Useful mathematics

A

A.1 Fourier Transforms

The Fourier Transform is commonly used to analyze the dynamics of a system. The Fourier Transform of a function $f(t)$ is

$$\tilde{f}(\omega) = \mathscr{F}\{f(t)\} = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt, \tag{A.1}$$

while the inverse Fourier Tranform is defined as

$$f(t) = \mathscr{F}^{-1}\{\tilde{f}(\omega)\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{f}(\omega)e^{i\omega t}d\omega. \tag{A.2}$$

Using integration by parts, it is straightforward to show that the Fourier Transform of $f'(t) = df/dt$ is

$$\int_{-\infty}^{\infty} f'(t)e^{i\omega t}dt = i\omega\tilde{f}(\omega). \tag{A.3}$$

Likewise, the Fourier Transform of $f''(t) = d^2f/dt^2$ is

$$\int_{-\infty}^{\infty} f''(t)e^{i\omega t}dt = -\omega^2\tilde{f}(\omega). \tag{A.4}$$

The Fourier Transforms and inverse transforms of many functions can be found in tables and classic texts like Bracewell (1986). The Fourier Transform of a convolution is particularly useful. The theorem states that Fourier Transform of the convolution of functions $f(t)$ and $g(t)$

$$f * g = \int_{-\infty}^{t} f(t')g(t-t')dt', \tag{A.5}$$

where $*$ denotes the convolution operation, is the product of the Fourier Transforms of those functions,

$$\int_{-\infty}^{\infty} (f * g)e^{i\omega t}dt = \tilde{f}(\omega)\tilde{g}(\omega). \tag{A.6}$$

Table A.1 summarizes several other useful Fourier-Transform pairs. However, many functions of interest to rheology do not have a Fourier Transform because eqn A.1 fails to converge at its infinite limits.

Table A.1 *Useful Fourier and Laplace Transform pairs.*

Fourier Transforms

Time domain	$f(t)$	**Frequency domain**	$\tilde{f}(\omega)$
Constant	a	Delta function	$2\pi a\delta(\omega)$
Harmonic	$ae^{i\omega_0 t}$	Delta function	$2\pi a\delta(\omega-\omega_0)$
Exponential	$ae^{-\lvert t\rvert/\tau}$	Lorentzian	$2a\frac{1/\tau}{\omega^2+(1/\tau)^2}$
Gaussian	$ae^{-(t/\tau)^2}$	Gaussian	$\sqrt{\pi}a\tau e^{-(\omega\tau/2)^2}$

Laplace Transforms

Time domain	$f(t)$	**Frequency domain**	$\tilde{f}(s)$
Differentiation	$f'(t)$		$sF(s)-f(0)$
Second derivative	$f''(t)$		$s^2F(s)-sf(0)-f'(0)$
	$tf(t)$	Differentiation	$F'(s)$
Linear (one sided)[1]	$t\cdot H(t)$		$\frac{1}{s^2}$
Exponential (one sided)	$e^{-at}\cdot H(t)$		$\frac{1}{s+a}$
Exponential	$e^{-a\lvert t\rvert}$		$\frac{a}{s^2+a^2}$
Sine	$\sin\omega t$		$\frac{\omega}{s^2+\omega^2}$
Cosine	$\cos\omega t$		$\frac{s}{s^2+\omega^2}$
Power law[2]	t^p		$\frac{\Gamma(p+1)}{s^{p+1}}$

[1] $H(t)$ is the Heaviside step function.
[2] $\Gamma(x)=\int_0^\infty e^r r^{x-1}dr$ is the Gamma function. If x is a positive integer, then $\Gamma(x+1)=x!$

A.1.1 Unilateral Fourier and Laplace Transform

The Laplace Transform is defined as

$$F(s)=\mathscr{L}\{f(t)\}=\int_0^\infty f(t)e^{-st}dt. \tag{A.7}$$

The transform converges in the upper limit by multiplying the function $f(t)$ a damping factor $\exp(-\sigma t)$ such that the Laplace Transform variable is a complex number $s=\sigma+i\omega$. The Laplace Transform is suited to *causal* functions for which the behavior of $f(t)$ for $t>0$ is of interest.

