Tutorial for Theoretical Optics SS 2022

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1 Dispersive medium

In the lecture, we discussed how material properties like nonlinearity, anisotropy, inhomogeneity, and a dispersion, can be described in Maxwell's equations. To study these phenomena we can consider a wave propagation through a medium that posses aforementioned material properties. Here we concentrate our discussion on the dispersive response of the materials to electromagnetic waves. For this purpose, we assume a linear, isotropic, homogeneous, and non-magnetic material with no external charge and current. The wave equation in terms of the polarization density vector $\mathbf{P}$ and the current density $\mathbf{J}$ (see the script for details) is then written as

$$\nabla^2 \mathbf{E}(\mathbf{r},t) = -\mu_0\varepsilon_0 \frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t) - \mu_0 \frac{\partial^2}{\partial t^2}\mathbf{P}(\mathbf{r},t) - \mu_0 \frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t). \tag{1}$$

The above wave equation is in time domain and using the Fourier transformation can be transformed into the frequency domain. Finally, with $\overline{\mathbf{P}}(\mathbf{r},\omega) = \varepsilon_0\chi(\omega)\overline{\mathbf{E}}(\mathbf{r},\omega)$[1] and $\overline{\mathbf{J}}(\mathbf{r},\omega) = \sigma(\omega)\overline{\mathbf{E}}(\mathbf{r},\omega)$, it takes the form of

$$\nabla^2 \overline{\mathbf{E}}(\mathbf{r},\omega) = \varepsilon_r(\omega)\frac{\omega^2}{c^2}\overline{\mathbf{E}}(\mathbf{r},\omega). \tag{2}$$

Here, the relative dielectric function $\varepsilon_r(\omega) = 1 + \chi(\omega) + i\frac{\sigma(\omega)}{\varepsilon_0\omega}$ is defined with the susceptibility $\chi(\omega)$ and conductivity $\sigma(\omega)$ that characterize the optical responses of material. As shown in Table 1, we differentiate four cases depending on $\overline{\mathbf{P}}$ and $\overline{\mathbf{J}}$.

	$\overline{\mathbf{P}}(\mathbf{r},\omega)$	$\overline{\mathbf{J}}(\mathbf{r},\omega)$	Model	Relative dielectric function
case I	$=0$	$=0$	Vacuum	$\varepsilon_r = 1$
case II	$\neq 0$	$=0$	Bound-electron model	$\varepsilon_r(\omega) = 1 + \chi(\omega)$
case III	$=0$	$\neq 0$	Free-electron model	$\varepsilon_r(\omega) = 1 + i\frac{\sigma(\omega)}{\varepsilon_0\omega}$
case IV	$\neq 0$	$\neq 0$	General material model	$\varepsilon_r(\omega) = 1 + \chi(\omega) + i\frac{\sigma(\omega)}{\varepsilon_0\omega}$

Table 1: Classification of different material models depending on $\overline{\mathbf{P}}$ and $\overline{\mathbf{J}}$

In what follows, we derive the relative dielectric functions for the second and third cases in Table 1, for each of which we assume that the material consists of an ensemble similar atoms with no coupling. Of course, such assumption is not fully realistic, but descriptive enough in many optical scenarios and insightful for understanding the physical mechanism behind. These assumptions allow us to describe all electrons in the same manner, and the overall response is just a superposition of the individual entities, *i.e.*, the single-atom multiplied by the density $N = n/V$ where n denotes the total number of interacting electrons in a material of volume V.

[1] $\mathbf{P}(\mathbf{r},t) = \varepsilon_0 \int_{-\infty}^{\infty} R(t-t')\mathbf{E}(\mathbf{r},t')dt' \rightarrow \overline{\mathbf{P}}(\mathbf{r},\omega) = \varepsilon_0\chi(\omega)\overline{\mathbf{E}}(\mathbf{r},\omega)$ via the convolution theorem.

1.1 Lorentz model

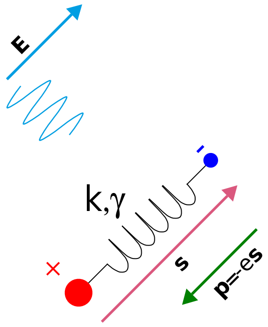

Figure 1: Forces acting on a bound electron. The displacement vector is represented by $\mathbf{s}$, and the polarization vector is defined as $\mathbf{p} = -e\mathbf{s}$.

The Lorentz model is a phenomenological model that describes the electromagnetic response of bound electrons in a material, e.g., dielectrics or semiconductors. In this model, the electron bound to a nucleus is treated as a harmonic oscillator (see Fig. 1) with a characteristic frequency ω_0, which can be determined either empirically or by the first-principle calculation of quantum mechanics. The mechanical motion of the bound electron for a given external electric field $\mathbf{E}$ can be described in terms of the displacement vector $\mathbf{s}$ from its equilibrium position. The equation of motion is written as

$$m_\mathrm{e}\frac{\mathrm{d}^2\mathbf{s}(\mathbf{r},t)}{\mathrm{d}t^2} = -m_\mathrm{e}\gamma\frac{\mathrm{d}\mathbf{s}(\mathbf{r},\mathbf{t})}{\mathrm{d}t} - K\mathbf{s}(\mathbf{r},\mathbf{t}) - e\mathbf{E}(\mathbf{r},\mathbf{t}),$$

where γ denotes damping, $K = \omega_0^2 m_\mathrm{e}$ is the spring constant, e represents the electric charge and m_e is the effective mass of the bound electron. This can be transformed into the frequency domain via the Fourier transformation, yielding

$$-\omega^2 m_\mathrm{e}\overline{\mathbf{s}}(\mathbf{r},\omega) = -i\omega m_\mathrm{e}\gamma\overline{\mathbf{s}}(\mathbf{r},\omega) - m_\mathrm{e}\omega_0^2\overline{\mathbf{s}}(\mathbf{r},\omega) - e\overline{\mathbf{E}}(\mathbf{r},\omega),$$

from which one gets

$$\overline{\mathbf{s}}(\mathbf{r},\omega) = \frac{-e/m_\mathrm{e}}{\omega_0^2 - \omega^2 - i\omega\gamma}\overline{\mathbf{E}}(\mathbf{r},\omega).$$

The polarization $\overline{\mathbf{p}}(\mathbf{r},\omega)$[2] induced for a single electron by the external field $\overline{\mathbf{E}}(\mathbf{r},\omega)$ can be written as

$$\overline{\mathbf{p}}(\mathbf{r},\omega) = -e\overline{\mathbf{s}}(\mathbf{r},\omega) = \frac{e^2/m_\mathrm{e}}{\omega_0^2 - \omega^2 - i\omega\gamma}\overline{\mathbf{E}}(\mathbf{r},\omega).$$

