtained in a simpler way by treating δ as a “formal function”:

$$\mathcal{F}[\delta](k) = \int_{\mathbb{R}} e^{-ikx} \delta(x) dx = e^{-ik0} = 1$$

This leads to an equivalent definition for the δ “function”:

$$\delta(x) = \mathcal{F}^{-1}[1](x) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{ikx} dk$$

Also, note that:

$$\mathcal{F}[1](k) = \int_{\mathbb{R}} e^{-ikx} dx = \int_{\mathbb{R}} e^{ikx} dx = \textcolor{red}{2\pi} \left(\frac{1}{\textcolor{red}{2\pi}} \int_{\mathbb{R}} e^{ikx} dx \right) = 2\pi \delta(k) \quad (1.9)$$

Heaviside transform

We can use the result for the δ to aid the computation of $\mathcal{F}[\theta]$, where $\theta(x)$ is the regular distribution defined from (1.6). We have already seen in (1.7) that $\theta' = \delta$. So, we can use the formula for the Fourier transform of a derivative (which naturally generalizes to distributions):

$$\mathcal{F}[T'] = ik\tilde{T} \quad (1.10) \quad \text{Fourier transform of a derivative}$$

In our case:

$$\mathcal{F}[\theta'] \stackrel{(1.7)}{=} \mathcal{F}[\delta] = 1 = ik\tilde{\theta} \quad (1.11)$$

However, (1.11) cannot be used to reconstruct $\tilde{\theta}$ by itself, that is we cannot just “solve by $\tilde{\theta}$ ” and write:

$$\tilde{\theta}(k) = \frac{1}{ik} \quad (1.12)$$

In fact, consider a different $\theta^*(x) \equiv \theta(x) + c$, with $c \in \mathbb{R}$ constant. Their derivatives coincide, and so formula (1.11) would give the same result for both of them. However:

$$\mathcal{F}[\theta^*(x)](k) = \mathcal{F}[\theta(x)](k) + \mathcal{F}[c](k) = \tilde{\theta}(k) + c\delta(k) \neq \tilde{\theta}(k)$$

So we are missing a δ term, meaning that the correct Fourier transform should be:

$$\tilde{\theta}(k) = \mathcal{P}\left(\frac{1}{ik}\right) + c\delta(k) \quad (1.13)$$

Inversion formula

for some constant c . \mathcal{P} denotes the Cauchy principal value, which needs to be used to “fix” the singularity at $k = 0$ (see the following green boxes for the details).

There are several ways to fix c in (1.13). One of the quickest is to reason *with symmetries*.

Let f be an even function (i.e. a gaussian). Symmetry is preserved by the Fourier transform, and so:

1. Fix c
(symmetries)

$$\langle \tilde{\theta}, \tilde{f} \rangle = \mathcal{P} \int_{\mathbb{R}} \frac{1}{ik} \tilde{f}(k) dk + c \langle \delta, \tilde{f} \rangle = c \tilde{f}(0) = c \int_{\mathbb{R}} f(x) dx \quad (1.14)$$

The principal value vanishes because \tilde{f} is even (as f is even). The corresponding scalar product without the Fourier transforms is:

$$\langle \theta, f \rangle = \int_0^{+\infty} f(x) dx \stackrel{(a)}{=} \frac{1}{2} \int_{\mathbb{R}} f(x) dx \quad (1.15)$$

where in (a) we again used the symmetry of f . Then, recalling (1.8), we have:

$$\langle \tilde{\theta}, \tilde{f} \rangle = 2\pi \langle \theta, f \rangle \Rightarrow c \int_{\mathbb{R}} f(x) dx = \frac{2\pi}{2} \int_{\mathbb{R}} f(x) dx \Rightarrow c = \pi$$

(Note that c depends on the choice we made for the normalization in the Fourier transforms).

A similar argument can be made noting that $\theta(x)$ is just a scaled and shifted sgn function, which is odd:

2. Fix c with
symmetries and
sgn(x)

$$\theta(x) = \frac{1}{2} + \frac{1}{2} \text{sgn}(x) \quad \text{sgn}(x) = \begin{cases} 1 & x > 0 \\ 0 & x = 0 \\ -1 & x < 0 \end{cases}$$

By linearity we have:

$$\tilde{\theta}(k) = \mathcal{F}\left(\frac{1}{2}\right) + \frac{1}{2} \mathcal{F}[\text{sgn}(x)](k) \quad (1.16)$$