The Unilateral Fourier Transform, also known as the Fourier–Laplace Transform or the one-sided Fourier Transform, is found by analytic continuation on the pure imaginary axis by the substitution

$$s=i\omega. \tag{A.8}$$

We denote the inverse Laplace Transform of the function as $f(t) = \mathscr{L}^{-1}\{\tilde{f}(s)\}$. Several useful Laplace Transforms are given in the Table A.1. The Laplace Transform also has the convolution theorem

$$f * g = \tilde{f}(s)\tilde{g}(s). \tag{A.9}$$

In Chapter 3 we use it to solve the Langevin equation.

A.1.2 Spatial Fourier Transform

The Fourier Transform may be generalized to functions defined in a three-dimensional space. The transform of a function is $f(\mathbf{r})$

$$\tilde{f}(\mathbf{q}) = \int f(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r}, \tag{A.10}$$

and the inverse transform

$$f(\mathbf{r}) = \frac{1}{(2\pi)^3}\int \tilde{f}(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{r}}d\mathbf{q}. \tag{A.11}$$

In Cartesian coordinates,

$$\tilde{f}(u, v, w) = \iiint_{-\infty}^{\infty} f(x, y, z)e^{-i(xu+yv+zw)}dxdydz \tag{A.12}$$

and the inverse transform is

$$f(x, y, z) = \frac{1}{(2\pi)^3}\iiint_{-\infty}^{\infty} \tilde{f}(u, v, w)e^{i(ux+vy+wz)}dudvdw. \tag{A.13}$$

Again, using integration by parts, it is straightforward to show that the Fourier Transform of $\nabla f(\mathbf{r})$ is

$$\int \nabla f(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r} = -iq\tilde{f}(\mathbf{q}). \tag{A.14}$$

Likewise, the Fourier Tranform of $\nabla^2 f(\mathbf{r})$ is

$$\int \nabla^2 f(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r} = -q^2\tilde{f}(\mathbf{q}). \tag{A.15}$$

These relationships are particularly useful for solving differential equations when the homogeneous solutions can be neglected (such as the long-time behavior of the Langevin equation).

Fourier Transforms are useful in the theory of spatial correlations of colloids (as well as molecular fluids and polymers,) especially in scattering experiments (x-ray, light and neutron).

A.1.3 Dirac delta function

In one dimension, the Dirac delta function is defined as the derivative of the Heaviside step function $H(x)$

$$\delta(x) = \frac{dH(x)}{dx} = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases} \tag{A.16}$$

The "sifting" property of the Dirac delta function is expressed as

$$f(0) = \int_{-\infty}^{\infty} f(x)\delta(x)dx. \tag{A.17}$$

In Cartesian space, the Dirac delta function may defined such that $\delta(\mathbf{r}) = 0$ if $\mathbf{r} \neq \mathbf{0}$ and $\delta(\mathbf{r}) = \infty$ if $\mathbf{r} = \mathbf{0}$.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(\mathbf{r})d^3r = 1. \tag{A.18}$$

A useful relationship of the delta function is that its Fourier Transform is unity,

$$\int \delta(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r} = 1. \tag{A.19}$$

A.2 Relating Fourier and Laplace Transforms

Consider a function $V(t)$ that is identially zero for $t < 0$, for which the Fourier Transform is

$$\tilde{V}(\omega) = \int_{-\infty}^{\infty} \tilde{V}(t)e^{-i\omega t}dt, \tag{A.20}$$

and inverse Fourier Transform

$$V(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{V}(\omega)e^{i\omega t}d\omega. \tag{A.21}$$

Important properties of $\tilde{V}$ emerge when this is performed via contour integration. When $t < 0$ (for which $V(t < 0) = 0$), the exponential in the inverse transform becomes $e^{-i\omega|t|}$, meaning that any ω with positive real part grows exponentially for negative t as $|\omega| \to \infty$. Therefore, we must close the contour around the *negative* imaginary plane of ω for all $t < 0$, so that the countour at infinity vanishes.