Then, the total polarization density $\overline{\mathbf{P}}(\mathbf{r},\omega)$ over the volume V for n identical electrons can be written as

$$\overline{\mathbf{P}}(\mathbf{r},\omega) = \frac{n}{V}\overline{\mathbf{p}}(\mathbf{r},\omega) = \varepsilon_0\frac{\frac{Ne^2}{m_\mathrm{e}\varepsilon_0}}{\omega_0^2 - \omega^2 - i\omega\gamma}\overline{\mathbf{E}}(\mathbf{r},\omega),$$

where $N = n/V$, and we define the constant quantity $f_0 = \frac{Ne^2}{m_\mathrm{e}\varepsilon_0}$ as the "oscillator strength". From the relation $\overline{\mathbf{P}}(\mathbf{r},\omega) = \varepsilon_0\chi(\omega)\overline{\mathbf{E}}(\mathbf{r},\omega)$, one can obtain the susceptibility $\chi(\omega)$ as

$$\chi(\omega) = \frac{f_0}{(\omega_0^2 - \omega^2) - i\omega\gamma},$$

whereby the relative permittivity $\varepsilon_r(\omega)$ is defined as $\varepsilon_r(\omega) = 1 + \chi(\omega) = \varepsilon_r' + i\varepsilon_r''$.

[2]For a single electron forming the dipole with its positive charge partner, The polarization vector $\mathbf{p}$ is defined as $\mathbf{p} = -e\mathbf{d}$, where q is the charge and d is the distance

Example

When a single-atomic gas or model is considered, it shows a single-resonance behavior as shown in Fig. 2. It presents the behavior of the real part $\varepsilon_r'(\omega)$, and the imaginary part $\varepsilon_r''(\omega)$ of the dielectric function $\varepsilon_r(\omega)$ around the resonant frequency ω_0. The plot of $\varepsilon_r''(\omega)$ shows a very pronounced absorption peak at the resonant frequency ω_0, and the width of the peak depends on the damping term γ. This graph depicts the "Lorentzian" dispersion model.

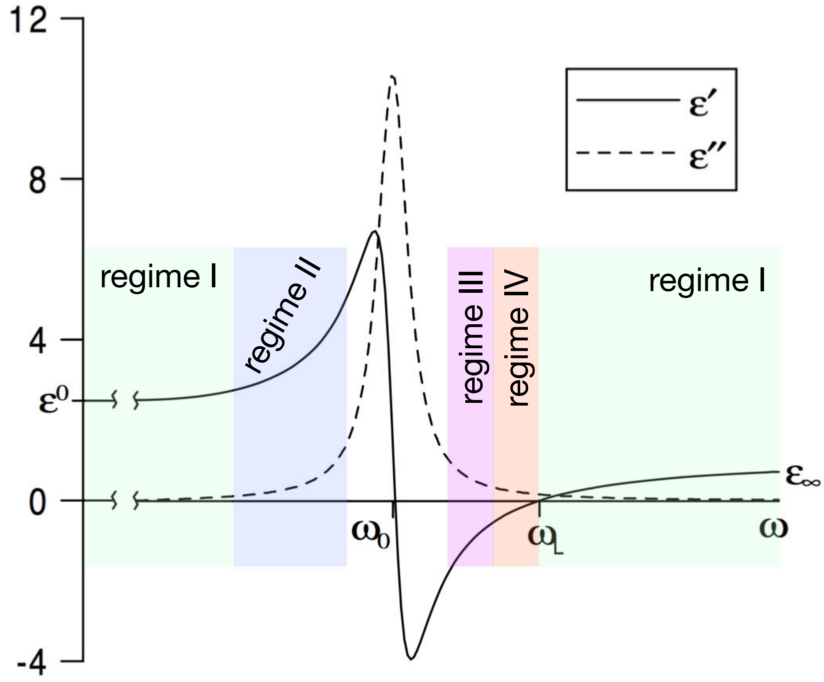

Figure 2: Real and imaginary parts of the permittivity $\varepsilon_r(\omega)$ of the Lorentz model

It is interesting to see that there are several regimes showing different optical behaviors with the frequency ω. Apart from the regimes near resonance ω_0 where $|\varepsilon_r''(\omega)| \gg |\varepsilon_r'(\omega)|$ and so a large absorption takes place, which is not very interesting in optics, we have four interesting regimes when the plane wave solutions are considered.

1. When $\varepsilon_r'(\omega) > 0$ and $\varepsilon_r''(\omega) \approx 0$, undamped homogeneous waves exist, or evanescent waves exist at interfaces.
2. When $\varepsilon_r'(\omega) > 0$ and $\varepsilon_r''(\omega) > 0$, weakly damped quasi-homogeneous waves exist.
3. When $\varepsilon_r'(\omega) < 0$ and $\varepsilon_r''(\omega) > 0$, strongly damped quasi-homogeneous waves exist.
4. When $\varepsilon_r'(\omega) < 0$ and $\varepsilon_r''(\omega) \approx 0$, evanescent waves exist at interfaces.

We do NOT explain the aforementioned regimes here in details since they require more mathematics and discussions, but please note that such a phenomenological model is very useful for understanding the physical mechanism that determines various optical responses of the material with an operating frequency.

1.2 Drude model

The Drude dielectric function describes the electromagnetic response of free electrons in a material, e.g., metals or excited semiconductors. In this case, the single electron is not bound to the nucleus (*i.e.*, no restoring force, $\omega_0 = 0$, when compared to the Lorentz model), but it is only subject to the external electromagnetic field, and the drag exerted by the ions in a metal. We use the same equation of motion used in the Lorentz model with $\omega_0 = 0$, but it is useful to formulate the equation of motion in terms of the velocity $\mathbf{v} = \frac{d\mathbf{s}}{dt}$ of the free electron:

$$m_{\mathrm{e}} \frac{\mathrm{d}\mathbf{v}(\mathbf{r}, t)}{\mathrm{d}t} = -m_{\mathrm{e}} \gamma \mathbf{v}(\mathbf{r}, \mathbf{t}) - e\mathbf{E}(\mathbf{r}, \mathbf{t}),$$

where the damping factor γ takes into account the scattering of the electrons by the ions. Via the Fourier transformation, the velocity reads in the frequency domain

$$\overline{\mathbf{v}}(\mathbf{r}, \omega) = \frac{-e/m}{-i\omega + \gamma} \overline{\mathbf{E}}(\mathbf{r}, \omega).$$