Noting that $\text{sgn}' = 2\delta$ and using (1.10) leads to:

$$2 = ik \mathcal{F}[\text{sgn}](k)$$

Inverting with (1.13), we have:

$$\mathcal{F}[\text{sgn}](k) = \mathcal{P}\left(\frac{2}{ik}\right) + c\delta(k) = \mathcal{P}\left(\frac{2}{ik}\right)$$

As this time c must be 0, otherwise $\mathcal{F}[\text{sgn}](k)$ wouldn't be odd (the δ is *even*). Substituting in (1.16) we have:

$$\tilde{\theta}(k) = \frac{1}{2} \underbrace{\mathcal{F}[1]}_{2\pi} + \frac{1}{2} \mathcal{P}\left(\frac{2}{ik}\right) = \mathcal{P}\left(\frac{1}{ik}\right) + \pi\delta(k)$$

Why is (1.12) wrong? There are two main reasons:

- $1/(ik)$ is not locally integrable (as it diverges for $k = 0$), so it cannot be used to define a distribution, such as $\tilde{\theta}$. This can be solved by using the *principal part* of $1/(ik)$ instead.
- The most general solution to the equation $xT = 1$, where T is a tempered distribution, is not just $T = \mathcal{P}(1/x)$, but:

$$T = \mathcal{P}\left(\frac{1}{x}\right) + c\delta$$

for some constant $c \in \mathbb{R}$.

First, to be precise, the product of a function, such as $f(x) = x$, with a distribution T is *defined* as the following distribution:

$$\langle f(x)T, \varphi \rangle \equiv \langle T, f(x)\varphi \rangle \quad (1.17)$$

where $f(x)$ must be such that $f(x)\varphi \in \mathcal{S} \forall \varphi \in \mathcal{S}$, which is indeed the case for any polynomial.

Now consider the *distributional* equation $xT = 1$. If we apply *both sides* to some test function φ , we have:

$$\langle T, x\varphi \rangle = \langle 1, \varphi \rangle = \int_{\mathbb{R}} \varphi(x) dx \quad (1.18)$$

The problem of *finding* T satisfying (1.18) is called the (distributional) **division problem**. To solve it, we want to reduce the equation to something in the form of $xT' = 0$, that can then be solved. So we rewrite the rhs as follows:

$$\int_{\mathbb{R}} \varphi(x) dx = \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R} \setminus [-\epsilon, \epsilon]} \varphi(x) dx = \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R} \setminus [-\epsilon, \epsilon]} \frac{x\varphi(x)}{x} dx$$

Then we define the **principal value distribution** $\mathcal{P}(1/x)$ as:

$$\langle \mathcal{P}\left(\frac{1}{x}\right), \varphi \rangle = \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R} \setminus [-\epsilon, \epsilon]} \frac{\varphi(x)}{x} dx$$

so that:

$$\int_{\mathbb{R}} \varphi(x) dx = \langle \mathcal{P}\left(\frac{1}{x}\right), x\varphi \rangle$$

Substituting back in (1.18) and rearranging we get:

$$\langle T, x\varphi \rangle = \langle \mathcal{P}\left(\frac{1}{x}\right), x\varphi \rangle \Rightarrow \langle T - \mathcal{P}\left(\frac{1}{x}\right), x\varphi \rangle = 0 \stackrel{(1.17)}{\Rightarrow} x \left[T - \mathcal{P}\left(\frac{1}{x}\right) \right] = 0$$

All that's left is to solve:

$$xT' = 0 \quad (1.19)$$

with $T' = T - \mathcal{P}(1/x)$. We will now see that the general solution of (1.19) is $T = c\delta$, for some constant c . This leads to:

$$T' = T - \mathcal{P}\left(\frac{1}{x}\right) = c\delta \Rightarrow T = \mathcal{P}\left(\frac{1}{x}\right) + c\delta$$

which indeed confirms (1.13).

So, let's see why $T' = c\delta$. In the following, we drop the $'$ for simplicity. First, we note that any test function $\varphi(x)$ can be written as:

$$\varphi(x) = \varphi(0) + x\psi(x)$$

for some $\psi(x) \in \mathcal{S}(\mathbb{R})$. Explicitly:

$$\begin{aligned} \varphi(x) &= \varphi(0) + \int_0^x \varphi'(t) dt \underset{u=\frac{t}{x}}{=} \varphi(0) + \int_0^1 x\varphi'(xu) du = \\ &= \varphi(0) + x \underbrace{\int_0^1 \varphi'(xu) du}_{\psi(x)} = \varphi(0) + x\psi(x) \end{aligned} \quad (1.20)$$

Note that if $\varphi(0) = 0$, then $\varphi(x) = x\psi(x)$.