Since that integral must be identically zero for $t < 0$, residue calculus requires $\tilde{V}(\omega)$ to be analytic on the lower-half plane.[3]

Taking the Laplace Transform of the inverse Fourier Transform will allow us to relate the two transforms.

$$\hat{V}(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{0}^{\infty}\tilde{V}(\omega)e^{i\omega t-st}dtd\omega \tag{A.22}$$

which is given by

$$\hat{V}(s) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\tilde{V}(\omega)}{i\omega - s}e^{-i\omega t-st}\Bigg|_{t=0}^{t=\infty} d\omega. \tag{A.23}$$

$$\hat{V}(s) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\tilde{V}(\omega)}{\omega + is}d\omega. \tag{A.24}$$

Since $\tilde{V}(\omega)$ is analytic on the lower-half plane, the only singularity in the integrand is the pole at $\omega = -is$. Consequently, we can push the contour down, picking up only the residue from the pole at $\omega = -is$, to give

$$\hat{V}(s) = \tilde{V}(\omega \to -is). \tag{A.25}$$

So, the Fourier and Laplace Transforms are related for causal functions (which are zero for $t < 0$).

Another way to show this is via analytic continuation. To see that, we start once again with the definition of the Fourier Transform

$$\tilde{V}(\omega) = \int_{-\infty}^{\infty} V(t)e^{-i\omega t}dt. \tag{A.26}$$

Because $V(t < 0) = 0$, the bilateral Fourier Transform is identical to the unilaterial Fourier Transform,

$$\tilde{V}(\omega) = \int_{0}^{\infty} V(t)e^{-i\omega t}dt. \tag{A.27}$$

We now allow ω to take a complex argument, with negative imaginary part (as required for eqn A.27 to converge)

$$\omega = a - is \tag{A.28}$$

and in fact, take $a = 0$, then the Fourier Transform becomes

$$\tilde{V}(\omega \to -is) = \int_{0}^{\infty} V(t)e^{-st}dt = \hat{V}(s). \tag{A.29}$$

Given a causal function (for which $V(t < 0) = 0$, the Laplace and Fourier Transforms are related. Namely, taking the Fourier Transform $\tilde{V}(\omega)$ and replacing $\omega = -is$ gives the Laplace Transform. This holds for all causal functions.

[3] If the Fourier Transform is defined with the opposite sign convention, then $\tilde{V}(\omega)$ must be analytic in the upper-half plane.

A.3 Kramers–Kronig relations

The Kramers–Kronig relations allow the real part of any Fourier-Transformed causal function to be determined from the imaginary part, and vice-versa. We will derive them for the complex modulus $G^*(\omega)$, which is the Fourier Transform of the memory function $m(t)$:

$$m(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G^*(\omega)e^{i\omega t}d\omega \qquad \text{(A.30)}$$

For all $t < 0$, the fact that $m(t)$ is causal requires

$$m(t < 0) = 0 = \frac{1}{2\pi}\int_{-\infty}^{\infty} G^*(\omega)e^{i\omega t}d\omega. \qquad \text{(A.31)}$$

This, in turn, requires that $G^*(\omega)$ be analytic in the lower-half plane.

We will now consider the integral

$$\int_C \frac{G^*(\omega)}{\omega - \omega_0}d\omega, \qquad \text{(A.32)}$$

We will consider a closed contour that proceeds along the real axis, making an infinitesimally small semicircular path below the pole at ω_0, then returns to $-\infty$ via a semicircular arc around the lower-half plane at infinity. Because $G^*(\omega)$ is analytic in the lower-half plane, this contour contains no singularities, and the contour integral must be zero.