If a free-electron distribution, "called free-electron gas", with density N is considered, the current density $\bar{\mathbf{J}}$ induced by such moving electrons can be written[3] as

$$\bar{\mathbf{J}}(\mathbf{r}, \omega) = -Ne\overline{\mathbf{v}}(\mathbf{r}, \omega) = \frac{Ne^2}{m_{\mathrm{e}}\gamma} \frac{1}{1 - i(\omega/\gamma)} \overline{\mathbf{E}}(\mathbf{r}, \omega) = \sigma(\omega)\overline{\mathbf{E}}(\mathbf{r}, \omega)$$

where $\sigma(\omega)$ is the "dynamic conductivity" of the electrons:

$$\sigma(\omega) = \frac{Ne^2}{m_{\mathrm{e}}\gamma} \frac{1}{1 - i(\omega/\gamma)} = \frac{\sigma_0}{1 - i(\omega/\gamma)},$$

where $\sigma_0 = \frac{Ne^2}{m_{\mathrm{e}}\gamma}$ is called "static conductivity" such that $\sigma(\omega) = \sigma_0$ for a static field, *i.e.*, when $\omega = 0$. The dielectric function for the free-electron gas is then given by

$$\varepsilon_r(\omega) = 1 + i\frac{\sigma(\omega)}{\varepsilon_0 \omega} = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)},$$

where $\omega_p = \left(\frac{Ne^2}{m_e \varepsilon_0}\right)^{1/2}$ is called "plasma frequency" of the free-electron gas.

[3] The current density is defined by the electric current per unit area of cross section, *i.e.*, $\mathbf{J} = \frac{\text{Current}}{\text{Area}} = \frac{\Delta Q}{A \Delta t} = -\frac{ne}{A\Delta l/\mathbf{v}} = -Ne\mathbf{v}$, where the total charge of n electrons, $\Delta Q = ne$, passes through the area A during the time Δt with an average speed of v.

Example: a plane wave illumination at a normal incidence

Let us consider a plane wave illumination at the interface between an air and the bulk metal described by the Drude model. From the Fresnel equations, the reflection coefficients r for s- and p-polarized incident waves are obtained in terms of the refractive indices (n_{air} and n_{metal}) and incident/transmitted angle (θ_i/θ_t) as

$$r_s = \frac{n_{\text{air}}\cos\theta_i - n_{\text{metal}}\cos\theta_t}{n_{\text{air}}\cos\theta_i + n_{\text{metal}}\cos\theta_t} \text{ and } r_p = \frac{n_{\text{air}}\cos\theta_t - n_{\text{metal}}\cos\theta_i}{n_{\text{air}}\cos\theta_t + n_{\text{metal}}\cos\theta_i}, \tag{3}$$

respectively. When $\theta_i = 0$, then $\theta_t = 0$, so the reflection coefficients exhibit the polarization-independent behavior as

$$r_s = r_p = \frac{1 - \sqrt{\varepsilon_r(\omega)}}{1 + \sqrt{\varepsilon_r(\omega)}}, \tag{4}$$

for which we use $n_{\text{air}} = 1$ and $n_{\text{metal}} = \sqrt{\varepsilon_r(\omega)}$. So the reflected intensity is $R = \left|\frac{\sqrt{\varepsilon_r(\omega)}-1}{\sqrt{\varepsilon_r(\omega)}+1}\right|^2$.

Figure 3(a) shows the permittivity $\varepsilon(\omega)$ of the free-electron gas, and one can see that the real part ε_r' is negative for $\omega < \omega_p$. This means that light cannot propagate through the free-electron gas in this frequency region, and therefore $R = 1$ in the absence of absorption. For $\omega > \omega_p$, light propagates through the metal and so R is no longer unity (see Fig. 3(b), where $\gamma = 0$ is assumed for simplicity).

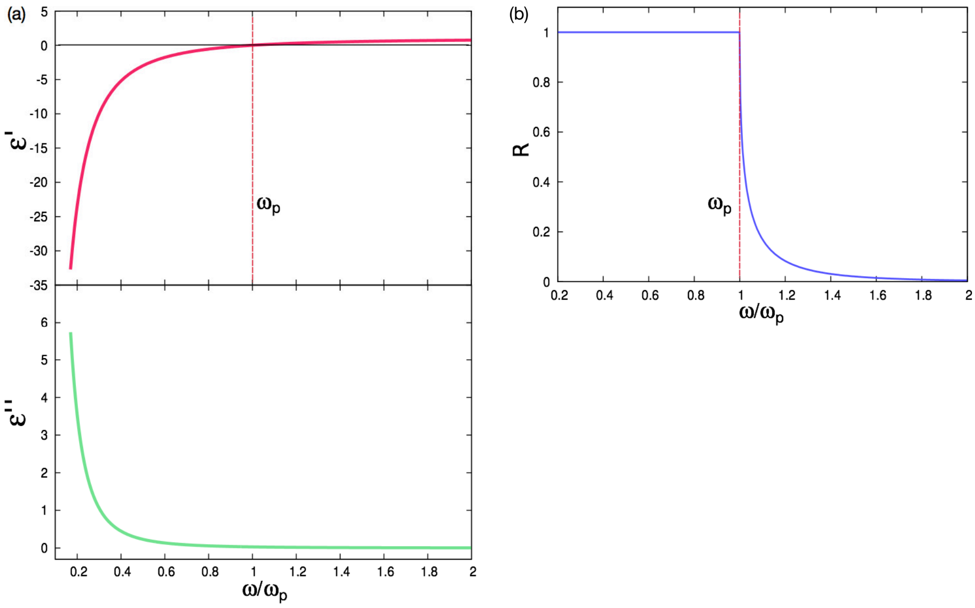

Figure 3: (a) Real and imaginary parts of the permittivity $\varepsilon_r(\omega)$ of sodium, an example of Drude metal. (b) Reflectivity of a Drude metal. $R = 1$ for $\omega < \omega_p$, for which the damping constant is set to $\gamma = 0$. When $\gamma \neq 0$, the abrupt drop of the curve at ω_{p} is smoothened.

2 Method of contour integration

Here we introduce the method of contour integration, useful for certain line integrals that are not easy to calculate based on the direct integration. The mathematical methods introduced in the following can be applied to all problems in the topics treated in the lecture on Theoretical Optics. First of all, we lay out several basic mathematical theorems from the complex analysis below and then we demonstrate a simple example to discuss how they can be used in practice.