Now, $xT = 0$ means that:

$$\langle xT, \varphi \rangle = 0 \quad \forall \varphi \in \mathcal{S}(\mathbb{R}) \quad (1.21)$$

To see what T is, we evaluate it on a test function $\varphi(x)$. The idea is to write $\varphi(x)$ as a sum of two test functions $a(x)$ and $b(x)$, choosing $b(x)$ so that it vanishes at 0, meaning that we can factor a x from it (1.20), and then use $\langle T, xb \rangle = \langle xT, b \rangle = 0$ (1.21).

Note that we can't just directly use (1.20), because while $x\psi(x)$ is indeed a test function, $\varphi(0) \notin \mathcal{S}(\mathbb{R})$ (it is a constant value, so it doesn't vanish for $x \rightarrow \infty$). So, the following is ill-defined:

$$\langle T, \varphi \rangle = \underbrace{\langle T, \varphi(0) \rangle}_{?} + \underbrace{\langle T, x\psi(x) \rangle}_0$$

as $\langle T, \varphi(0) \rangle$ can't be done, because distributions act *only* on elements of $\mathcal{S}(\mathbb{R})$.

The idea is to *convert* $\varphi(0)$ to a test function by multiplying it with another test function $\chi(x) \in \mathcal{S}(\mathbb{R})$, that we choose (for simplicity) so that $\chi(0) = 1$. Then we

write $\varphi(x)$ as:

$$\begin{aligned}\varphi(x) &= \varphi(x) + \varphi(0)\chi(x) - \varphi(0)\chi(x) = \\ &= \underbrace{\varphi(0)\chi(x)}_{a(x)} + \underbrace{[\varphi(x) - \varphi(0)\chi(x)]}_{b(x)}\end{aligned}$$

Note that now $a(x) \in \mathcal{S}(\mathbb{R})$, meaning that $\langle T, a \rangle$ is properly defined. Moreover, as we chose $\chi(0) = 1$, $b(x)$ is a test function that vanishes at 0:

$$b(0) = \varphi(0) - \varphi(0)\chi(0) = \varphi(0) - \varphi(0) = 0$$

And so we can use (1.20) to write $b(x) = x\psi(x)$ for some $\psi(x) \in \mathcal{S}(\mathbb{R})$. Finally, we are able to apply T to $\varphi(x)$:

$$\begin{aligned}\langle T, \varphi \rangle &= \langle T, \varphi(0)\chi + x\psi \rangle = \\ &= \varphi(0) \underbrace{\langle T, \chi \rangle}_c + \underbrace{\langle xT, \psi \rangle}_0 = \\ &= c\varphi(0) = \langle c\delta, \varphi \rangle\end{aligned}$$

where we denoted with c the result of $\langle T, \chi \rangle$. This proves that the general solution is indeed $T = c\delta$.

Some references on these derivations can be found in:

- <https://see.stanford.edu/materials/lsoftae261/book-fall-07.pdf>
- <https://math.stackexchange.com/questions/678457/distribution-solution-to-xt-0-in-schwartz-space>
- <https://math.stackexchange.com/questions/2962209/solve-the-distribution-equation-xt-1>

Explicit computation. It is also possible to compute $\tilde{\theta}$ *directly*, at the cost of a longer derivation. The idea is to use a *limit representation* $\theta_\epsilon(x)$ for $\theta(x)$, so that $\theta_\epsilon(x)$ has the same discontinuity of $\theta(x)$ at $x = 0$, and $\lim_{\epsilon \rightarrow 0^+} \theta_\epsilon(x) = \theta(x)$. One possible choice is:

$$\theta_\epsilon(x) = \begin{cases} e^{-\epsilon x} & x > 0 \\ 0 & x < 0 \end{cases}$$

When $\epsilon \rightarrow 0^+$, $e^{-\epsilon x} \rightarrow 1$, reconstructing the Heaviside function. So:

$$\begin{aligned}\tilde{\theta}(k) &= \int_{\mathbb{R}} \theta(x) e^{-ikx} dx = \lim_{\epsilon \rightarrow 0^+} \int_0^{+\infty} e^{-\epsilon x} e^{-ikx} dx = \lim_{\epsilon \rightarrow 0^+} -\frac{1}{\epsilon + ik} [e^{-\infty} - 1] = \\ &= \lim_{\epsilon \rightarrow 0^+} \frac{1}{\epsilon + ik} \frac{-i^2}{-i^2} = \lim_{\epsilon \rightarrow 0^+} \frac{-i}{k - i\epsilon}\end{aligned}$$