$$\int_{-\infty}^{\omega_0-\rho} \frac{G^*(\omega)}{\omega - \omega_0}d\omega + \int_{\omega_0+\rho}^{\infty} \frac{G^*(\omega)}{\omega - \omega_0}d\omega + \int_{\rho} \frac{G^*(\omega)}{\omega - \omega_0}d\omega = 0, \qquad \text{(A.33)}$$

where the final integral is an infinitesimally small semicircle, wrapping around the pole at ω_0 in the positive direction, contributing half of that pole's residue. The first two integrals, in the limit $\rho \to 0$, represent the Cauchy Principle value of the integral, leaving

$$\mathscr{P}\int_{-\infty}^{\infty} \frac{G^*(\omega)}{\omega - \omega_0}d\omega + i\pi G^*(\omega_0) = 0. \qquad \text{(A.34)}$$

Separating the real and imaginary parts of $G^*(\omega) = G'(\omega) + iG''(\omega)$ gives

$$\mathscr{P}\int_{-\infty}^{\infty} \frac{G'(\omega) + iG''(\omega)}{\omega - \omega_0}d\omega + i\pi G'(\omega_0) - \pi G''(\omega_0) = 0. \qquad \text{(A.35)}$$

The real and imaginary parts of this equation must be satisfied independently, thus yielding the Kramers–Kronig relations

$$G'(\omega_0) = -\frac{1}{\pi}\mathscr{P}\int_{-\infty}^{\infty}\frac{G''(\omega)}{\omega-\omega_0}d\omega \tag{A.36}$$

$$G''(\omega_0) = \frac{1}{\pi}\mathscr{P}\int_{-\infty}^{\infty}\frac{G'(\omega)}{\omega-\omega_0}d\omega. \tag{A.37}$$

Note that choosing the opposite sign convention for Fourier Transforms, as Landau *et al.* (1986) do, renders $G^*(\omega)$ analytic in the upper-half plane, so that the contour must go above ω_0. This is in the negative direction, and would reverse the signs on the right-hand side of eqns A.36–A.37.

A.4 Vector harmonic solutions to Stokes equations

The use of harmonic functions is particularly elegant when deriving the solution to creeping-flow equations like Stokes flow around a sphere. Leal (2007) presents an excellent introduction to the topic, including solutions for rotating spheres and spheres in general linear flows. In this section, we derive the velocity and pressure fields around a sphere translating through a quiescent fluid.

A.4.1 Harmonic functions

Harmonic functions are solutions to the differential equation

$$\nabla^2\psi = 0. \tag{A.38}$$

The harmonic functions consist of *decaying* and *growing* harmonics. The decaying harmonics are conveniently represented by taking higher-order derivatives of $1/r$,

$$\frac{1}{r} \tag{A.39}$$

$$\nabla\left(\frac{1}{r}\right) \to -\frac{x_i}{r^3} \tag{A.40}$$

$$\nabla\left(\frac{\mathbf{x}}{r^3}\right) \to \frac{\delta_{ij}}{r^3} - 3\frac{x_i x_j}{r^5} \tag{A.41}$$

$$\nabla\left(\frac{\boldsymbol{\delta}}{r^3} - 3\frac{\mathbf{xx}}{r^5}\right) \to 15\frac{x_i x_j x_k}{r^7} - 3\frac{x_i\delta_{jk} + x_j\delta_{ik} + x_k\delta_{ij}}{r^5} \tag{A.42}$$

Written in index notation, the functions are

$$\frac{1}{r} \tag{A.43}$$

$$\frac{x_i}{r^3} \tag{A.44}$$

$$\frac{x_i x_j}{r^5} - \frac{\delta_{ij}}{3r^3} \tag{A.45}$$

$$\frac{x_i x_j x_k}{r^7} - \frac{x_i \delta_{jk} + x_j \delta_{ik} + x_k \delta_{ij}}{5r^5} \tag{A.46}$$

or

$$\phi_{-(n+1)} = \frac{(-1)^n}{1 \cdot 3 \cdot 5 \cdots (2n-1)} \frac{\partial^n}{\partial x_i \partial x_j \partial x_k \cdots} \left(\frac{1}{r} \right), \quad n = 0, 1, 2, \ldots \tag{A.47}$$