■ Analyticity of a function and the Cauchy-Riemann equations

In mathematics, a *holomorphic* function is a complex-valued function of complex variables, *complex differentiable* in a neighborhood of every point in its domain. The existence of a complex derivative in a neighborhood is a very strong condition, for it implies that any holomorphic function is actually infinitely differentiable and equal to its own Taylor series (analytic). Though the term *analytic* function is often used interchangeably with "holomorphic function", the word "analytic" is defined in a broader sense to denote any function (real, complex, or of more general type) that can be written as a *convergent power series* in a neighborhood of each point in its domain. Note that all holomorphic functions are complex analytic functions, and vice versa. In addition, the phrase "holomorphic at a point z_0" means not just differentiable at z_0, but differentiable everywhere within some neighborhood of z_0 in the complex plane.

The condition of complex differentiability of a function $f(z) = u(z) + iv(z)$ in a neighborhood of a point $z_0 = x_0 + iy_0$ implies that the limit:

$$\mathrm{L} = \lim_{|\delta|\to 0} \frac{f(z_0 + |\delta|e^{i\phi}) - f(z_0)}{|\delta|e^{i\phi}} \tag{5}$$

exists and is the same for any angle $\phi \in [0, 2\pi]$. This means that the limit L is the same independent of the direction that we approach the point z_0. By making use of the Wirtinger derivative $\frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)$ it is straightforward to show that approaching z_0 along the two axis we get the following:

$$\mathrm{L} = \frac{1}{2}\left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right)\bigg|_{z_0}, \qquad \text{for } \phi = 0, \quad \text{i.e.} \frac{\partial}{\partial y} = 0, \tag{6}$$

$$\mathrm{L} = \frac{1}{2}\left(\frac{\partial v}{\partial y} - i\frac{\partial u}{\partial y}\right)\bigg|_{z_0}, \qquad \text{for } \phi = \pi/2, \quad \text{i.e.} \frac{\partial}{\partial x} = 0. \tag{7}$$

Equating the two results gives the Cauchy-Riemann equations:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \text{ and } \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}. \tag{8}$$

It can by shown that the Cauchy-Riemann equations guarantee the existence of the limit L for any approaching direction, i.e. for any angle ϕ. That is to say that they are sufficient conditions for the function f to be complex differentiable, i.e. holomorphic, around z_0.

■ Cauchy's integral theorem

The theorem says that if a function $f(z)$ is *holomorphic* everywhere inside a domain D of the complex plane that is enclosed by a contour C, then the following property holds true:

$$\oint_C f(z)\,\mathrm{d}z = 0. \tag{9}$$

Simple proof. Writing z as $z = x + iy$ and $f(z)$ as $f(z) = u + iv$ then gives

$$\oint_C f(z)\,\mathrm{d}z = \oint_C (u+iv)(\mathrm{d}x + i dy) = \oint_C (u\,\mathrm{d}x - v\,dy) + i\oint_C (v\,\mathrm{d}x + u\,dy)\,. \tag{10}$$

Making use of the Green's theorem we have that

$$\oint_C f(x,y)\mathrm{d}x \pm g(x,y)dy = \pm \iint_D \left(\frac{\partial g}{\partial x} \mp \frac{\partial f}{\partial y}\right)\mathrm{d}x dy. \tag{11}$$

We may then replace the integrals around the closed contour C with an area integral throughout the domain D that is enclosed by C as follows

$$\oint_C f(z)\,\mathrm{d}z = -\iint_D \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\mathrm{d}x dy + i\iint_D \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)\mathrm{d}x dy. \tag{12}$$

However, since we assumed that $f(z)$ is holomorphic everywhere in D, we have that the Cauchy-Riemann equations (Eq. (8)) apply everywhere in D. This makes the surface integrals on the right hand side of the previous equation vanish, finally giving Cauchy's integral theorem: $\oint_C f(z)\,\mathrm{d}z = 0$.

■ Laurent series expansion and Cauchy's integral formula

Any complex function $f(z)$ that is *holomorphic* everywhere inside an annulus (ring) centered at z_0, defined by $z:\ \mathrm{R}^- < |z - z_0| < \mathrm{R}^+$, can be expanded there into a convergent power series. Such a so called Laurent series expansion of $f(z)$ around z_0 reads as:

$$f(z) = \sum_{n=-\infty}^{+\infty} a_n(z_0)(z-z_0)^n. \tag{13}$$

- If $f(z)$ is an *entire* function, i.e. if it is holomorphic everywhere in the complex plane, then we have that $a_n(z_0) = 0$ for all negative integer terms with $n < 0$. Such is also the case if just $f(z)$ is holomorphic in the neighborhood of z_0.
- If $\mathrm{R}^- \to 0$ and $a_n(z_0) = 0$ for all $n < -\mathrm{N} - 1$, then we say that $f(z)$ has a *pole* (or else a *removable singularity*) of order N at z_0.
- If $\mathrm{R}^- \to 0$ and the sum of the Laurent series extends infinitely to $n = -\infty$, then we say that $f(z)$ has an *essential singularity* at z_0.
- It is straightforward to show from the above definition that if $f(z)$ is holomorphic in the neighborhood of z_0, then we have that:

$$a_n(z_0) = \frac{f^{(n)}(z_0)}{n!}. \tag{14}$$

- An alternative way to calculate the coefficients $a_n(z_0)$ is provided by *Cauchy's integral formula*. Instead of differentiation at z_0, this time we make use of a (counter-clockwise) contour integral over a closed contour C (with winding number one) that encloses a domain D on the complex plane where $f(z)$ is holomorphic everywhere, and, also, the point z_0 is located inside D. Then it can be shown that:

$$a_n(z_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-z_0)^{n+1}}\mathrm{d}z. \tag{15}$$

  We can prove the above generalized Cauchy's integral formula by working as follows. First, since $f(z)$ is holomorphic everywhere inside D, we can make use of Cauchy's integral theorem and change the contour of integration into a circle C_R with radius R centered at z_0 and being enclosed inside C, with the integral in the right hand side of the equation remaining unchanged since $f(z)$ is holomorphic everywhere between C and $C_{\rm R}$. Hence, we have:

$$\frac{1}{2\pi i}\oint_C \frac{f(z)}{(z-z_0)^{n+1}}\mathrm{d}z = \frac{1}{2\pi i}\oint_{C_{\rm R}} \frac{f(z)}{(z-z_0)^{n+1}}\mathrm{d}z. \tag{16}$$