To manipulate this expression we need to treat it in the context of distributions, meaning that we need to apply it to a test function $\varphi(x)$ and see what happens:

$$\begin{aligned}\langle \tilde{\theta}, \varphi \rangle &= \int_{\mathbb{R}} \tilde{\theta}(k) \varphi(k) dk = \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}} \frac{-i}{k - i\epsilon} \frac{k + i\epsilon}{k + i\epsilon} \varphi(k) dk = \\ &= -i \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}} \frac{k + i\epsilon}{k^2 + \epsilon^2} \varphi(k) dk = \\ &\stackrel{(a)}{=} -i \left[\lim_{\epsilon \rightarrow 0^+} \underbrace{\int_{\mathbb{R}} \frac{k}{k^2 + \epsilon^2} \varphi(k) dk}_{A(\epsilon)} + i \lim_{\epsilon \rightarrow 0^+} \underbrace{\int_{\mathbb{R}} \frac{\epsilon}{k^2 + \epsilon^2} \varphi(k) dk}_{B(\epsilon)} \right]\end{aligned}$$

where in (a) we split the real and imaginary part. We then examine each of them separately:

$$\begin{aligned}A(\epsilon) &= \int_{\mathbb{R}} \frac{k}{k^2 + \epsilon^2} \varphi(k) dk = \int_{\mathbb{R}} \left(\frac{d}{dk} \frac{1}{2} \ln(k^2 + \epsilon^2) \right) \varphi(k) dk = \\ &\stackrel{(b)}{=} \cancel{a\varphi} \Big|_{\mathbb{R}} - \frac{1}{2} \int_{\mathbb{R}} \ln(k^2 + \epsilon^2) \varphi'(k) dk \\ &\xrightarrow{\epsilon \rightarrow 0^+} -\frac{1}{2} \int_{\mathbb{R}} \underbrace{\ln(k^2)}_{2 \ln |k|} \varphi'(k) dk = - \int_{\mathbb{R}} \ln |k| \varphi'(k) dk\end{aligned}$$

$$\begin{aligned}B(\epsilon) &= \int_{\mathbb{R}} \frac{\epsilon}{k^2 + \epsilon^2} \varphi(k) dk = \int_{\mathbb{R}} \frac{1}{\epsilon} \frac{1}{1 + \frac{k^2}{\epsilon^2}} \varphi(k) dk = \\ &= \int_{\mathbb{R}} \left[\frac{d}{dk} \arctan \left(\frac{k}{\epsilon} \right) \right] \varphi(k) dk = \\ &\stackrel{(c)}{=} \cancel{b\varphi} \Big|_{\mathbb{R}} - \int_{\mathbb{R}} \arctan \left(\frac{k}{\epsilon} \right) \varphi'(k) dk \\ &\xrightarrow{\epsilon \rightarrow 0^+} - \int_0^{+\infty} \frac{\pi}{2} \varphi'(k) dk - \int_{-\infty}^0 \left(-\frac{\pi}{2} \right) \varphi'(k) dk = \\ &= -\frac{\pi}{2} \int_{\mathbb{R}} \text{sgn}(k) \varphi'(k) dk \stackrel{(d)}{=} \frac{\pi}{2} \int_{\mathbb{R}} \underbrace{\text{sgn}'(k)}_{\mathcal{J}\delta(k)} \varphi(k) dk\end{aligned}$$

where in (b), (c) and (d) we performed integrations by parts. Then we note that:

$$\lim_{\epsilon \rightarrow 0^+} \langle B(\epsilon), \varphi \rangle = \pi \langle \delta, \varphi \rangle$$

$$\lim_{\epsilon \rightarrow 0^+} A(\epsilon) = - \int_{\mathbb{R}} \ln |k| \varphi'(k) dk \stackrel{(e)}{=} \mathcal{P} \int_{\mathbb{R}} \frac{1}{k} \varphi(k) dk$$

with a final integration by parts in (e). Putting it all together we arrive at the desired result:

$$\tilde{\theta}(k) = -i\mathcal{P}\left(\frac{1}{k}\right) + \pi\delta(k) = \mathcal{P}\left(\frac{1}{ik}\right) + \pi\delta(k)$$

Reference: <https://math.stackexchange.com/questions/269809/heaviside-step-function-fourier-transform-and-principal-values>

1.2 Fresnel integral

An important complex integral, appearing for example in the Schrödinger equation, is the Fresnel integral:

$$I(a, b) \equiv \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \exp(-iak^2 - ibk) = \frac{1}{\sqrt{4\pi ai}} \exp\left(\frac{ib^2}{4a}\right)$$

It is similar to a Gaussian integral, but with complex mean and variance.