The *growing harmonics* are

$$1 \tag{A.48}$$

$$x_i \tag{A.49}$$

$$x_i x_j - \frac{r^2}{3} \delta_{ij} \tag{A.50}$$

$$x_i x_j x_k - \frac{r^2}{5} x_i \delta_{jk} + x_j \delta_{ik} + x_k \delta_{ij}. \tag{A.51}$$

and may be expressed in terms of the decaying harmonics by

$$r^{2n+1} \phi_{-(n+1)}. \tag{A.52}$$

A.4.2 A sphere translating in a quiescent fluid

We seek solutions to the Stokes flow for an incompressible Newtonian fluid

$$\eta \nabla^2 \mathbf{v} - \nabla P = 0 \tag{A.53}$$

and

$$\nabla \cdot \mathbf{v} = 0. \tag{A.54}$$

First, we re-write the Stokes equations in a harmonic form. Taking the divergence of Stokes equation,

$$\nabla \cdot \left(\eta \nabla^2 \mathbf{v} - \nabla p \right) = 0 \tag{A.55}$$

where

$$\nabla^2 p = 0. \tag{A.56}$$

Next, we write the velocity field as

$$\mathbf{v} = \frac{\mathbf{x}}{2\eta} p + \mathbf{v}^H \tag{A.57}$$

which is a solution to eqn A.55 where $\mathbf{v}^H$ is a harmonic function,

$$\nabla^2 \mathbf{v}^H = 0. \tag{A.58}$$

Continuity requires that

$$\nabla \cdot \mathbf{v}^H = -\frac{1}{2\eta} \left(3p + \mathbf{x} \cdot \nabla p\right). \tag{A.59}$$

For a velocity of the sphere $\mathbf{V}$ we can construct a solution beginning with the pressure. The pressure is constructed from harmonic solutions that are linear in $\mathbf{V}$ and $\mathbf{x}$ only, therefore

$$p = C_1 \frac{\mathbf{V} \cdot \mathbf{x}}{r^3} \tag{A.60}$$

and now

$$\mathbf{v} = \frac{\mathbf{x}}{2\eta} \left(C_1 \frac{\mathbf{V} \cdot \mathbf{x}}{r^3}\right) + \mathbf{v}^H. \tag{A.61}$$

We are left to find solutions for $\mathbf{v}^H$. These must be decaying functions that are linear in $\mathbf{V}$ and are real vectors (same tensorial rank) and same tensorial parity. There are two terms constructed from $\mathbf{V}$ and the harmonic functions

$$\mathbf{v}^H = C_2 \frac{\mathbf{V}}{r} + C_3 \mathbf{V} \cdot \left(\frac{\mathbf{xx}}{r^5} - \frac{\boldsymbol{\delta}}{3r^3}\right) \tag{A.62}$$

that satisfy the criteria.

Next, we find the constants C_1, C_2, and C_3 in the equation

$$\mathbf{v} = \frac{\mathbf{x}}{2\eta} \left(C_1 \frac{\mathbf{V} \cdot \mathbf{x}}{r^3}\right) + C_2 \frac{\mathbf{V}}{r} + C_3 \mathbf{V} \cdot \left(\frac{\mathbf{xx}}{r^5} - \frac{\boldsymbol{\delta}}{3r^3}\right). \tag{A.63}$$

First, continuity requires that

$$C_2 = \frac{C_1}{2\eta}. \tag{A.64}$$

Now

$$\mathbf{v}^H = \frac{C_1}{2\eta}\frac{\mathbf{V}}{r} + C_3\mathbf{V}\cdot\left(\frac{\mathbf{xx}}{r^5} - \frac{\boldsymbol{\delta}}{3r^3}\right) \tag{A.65}$$

and

$$\mathbf{v} = \frac{\mathbf{x}}{2\eta}\left(C_1\frac{\mathbf{V}\cdot\mathbf{x}}{r^3}\right) + \frac{C_1}{2\eta}\frac{\mathbf{V}}{r} + C_3\mathbf{V}\cdot\left(\frac{\mathbf{xx}}{r^5} - \frac{\boldsymbol{\delta}}{3r^3}\right) \tag{A.66}$$

which can be rearranged to

$$\mathbf{v} = \frac{\mathbf{x}(\mathbf{V}\cdot\mathbf{x})}{r^3}\left(\frac{C_1}{2\eta} + \frac{C_3}{r^2}\right) + \frac{\mathbf{V}}{r}\left(\frac{C_1}{2\eta} - \frac{C_3}{3r^2}\right). \tag{A.67}$$