Then we parametrize $C_{\rm R}$ by introducing the angle/variable ϕ. On $C_{\rm R}$ we have that $z = z_0 + {\rm R}e^{i\phi}$, with $\phi \in [0, 2\pi]$ and $\mathrm{d}z = i{\rm R}e^{i\phi}d\phi$. Then we take the following:

$$\frac{1}{2\pi i}\oint_{C_{\rm R}} \frac{f(z)}{(z-z_0)^{n+1}}\mathrm{d}z = \frac{1}{2\pi}\int_0^{2\pi} \frac{f(z_0+{\rm R}e^{i\phi})}{({\rm R}e^{i\phi})^n}d\phi. \tag{17}$$

Then we expand $f(z)$ in Laurent series around z_0 (Eq. (13)) and we finally take the desired result as follows:

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{f(z_0+{\rm R}e^{i\phi})}{({\rm R}e^{i\phi})^n}d\phi = \frac{1}{2\pi}\int_0^{2\pi}\sum_{n'=0}^{+\infty} a_{n'}(z_0)({\rm R}e^{i\phi})^{n'-n}d\phi = \sum_{n'=0}^{+\infty} a_{n'}(z_0)\delta_{nn'} = a_n(z_0). \tag{18}$$

Note that $\delta_{nn'}$ is the Kronecker delta and the sum over n' here starts from zero since $f(z)$ is holomorphic around z_0 and, therefore, all the negative terms in the series are zero.

■ Residues of a meromorphic function

Let's consider now a complex function $f(z)$ which is *meromorphic*. That is to say $f(z)$ is holomorphic everywhere in the complex plane apart from a countable set of discrete points where it has isolated poles. Let N be the total number of the poles and z_j, o_j (with $j = 1, ..., N$) be the position and the order of each such pole respectively. As the *residue* of f at z_j, ${\rm Res}(f, z_j)$, we define to be the coefficient $a_{-1}(z_j)$ of the Laurent series expansion of f around z_j:

$${\rm Res}(f, z_j) \triangleq a_{-1}(z_j). \tag{19}$$

Next, let us prove the following two equivalent definitions of the residues:

$${\rm Res}(f, z_j) \triangleq a_{-1}(z_j) \;\equiv\; \frac{1}{2\pi i}\oint_{S_j} f(z)\mathrm{d}z \;\equiv\; \frac{1}{(o_j-1)!}\lim_{z\to z_j}\left[\frac{d^{o_j-1}}{\mathrm{d}z^{o_j-1}}(z-z_j)^{o_j}f(z)\right]. \tag{20}$$

The first alternative definition of the residue ${\rm Res}(f, z_j)$ involves a (counter-clockwise) integration along the contour S_j of a circle with center $z = z_j$ and radius R_j that is small enough so that there is no other pole enclosed inside the circle apart from the one at its center. In order to prove the equivalence we will work as follows. Expanding $f(z)$ in Laurent series around the pole of order o_j located at $z = z_j$, and parametrizing again the contour of the integral S_j by introducing the angle/variable ϕ and writing $z = z_j + R_je^{i\phi}$, we get:

$$\begin{aligned}\frac{1}{2\pi i}\oint_{S_j} f(z)\mathrm{d}z &= \frac{1}{2\pi i}\oint_{S_j}\sum_{n=-o_j}^{+\infty} a_n(z_j)(z-z_j)^n\mathrm{d}z \\ &= \frac{1}{2\pi}\int_0^{2\pi}\sum_{n=-o_j}^{+\infty} a_n(z_j)(R_je^{i\phi})^{n+1}d\phi \\ &= \sum_{n=-o_j}^{+\infty} a_n(z_j)\delta_{n,-1} \\ &= a_{-1}(z_j). \end{aligned} \tag{21}$$

The second alternative definition of the residue $\text{Res}(f, z_j)$ involves a differentiation at $z = z_j$. Expanding $f(z)$ in Laurent series around the pole of order o_j located at $z = z_j$ we get that:

$$\begin{aligned}
\frac{1}{(o_j-1)!}\lim_{z\to z_j}\left[\frac{d^{o_j-1}}{\mathrm{d}z^{o_j-1}}(z-z_j)^{o_j}f(z)\right] &= \frac{1}{(o_j-1)!}\lim_{z\to z_j}\left[\frac{d^{o_j-1}}{\mathrm{d}z^{o_j-1}}(z-z_j)^{o_j}\sum_{n=-o_j}^{+\infty}a_n(z_j)(z-z_j)^n\right] \\
&= \frac{1}{(o_j-1)!}\sum_{n=-o_j}^{+\infty}a_n(z_j)\lim_{z\to z_j}\left[\frac{d^{o_j-1}}{\mathrm{d}z^{o_j-1}}(z-z_j)^{n+o_j}\right] \\
&= \frac{1}{(o_j-1)!}\sum_{n=-o_j}^{+\infty}a_n(z_j)(o_j-1)!\delta_{n,-1} \\
&= a_{-1}(z_j). \qquad (22)
\end{aligned}$$

■ Cauchy's residue theorem

Cauchy's residue theorem is a powerful method when it comes to calculating contour integrals of complex meromorphic functions. For $f(z)$ being a meromorphic function and C being a positively oriented (i.e. counter-clockwise oriented) simple closed curve (non-self-intersected) that encloses a number of N isolated poles of order o_j and position z_j, with $j = 1, ..., N$, Cauchy's residue theorem states that:

$$\oint_C f(z)\mathrm{d}z = 2\pi i\sum_{j=1}^{N}\text{Res}(f, z_j). \qquad (23)$$

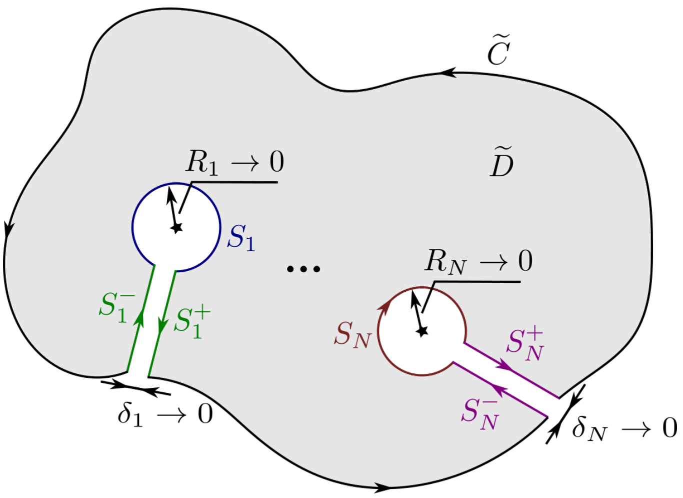

Figure 4: Contour integration in the complex plane for the proof of the residue theorem