To compute it, the idea is to *rotate it* so that it is not entirely along the imaginary axis. Explicitly, we rewrite the i multiplying the a in the exponential argument as:

$$i = \exp\left(i\frac{\pi}{2}\right)$$

And then we subtract an angle ϵ , and consider the limit $\epsilon \rightarrow 0^+$:

$$i = \lim_{\epsilon \rightarrow 0^+} \exp\left[i\left(\frac{\pi}{2} - \epsilon\right)\right]$$

Then, we evaluate the integral over one segment $[-R, R]$ of the real line, and take the limit $R \rightarrow \infty$:

$$I(a, b) = \lim_{\epsilon \rightarrow 0^+} I_{\epsilon}(a, b)$$

$$I_{\epsilon}(a, b) = \lim_{R \rightarrow \infty} \int_{-R}^{+R} \frac{dk}{2\pi} \exp\left(- \underbrace{a k^2 \exp\left[i\left(\frac{\pi}{2} - \epsilon\right)\right]}_{z^2} - ibk\right) \quad a, b \in \mathbb{R}$$

“Regularized”
Fresnel integral

Suppose that $a > 0$. We make the change of variables:

$$z^2 \equiv k^2 \exp\left[i\left(\frac{\pi}{2} - \epsilon\right)\right] \Rightarrow z = k \exp\left[i \underbrace{\left(\frac{\pi}{4} - \frac{\epsilon}{2}\right)}_{\phi_{\epsilon}}\right] = k e^{i\phi_{\epsilon}} \Rightarrow k = z e^{-i\phi_{\epsilon}}$$

1. Change of
variables

And $dk = dz e^{-i\phi_\epsilon}$. Note that:

$$\phi_\epsilon < \frac{\pi}{4} \quad (1.22)$$

definitely when $\epsilon \rightarrow 0^+$.

This change of variables has removed the i multiplying the z^2 , meaning that now we have a “standard” Gaussian integral. However, the integration path is now $\gamma_R = \{|z| \leq R, \arg z = \phi_\epsilon\}$, i.e. a segment of length $2R$, centred at the origin and forming an angle ϕ_ϵ with the real line. So the integral becomes:

$$\begin{aligned} I_\epsilon(a, b) &= \lim_{R \rightarrow \infty} \int_{\gamma_R} \frac{dz}{2\pi} e^{-i\phi_\epsilon} \exp\left(-az^2 - iz \underbrace{be^{-i\phi_\epsilon}}_{b'}\right) \quad b' = be^{-i\phi_\epsilon} \\ &= \lim_{R \rightarrow \infty} \int_{\gamma_R} \frac{dz}{2\pi} e^{-i\phi_\epsilon} \exp(-az^2 - ib'z) \end{aligned}$$

We want to *relate* this integral to its version *on the real line*, that we know how to compute. To do this, as always, we *close* the path of integration and use the Cauchy integral theorem, following the schema in fig. 1.1.

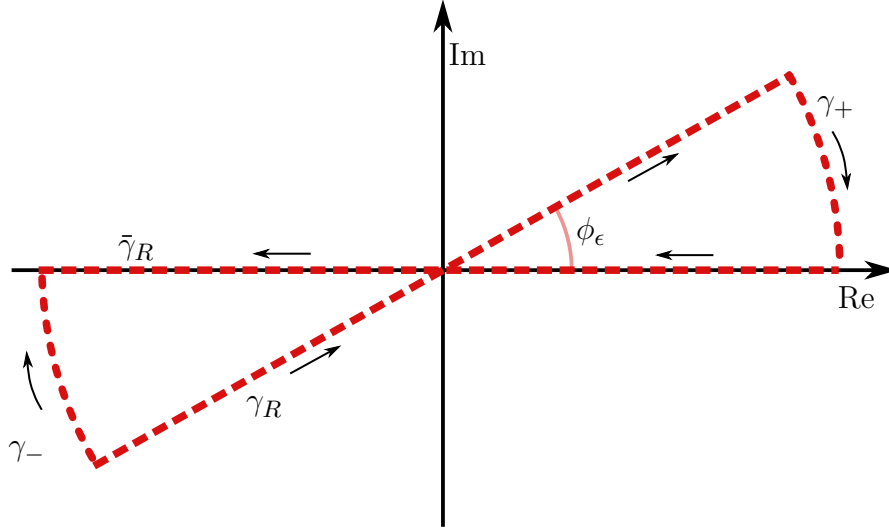


Figure (1.1) – Integration path for the Fresnel integral

Explicitly, consider the closed curve Γ_R defined by:

$$\Gamma_R = \gamma_R + \gamma_+ + \bar{\gamma}_R + \gamma_-$$

where:

$$\begin{aligned} \gamma_+ &= \{z = Re^{i\theta} : \theta \in [0, \phi_\epsilon]\} \\ \gamma_- &= \{z = Re^{i\theta} : \theta \in [\pi, \pi + \phi_\epsilon]\} \\ \gamma_R &= \{|z| \leq R, \arg z = \phi_\epsilon\} \\ \bar{\gamma}_R &= [-R, R] \end{aligned}$$

2. Contour
integration

As the integrand has no poles inside Γ_R , we have:

$$\lim_{R \rightarrow \infty} \int_{\Gamma_R} \frac{dz}{2\pi} e^{-i\phi_\epsilon} \exp(-az^2 - ib'z) = 0$$

Moreover, the integral over γ_+ and γ_- vanish. We show this explicitly only for the γ_+ case:

3. Integrals over γ_\pm vanish

$$\left| \int_{\gamma_+} \frac{dz}{2\pi} e^{-i\phi_\epsilon} \exp(-az^2 - ibze^{-i\phi_\epsilon}) \right| \quad (1.23)$$

We use the parameterization of γ_+ to change variables:

$$z = Re^{i\theta} \Rightarrow dz = iRe^{i\theta} d\theta$$

leading to:

$$\begin{aligned} (1.23) &= \left| \int_0^{\phi_\epsilon} \frac{d\theta}{2\pi} iRe^{i\theta} e^{-i\phi_\epsilon} \exp(-aR^2 e^{2i\theta} - ibRe^{i\theta} e^{-i\phi_\epsilon}) \right| = \\ &= \underbrace{\left| \frac{iR}{2\pi} e^{-i\phi_\epsilon} \right|}_{R/(2\pi)} \left| \int_0^{\phi_\epsilon} d\theta e^{i\theta} \exp(-aR^2 e^{2i\theta} - ibRe^{i(\theta-\phi_\epsilon)}) \right| \leq \\ &\leq \frac{R}{2\pi} \int_0^{\phi_\epsilon} d\theta \left| \exp(i\theta - aR^2 e^{2i\theta} - ibRe^{i(\theta-\phi_\epsilon)}) \right| = \\ &= \frac{R}{2\pi} \int_0^{\phi_\epsilon} d\theta \underbrace{|e^{i\theta}|}_1 |e^{-aR^2(\cos 2\theta + i \sin 2\theta)}| |e^{-ibR(\cos(\theta-\phi_\epsilon) + i \sin(\theta-\phi_\epsilon))}| = \\ &= \frac{R}{2\pi} \int_0^{\phi_\epsilon} d\theta e^{-aR^2 \cos 2\theta + Rb \sin(\theta-\phi_\epsilon)} \xrightarrow{R \rightarrow \infty} 0 \end{aligned}$$

As the integral is over θ in $[0, \phi_\epsilon]$, we have:

$$0 < \theta < \phi_\epsilon \underbrace{\leq \frac{\pi}{4}}_{(1.22)} \Rightarrow 0 < 2\theta < \frac{\pi}{2} \Rightarrow \cos(2\theta) > 0$$

So, as we assumed $a > 0$, the integrand decays exponentially fast when $R \rightarrow \infty$, making the integral vanish.

Finally, as the integral over γ_+ and γ_- vanish, then:

$$I_{\gamma_R} + I_{\bar{\gamma}_R} = 0 \Rightarrow I_{\gamma_R} = -I_{\bar{\gamma}_R}$$

where $I_{\bar{\gamma}_R}$ is the integral over the real line, that we can compute:

4. Integral over the real line

$$\begin{aligned} I_{\gamma_R} &= - \int_{-R}^R \frac{dz}{2\pi} e^{-i\phi_\epsilon} \exp(-az^2 - ib'z) \xrightarrow{R \rightarrow \infty} \frac{e^{-i\phi_\epsilon}}{2\pi} \sqrt{\frac{\pi}{a}} \exp\left(-\frac{(b')^2}{4a}\right) = \\ &= \frac{1}{\sqrt{4\pi a}} e^{-i\phi_\epsilon} \exp\left(-\frac{(b')^2}{4a}\right) \end{aligned}$$