Satisfying the boundary condition that $\mathbf{v} = \mathbf{V}$ at $\mathbf{x} = \hat{\mathbf{n}}a$, or equivalently, at $|\mathbf{x}| = r = a$, leads to

$$\mathbf{V} = a^2\frac{\hat{\mathbf{n}}(\mathbf{V}\cdot\hat{\mathbf{n}})}{a^3}\left(\frac{C_1}{2\eta} + \frac{C_3}{a^2}\right) + \frac{\mathbf{V}}{a}\left(\frac{C_1}{2\eta} - \frac{C_3}{3a^2}\right) \tag{A.68}$$

and the following two equations that determine the constants C_1 and C_3:

$$\frac{C_1}{2\eta} + \frac{C_3}{a^2} = 0 \tag{A.69}$$

$$\frac{C_1}{2\eta a} - \frac{C_3}{3a^3} = 1 \tag{A.70}$$

These give us

$$C_1 = \frac{3\eta a}{2} \tag{A.71}$$

$$C_3 = -\frac{3a^3}{4} \tag{A.72}$$

and

$$\mathbf{v} = \mathbf{x}(\mathbf{V}\cdot\mathbf{x})\left(\frac{3}{4}\frac{a}{r^3} - \frac{3}{4}\frac{a^3}{r^5}\right) + \mathbf{V}\left(\frac{3}{4}\frac{a}{r} + \frac{1}{4}\frac{a^3}{r^3}\right). \tag{A.73}$$

The corresponding pressure distribution is

$$p(\mathbf{x}) = \frac{3\eta a^2}{2}\frac{\mathbf{V}\cdot\mathbf{x}}{r^3}, \tag{A.74}$$

which appear as eqns 2.70 and 2.71 in Section 2.5.

A.5 Dynamics of an oscillating particle

The equation governing the motion of an optically trapped sphere (eqn 9.38) is

$$\zeta \dot{x} + \kappa_t x = \kappa_t x_t \tag{A.75}$$

where $x_t = A \cos \omega t$. Here, we show that the general solution is

$$x(t) = D(\omega) e^{i[\omega t - \delta(\omega)]}. \tag{A.76}$$

We rewrite the equation of motion,

$$\zeta \dot{x} + \kappa_t x = \kappa_t A e^{i\omega t} \tag{A.77}$$

recognizing that $x(t)$ is the real part of the solution.

We assume the solution $x = D' e^{i\omega t}$, which upon substituting into eqn A.77, gives

$$D'(\omega) = \frac{\kappa_t A}{\kappa_t + i\omega\zeta}. \tag{A.78}$$

In polar coordinates,

$$\kappa_t + i\omega\zeta = \sqrt{\kappa_t^2 + \omega^2\zeta^2}\, e^{i\delta} \tag{A.79}$$

where

$$\tan \delta = \omega\zeta / \kappa_t \tag{A.80}$$

so

$$D'(\omega) = \frac{\kappa_t A}{\sqrt{\kappa_t^2 + \omega^2\zeta^2}} e^{-i\delta}. \tag{A.81}$$

Thus, the solution is of the form

$$x(t) = D(\omega) e^{i[\omega t - \delta(\omega)]} \tag{A.82}$$

with

$$D(\omega) = \frac{\kappa_t A}{\sqrt{\kappa_t^2 + \omega^2\zeta^2}}. \tag{A.83}$$

Taking the real part, we find

$$x(t) = D(\omega) \cos[\omega t - \delta(\omega)]. \tag{A.84}$$