Let us prove the theorem now. We start by applying Cauchy's integral theorem over the simple closed contour $\tilde{C} \cup S$, where $S = S_1^- \cup S_1 \cup S_1^+ \cup \cdots \cup S_N^- \cup S_N \cup S_N^+$ is the union of introduced detours around the poles (see the figure above), that encloses the space $\tilde{D}$, which is holomorphic since it excludes the set of poles that are inside C. Hence, we have that:

$$\oint_{\tilde{C}\cup S} f(z)\mathrm{d}z = 0. \qquad (24)$$

But we also have that:

$$
\begin{aligned}
\oint_C f(z)\mathrm{d}z &= \lim_{\delta_j\to 0,\forall j}\int_{\tilde{C}} f(z)\mathrm{d}z \\
&= \lim_{\delta_j\to 0,\forall j}\oint_{\tilde{C}\cup S} f(z)\mathrm{d}z - \lim_{\delta_j\to 0,\forall j}\int_S f(z)\mathrm{d}z \\
&= -\lim_{\delta_j\to 0,\forall j}\int_S f(z)\mathrm{d}z \\
&= -\sum_{j=1}^{N}\lim_{R_j\to 0}\int_{S_j} f(z)\mathrm{d}z \\
&= 2\pi i\sum_{j=1}^{N}\mathrm{Res}(f,z_j), \qquad (25)
\end{aligned}
$$

which proves the residue theorem. For the third equation above we made use of Eq. (24), whereas for the fourth equation we made use of the property $\lim_{\delta_j\to 0}\int_{S_j^-\cup S_j^+} f(z)\mathrm{d}z = 0$ and for the last equation we made use of Eq. (20).

■ Cauchy's principal value

Cauchy's principal value is a method for assigning values to improper integrals that otherwise would be undefined. For our purposes, Cauchy's principal value is useful when we are called to do integrations along contours that have a finite set of singularities at several points on top of them. In order to perform such integrations properly, Cauchy's principal value is the limit of integration along the original contour, having removed infinitely small segments around the singularities that interfere along the path of the original integration contour. Therefore we have the following definition of Cauchy's principal value of an integral:

$$
\mathrm{P.V.}\left\{\int_C f(z)\mathrm{d}z\right\} = \lim_{\varepsilon\to 0^+}\int_{C_\varepsilon^-} f(z)\mathrm{d}z \qquad (26)
$$

where C is the original contour and C_ε^- is the original contour after we removed infinitely small segments of length ε around each singularity that lies on C.

Let us consider, for example, a function $f(x)$ that has a singularity at point b with $a < b < c$. In such a case, Cauchy's principal value of the integral from a to c takes the form:

$$
\mathrm{P.V.}\left\{\int_a^c f(x)\mathrm{d}x\right\} = \lim_{\varepsilon\to 0^+}\left[\int_a^{b-\varepsilon/2} f(x)\mathrm{d}x + \int_a^{b+\epsilon/2} f(x)\mathrm{d}x\right]. \qquad (27)
$$

Example of contour integration

Let us calculate the following integral

$$\int_{-\infty}^{\infty} \frac{e^{itx}}{x^2+1} \mathrm{d}x. \text{ (t is a real number)} \tag{28}$$

How can we calculate this? It may be possible to calculate by using a direct integration, but it is non-trivial. Alternatively the use of the aforementioned mathematical theorems renders the calculation much easier. To this end, let us transform the problem to complex plane, where $f(z)$ is a complex valued function with a complex variable z. Then consider an arbitrary contour that includes the horizontal axis, corresponding to the real value of z.

Let us first suppose $t > 0$, for which we define the contour as the upper half circle. The reason why we consider the upper half circle will be clear later. For this contour C, we apply *Cauchy's residue theorem* and then get

$$\oint_C \frac{e^{itz}}{z^2+1} \mathrm{d}z = \oint_C \frac{e^{itz}}{(z+i)(z-i)} \mathrm{d}z = 2\pi i \frac{e^{itz}}{z+i}\Big|_{z=i} = \pi e^{-t}. \tag{29}$$

This contour can be decomposed into two parts, the upper arc and the line along horizontal axis as follows,

$$\oint_C \frac{e^{itz}}{z^2+1} \mathrm{d}z = \int_{-a}^{a} \frac{e^{itx}}{x^2+1} \mathrm{d}x + \int_{\text{arc}} f(z) \mathrm{d}z \tag{30}$$

So, the original integration can be evaluated, by the *Cauchy's principal value*, as

$$\text{P.V.} \left\{ \int_{-\infty}^{\infty} \frac{e^{itx}}{x^2+1} \mathrm{d}x \right\} = \lim_{a\to\infty} \int_{-a}^{a} \frac{e^{itx}}{x^2+1} \mathrm{d}x = \pi e^{-t} - \lim_{a\to\infty} \int_{\text{arc}} f(z) \mathrm{d}z. \tag{31}$$

Therefore, the later term above needs to be calculated. For this last term, we simply use the direct integration method as follows,

$$\lim_{a\to\infty} \int_{\text{arc}} f(z) \mathrm{d}z = \lim_{a\to\infty} \int_0^{\pi} \frac{e^{itae^{i\theta}}}{a^2 e^{2i\theta}+1} iae^{i\theta} d\theta, \text{ (via the coord. transformation } z = re^{i\theta}) \tag{32}$$

$$= \lim_{a\to\infty} \int_0^{\pi} \frac{ae^{ita(\cos\theta + i\sin\theta)} e^{i\theta}}{a^2 e^{2i\theta}+1} i d\theta \tag{33}$$

$$= \lim_{a\to\infty} \int_0^{\pi} \underbrace{\frac{ae^{-ta\sin\theta}}{a^2 e^{2i\theta}+1}}_{=\mathrm{X}(\theta),\text{ with } \lim_{a\to\infty} |\mathrm{X}(\theta)|=0,\text{ for } t>0} \underbrace{e^{ita\cos\theta + i\theta}}_{\text{bounded oscillating term}} i d\theta \tag{34}$$

$$= 0 \tag{35}$$

As a result,

$$\int_{-\infty}^{\infty} \frac{e^{itx}}{x^2+1} \mathrm{d}x = \pi e^{-t} \tag{36}$$