Inserting back $b' = be^{-i\phi_\epsilon}$, and taking the limit $\epsilon \rightarrow 0^+$, we have:

$$\phi_\epsilon \xrightarrow{\epsilon \rightarrow 0^+} \frac{\pi}{4} \Rightarrow e^{-i\phi_\epsilon} \xrightarrow{\epsilon \rightarrow 0^+} \frac{1}{\sqrt{i}} \Rightarrow b' \xrightarrow{\epsilon \rightarrow 0^+} \frac{b}{\sqrt{i}}$$

and $(b')^2 \rightarrow -ib^2$, so that:

$$I(a, b) = \frac{1}{\sqrt{4\pi ai}} \exp\left(\frac{ib^2}{4a}\right)$$

which is the desired result.

For $a < 0$, observe that $I(a, b) = I^*(-a, -b)$, with $-ia = (ia)^*$ and $b^2 = (b^2)^*$, and the same result follows.

1.2.1 Schrödinger Equation

A possible application of the Fresnel integration is solving the Schrödinger equation for a *free* particle:

Example of application

$$i\hbar\partial_t\psi(x, t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x, t) \quad (1.24)$$

In the following, we will take $\hbar = 1$ for simplicity. Note that (1.24) is very similar to the diffusion equation, and in fact we can solve it in the same way, by applying a Fourier transform to both sides:

$$\begin{aligned} i\partial_t\tilde{\psi}(p, t) &\stackrel{(a)}{=} -\frac{1}{2m} \int_{\mathbb{R}} dx \partial_x^2\psi(x, t)e^{-ixp} = \\ &= \frac{p^2}{2m} \underbrace{\int_{\mathbb{R}} dx \psi(x, t)e^{-ipx}}_{\tilde{\psi}(p, t)} = \frac{p^2}{2m} \tilde{\psi}(p, t) \end{aligned}$$

where in (a) we performed two integrations by parts, using the fact that $\psi(x, t)$ vanishes at infinity to remove the boundary terms.

We are left with a first order ODE that can be solved by separation of variables:

$$i\partial_t\tilde{\psi} = \frac{p^2}{2m}\tilde{\psi} \Rightarrow \frac{d\tilde{\psi}}{\tilde{\psi}} = -i\frac{p^2}{2m} dt = -\frac{ip^2}{2m} dt \Rightarrow \tilde{\psi}(p, t) = \tilde{\psi}(p, 0) \exp\left(-\frac{ip^2 t}{2m}\right)$$

If we assume the particle to be initially localized at $x = 0$, meaning that $\psi(x, 0) = \delta(x)$, we have $\tilde{\psi}(p, 0) = 1$, and so:

$$\tilde{\psi}(p, t) = \exp\left(-i\frac{p^2 t}{2m}\right)$$

All that's left is to “go back to *position* space” with an inverse Fourier transform, which involves a Fresnel integral:

$$\psi(x, t) = \frac{1}{2\pi} \int_{\mathbb{R}} dp \exp\left(-\frac{ip^2 t}{2m}\right) e^{ipx} = \frac{1}{\sqrt{4\pi ai}} \exp\left(\frac{ib^2}{4a}\right)$$

with $a = t/(2m)$ and $b = -x$, leading to:

$$\psi(x, t) = \sqrt{\frac{m}{2\pi i t}} \exp\left(-\frac{mx^2}{2it}\right)$$

To reinsert \hbar we substitute $t \rightarrow t\hbar$:

$$\psi(x, t) = \sqrt{\frac{m}{2\pi\hbar i t}} \exp\left(-\frac{mx^2}{2\hbar i t}\right)$$

This is the Schrödinger **propagator** for a one-dimensional free particle.

1.3 Indented Integrals

Sometimes it is needed to compute integrals with *singularities* on the path of integration. Note that this integrals *do not exist*, meaning that there is not a unique way to compute them. Nonetheless, there are several *rules* (or *prescriptions*) that can be used to assign some result (possibly of physical significance) to these integrals.