When $t < 0$, we can apply the same method but with the lower half circle, and one gets

$$\int_{-\infty}^{\infty} \frac{e^{itx}}{x^2+1} \mathrm{d}x = \pi e^{t}. \tag{37}$$

When $t = 0$, we can directly calculate the integral to get

$$\int_{-\infty}^{\infty} \frac{1}{x^2+1} \mathrm{d}x = \pi. \tag{38}$$

Combining the above results, we get

$$\int_{-\infty}^{\infty} \frac{e^{itx}}{x^2+1} \mathrm{d}x = \pi e^{-|t|}. \tag{39}$$

3 Fourier transform of Heaviside function

Here we show that the Fourier transformation of the Heaviside function $\Theta(t)$ defined as

$$\Theta(t) = \begin{cases} 1, & \text{if } t > 0 \\ 1/2 & \text{if } t = 0 \\ 0, & \text{if } t < 0, \end{cases}$$

is given by

$$\overline{\Theta}(\omega) = \frac{i}{2\pi\omega} + \frac{\delta(\omega)}{2}.$$

The Fourier transformation of the Heaviside function from the time to the frequency domain is considerably cumbersome. Alternatively, we show the above relationship reversely, *i.e.*, from the frequency to the time domain, which we can write as follows,

$$\begin{aligned}
\Theta(t) &= \int_{-\infty}^{\infty} \overline{\Theta}(\omega) e^{-i\omega t} \mathrm{d}\omega \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{i}{\omega} e^{-i\omega t} \mathrm{d}\omega + \frac{1}{2} \int_{-\infty}^{+\infty} \delta(\omega) e^{-i\omega t} \mathrm{d}\omega, \\
&= \frac{i}{2\pi} \mathrm{PV} \int_{-\infty}^{+\infty} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \frac{1}{2},
\end{aligned}$$

where PV indicates the *Cauchy Principal Value* of the integral, useful method for assigning the value to an improper integral, defined as

$$\mathrm{PV} \int_{-\infty}^{+\infty} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega = \lim_{\varepsilon \to 0^+} \left[\int_{-\infty}^{-\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \int_{+\varepsilon}^{+\infty} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega \right] \equiv f(t). \tag{1}$$

We will focus now on the integral in (1), which we will indicate with $f(t)$, and then consider three regimes for t as (i) $t = 0$, (ii) $t < 0$, and (iii) $t > 0$.

(i) When $t = 0$, it is written

$$f(0) = \lim_{\varepsilon \to 0^+} \left[\int_{-\infty}^{-\varepsilon} \frac{1}{\omega} \mathrm{d}\omega + \int_{+\varepsilon}^{+\infty} \frac{1}{\omega} \mathrm{d}\omega \right] = 0,$$

due to the fact that the function $\frac{1}{\omega}$ is an odd function. So, $\Theta(t = 0) = \frac{1}{2}$. Q.E.D.

(ii) When $t < 0$, the value of $f(t)$ can be obtained by applying the *Cauchy Residue Theorem*. To this extent, we can extend the integration domain to the complex plane, and notice that the function in the integrand,

$$\Phi(\omega) = \frac{e^{-i\omega t}}{\omega}, \tag{2}$$

has only one pole at $\omega = 0$. For $0 < \varepsilon < R$, let C_ε and C_R be the semicircles in Fig. 1. Using the residue theorem, the integral of (2) along the path indicated by Fig. 1 vanishes, since there are no poles of the integrand inside the contour, *i.e.*,

$$\int_{-R}^{-\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \int_{C_\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \int_{+\varepsilon}^{R} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \int_{C_R} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega = 0. \qquad (3)$$

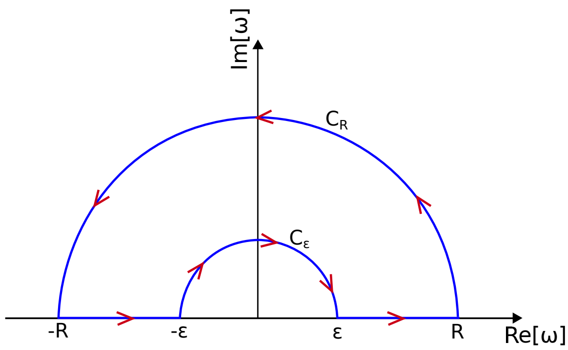

Figure 1: The contour for calculating $f(t)$ for $t < 0$.

We can now notice that $f(t)$ can be written as

$$f(t) = \lim_{\substack{\varepsilon \to 0^+ \\ R \to +\infty}} \left[\int_{-R}^{-\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega + \int_{+\varepsilon}^{+R} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega \right],$$

and Eq. (3) allows to transform this expression into an integral along C_ε and C_R,

$$f(t) = \lim_{\substack{\varepsilon \to 0^+ \\ R \to +\infty}} \left[-\int_{C_\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega - \int_{C_R} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega \right].$$

In order to calculate the integrals along the semicircles, we can write ω in polar coordinates $\omega = \rho e^{i\phi}$, with $\phi \in [0, \pi]$, and ρ is the radius of the circle that we consider. The length of arc becomes $\mathrm{d}\omega = i\rho e^{i\phi} \mathrm{d}\phi$. The integral along the path C_ε reads

$$\lim_{\varepsilon \to 0^+} \left[-\int_{C_\varepsilon} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega \right] = -\lim_{\varepsilon \to 0^+} \left[\int_{\pi}^{0} \frac{i\varepsilon e^{i\phi}}{\varepsilon e^{i\phi}} e^{-i\varepsilon(\cos(\phi) + i\sin(\phi))t} \mathrm{d}\phi \right] = i\pi,$$

whereas the integral along C_R reads

$$\lim_{R \to \infty} \left[\int_{C_R} \frac{1}{\omega} e^{-i\omega t} \mathrm{d}\omega \right] = \lim_{R \to \infty} \left[\int_{0}^{\pi} \frac{iRe^{i\phi}}{Re^{i\phi}} e^{-iRt\cos(\phi)} e^{Rt\sin(\phi)} \mathrm{d}\phi \right] = 0$$

since $e^{Rt \sin\phi} \to 0$ as $R \to +\infty$. As a result, we have $f(t < 0) = i\pi$, so that $\Theta(t < 0) = 0$.

Q.E.D.

(iii) When $t > 0$, the value of $f(t)$ can be obtained by applying the same argument, but the integration must be performed in the lower half-plane. This ensures the convergence of the integral along the circle of radius R when $R \to \infty$. The final result is $f(t > 0) = -i\pi$, so that $\Theta(t > 0) = 1$. Q.E.D.

3.1 Alternative approach

Using the conventions presented in the lecture notes:

1. $\mathcal{F}[f] \rightarrow$ Fourier transform ($\mathcal{FT}$) of the function f

2. $\frac{\mathrm{d}}{\mathrm{d}t} \xrightarrow{\mathcal{FT}} -i\omega$

3. $\mathcal{F}[\delta(t-t_0)] = \frac{1}{2\pi}\int_{-\infty}^{\infty} \delta(t-t_0)e^{i\omega t}\mathrm{d}t = \frac{1}{2\pi}e^{i\omega t_0}$

we introduce at this point an alternative approach to derive the Fourier transform of the Heaviside step function of the form:

$$\Theta(t) = \begin{cases} 1, & \text{if } t > 0 \\ \frac{1}{2}, & \text{if } t = 0 \\ 0, & \text{if } t < 0 \end{cases}$$

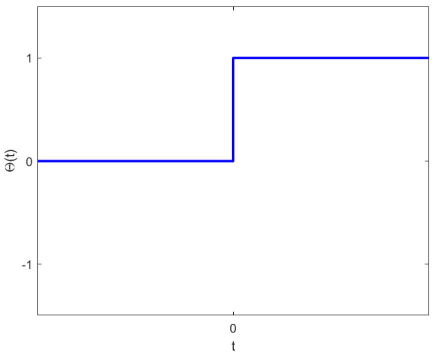

Figure 5: Unit Step Function

We see that integrating $\Theta(t)$ over the entire space does not give a finite integral value $\int_{-\infty}^{\infty} \Theta(t)dt = \infty$ and so the function intrinsically does not have a Fourier transformation. Alternatively we can represent the Heaviside function $\Theta(t) = \frac{1+\mathrm{sgn}(t)}{2} = \frac{1}{2} + \frac{\mathrm{sgn}(t)}{2}$ in terms of the **signum (sgn)** function and then formulate the Fourier transform for the Heaviside function.

The signum function is given as :

$$\mathrm{sgn}(t) = \begin{cases} 1, & \text{if } t > 0 \\ 0, & \text{if } t = 0 \\ -1, & \text{if } t < 0 \end{cases}$$

It is obvious from the nature of sgn(t) that the $\frac{\mathrm{d}}{\mathrm{d}t}(\frac{\mathrm{sgn}(t)}{2}) = \delta(t)$. So here we exploit this nature of the derivative of signum function and apply Fourier transform to get

$$\mathcal{F}\left[\frac{d}{dt}\left(\frac{\mathrm{sgn}(t)}{2}\right)\right] = -i\omega\left[\frac{d}{dt}\left(\frac{\mathrm{sgn}(t)}{2}\right)\right] = \mathcal{F}\left[\delta(t)\right]$$

$$\Rightarrow \mathcal{F}\left[\frac{\mathrm{sgn}(t)}{2}\right] = -\frac{1}{i\omega}\mathcal{F}\left[\delta(t)\right]$$

$$\mathcal{F}\left[\mathrm{sgn}(t)\right] = -\frac{1}{i\pi\omega}$$

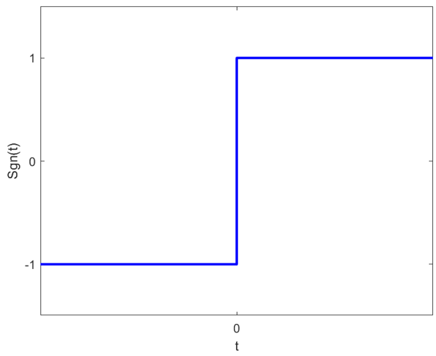

Figure 6: Signum Function

and substituting this result in $\Theta(t)$ gives

$$\begin{aligned} \mathcal{F}\left[\Theta(t)\right] &= \pi\mathcal{F}\left[\delta(t)\right] + \frac{1}{2}\mathcal{F}\left[\text{sgn}(t)\right], \\ \bar{\Theta}(\omega) &= \pi\delta(\omega) + \frac{i}{2\pi\omega}. \end{aligned}$$

The more rigorous approach in achieving these results is to use a weak formulation approach. In this approach we use a test function (preferably an exponential decay function) that convolutes with the signum function and ensures finite value for the full space integration. Later imposing appropriate limits requires the test function to vanish leaving behind the signum function. For instance, the test function g(t) can be defined as

$$g(t) = \begin{cases} e^{-at}, & \text{if } t > 0 \\ 0, & \text{if } t = 0 \\ e^{at}, & \text{if } t < 0 \end{cases}$$

with a being a real number.

Then, defining the convolution $u(t) = \text{sgn}(t)g(t)$ leads to

$$u(t) = \begin{cases} e^{-at}, & \text{if } t > 0 \\ 0, & \text{if } t = 0 \\ -e^{at}. & \text{if } t < 0 \end{cases}$$

Note that

$$\lim_{a \to 0} u(t) = \text{sgn}(t).$$

Applying the Fourier transform on $u(t)$ yields

$$\begin{aligned} \mathcal{F}\left[u(t)\right] &= \frac{1}{2\pi}\left(\int_{-\infty}^{0} u(t)e^{i\omega t}\text{d}t + \int_{0}^{\infty} u(t)e^{i\omega t}\text{d}t\right) \\ &= \frac{1}{2\pi}\left(-\int_{-\infty}^{0} e^{(a+i\omega)t}\text{d}t + \int_{0}^{\infty} e^{(-a+i\omega)t}\text{d}t\right) \\ &= \frac{1}{2\pi}\left(-\frac{1}{a+i\omega} + \frac{1}{a-i\omega}\right) \\ &= \frac{2i\omega}{2\pi\left(a^2+\omega^2\right)}. \end{aligned}$$

Limiting the value of a we have

$$\lim_{a\to 0} \mathcal{F}[u(t)] = \lim_{a\to 0} \frac{i\omega}{\pi\left(a^2+\omega^2\right)} = \frac{-1}{i\pi\omega}.$$

Substituting this result in $\Theta(t)$ gives us again

$$\begin{aligned}
\mathcal{F}\left[\Theta(t)\right] &= \pi\mathcal{F}\left[\delta(t)\right] + \frac{1}{2}\mathcal{F}\left[\operatorname{sgn}(t)\right], \\
\bar{\Theta}(\omega) &= \pi\delta(\omega) + \frac{i}{2\pi\omega}.
\end{aligned}$$