Compute integrals that do not exist

Consider, for example, an analytic function $f(z)$, and the following integral:

$$I = \int_{\mathbb{R}} dx \frac{f(x)}{x - x_0}$$

The integrand has a pole at x_0 , which lies in the path of integration. So I does not exist. However, we could integrate “symmetrically”, hoping that the diverging term from one side “cancels” with the one from the other. This is the gist of the **Cauchy Principal Value**:

1. Symmetrical integration

$$\mathcal{P} \int_{\mathbb{R}} dx \frac{f(x)}{x - x_0} = \lim_{\delta \rightarrow 0} \left[\int_{-\infty}^{x_0 - \delta} \frac{f(x)}{x - x_0} dx + \int_{x_0 + \delta}^{\infty} \frac{f(x)}{x - x_0} dx \right]$$

Cauchy Principal Value

For example, this works for $f(x) = 1/x^2$ and $x_0 = 0$:

$$\mathcal{P} \int_{\mathbb{R}} \frac{1}{x^3} dx = \lim_{\delta \rightarrow 0} \left[\int_{-\infty}^{-\delta} \frac{1}{x^3} dx + \int_{\delta}^{\infty} \frac{1}{x^3} dx \right] \stackrel{(a)}{=} \lim_{\delta \rightarrow 0} 0 = 0$$

where in (a) we used the *symmetry* of $1/x^3$ to cancel the two integrals.

Another possibility is to *deform* the integration path from the real line to a curve γ_ϵ that avoids the singularity, as can be seen in the bottom half of fig. 1.2. Doing so produces a *different* result from the one of the Cauchy Principal Value, because now we are accounting for half a small circle $C_\epsilon = \{z = x_0 + \epsilon e^{i\theta} : \theta \in [-\pi, 0]\}$ around the singularity:

2. Path deformation

$$\lim_{\epsilon \rightarrow 0} \int_{\gamma_\epsilon} \frac{f(x)}{x - x_0} dx = \mathcal{P} \int_{\mathbb{R}} \frac{f(x)}{x - x_0} dx + \lim_{\epsilon \rightarrow 0} \int_{C_\epsilon} \frac{f(x)}{x - x_0} dx \quad (1.25)$$

And the difference amounts to:

$$\lim_{\epsilon \rightarrow 0} \int_{C_\epsilon} dz \frac{f(z)}{z - a} \stackrel{(a)}{=} \lim_{\epsilon \rightarrow 0} \int_{-\pi}^0 d\theta (i\epsilon e^{i\theta}) \frac{f(x_0 + \epsilon e^{i\theta})}{\epsilon e^{i\theta}} = i \lim_{\epsilon \rightarrow 0} d\theta f(x_0 + \epsilon e^{i\theta}) = i\pi f(x_0)$$

where in (a) we changed variables using the parameterization of C_ϵ .

Integrating over γ_ϵ that passes *to the right* of the singularity is equivalent to not deforming at all the integration path and moving the singularity “up” instead, as can be seen in fig. 1.2. This is the idea of the **prescription $\pm i\epsilon$** :

3. Moving the singularity

$$\int_{\mathbb{R}} dx \frac{f(x)}{x - (x_0 + i\epsilon)} = \int_{\gamma_\epsilon} dx \frac{f(x)}{x - x_0} = \mathcal{P} \int_{\mathbb{R}} \frac{f(x)}{x - x_0} dx + i\pi f(x_0)$$

Equivalently, it is possible to show that integrating over a path γ_ϵ^- that passes *to the left* of the singularity equates to moving the singularity “down”:

$$\int_{\mathbb{R}} dx \frac{f(x)}{x - (x_0 - i\epsilon)} = \int_{\gamma_\epsilon^-} dx \frac{f(x)}{x - x_0} = \mathcal{P} \int_{\mathbb{R}} \frac{f(x)}{x - x_0} dx - i\pi f(x_0)$$

We can summarize these facts as an equation between *operators*:

$$\lim_{\epsilon \rightarrow 0} \frac{1}{x - x_0 \mp i\epsilon} = \mathcal{P} \frac{1}{x - x_0} \mp i\pi \delta(x - x_0)$$

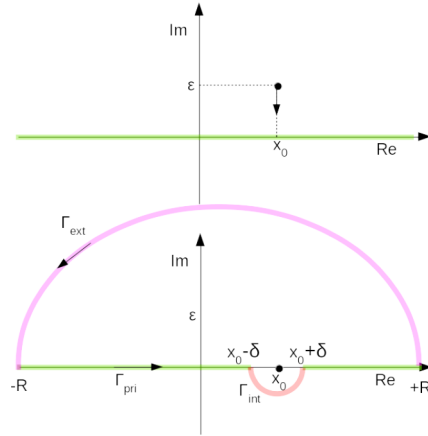


Figure (1.2) – Integration path for an indented integral