11 Integral Transforms

Many pairs of functions $F(k)$ and $f(x)$ can be related by expressions of the form

$$F(k) = \int_{-\infty}^{\infty} f(x) K(k, x) \, \mathrm{d}x, \tag{1}$$

where the function $K(k, x)$ is known as the kernel. The function $F(k)$ is called the integral transform of the function $f(x)$ by the kernel $K(k, x)$. The operation described by Eq. (1) is sometimes referred to as the mapping of the function $f(x)$ in x space into another function $F(k)$ in k space. It is important to note that the variables x and k have reciprocal dimensions. Thus, for example if x has dimensions of frequency, k has dimensions of time in this case. Similarly, if x is a distance, say, in a crystal, k is a "distance" in the reciprocal lattice (see Section 4.6).

11.1 THE FOURIER TRANSFORM

By far the most useful integral transform in chemistry and physics is that of Fourier, *viz.*

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{2\pi i k x} \, \mathrm{d}x, \tag{2}$$

where $i \equiv \sqrt{-1}$. Here, the kernel is complex, as given by Eulers's relation [Eq. (1-32)]. As any function of a real variable can be expressed as the sum of even and odd functions, *viz.*

$$f(x) = f_{\text{even}}(x) + f_{\text{odd}}(x), \tag{3}$$

where $f_{\text{even}}(x) = f_{\text{even}}(-x)$ and $f_{\text{odd}}(x) = -f_{\text{odd}}(-x)$, Eq. (2) becomes

$$F(k) = \int_{-\infty}^{\infty} f_{\text{even}}(x) \, cos(2\pi k x) \, \mathrm{d}x + i \int_{-\infty}^{\infty} f_{\text{odd}}(x) \, sin(2\pi k x) \, \mathrm{d}x \tag{4}$$

and $F(k)$ is complex. Clearly, as the functions sine and cosine are used to describe wave phenomena, Eq. (4) is employed in their analyses.

Other integral transforms are obtained with the use of the kernels e^{-kx} or x^{k-1}, among the infinite number of possibilities. The former yields the Laplace transform, which is of particular importance in the analysis of electrical circuits and the solution of certain differential equations. The latter was already introduced in the discussion of the gamma function (Section 5.5.4).

It is assumed that a given Fourier-transform operation, represented by

$$F(k) = \mathcal{F} f(x), \tag{5}$$

possesses an inverse such that

$$f(x) = \mathcal{F}^{-1} F(k). \tag{6}$$

Two functions that are related by Eqs. (5) and (6) are known as a transform pair. Thus, for example, the inverse of Eq. (2) is given by

$$f(x) = \int_{-\infty}^{\infty} F(k) e^{-2\pi ikx}\, dk, \tag{7}$$

which is also a Fourier transform. It should be noted that a Fourier transform and its inverse, as defined here, are symmetrical – aside from the differing signs in the exponents.*

11.1.1 Convolution

The Fourier transform of the product of two functions is given by

$$\mathcal{G}(k) = \int_{-\infty}^{\infty} f(x) g(x) e^{2\pi ikx}\, dx. \tag{8}$$

The Fourier transform of $f(x)$ can be written as

$$F(h) = \int_{-\infty}^{\infty} f(x) e^{2\pi ihx}\, dx, \tag{9}$$

and its inverse as

$$f(x) = \int_{-\infty}^{\infty} F(h) e^{-2\pi ihx}\, dh. \tag{10}$$

The substitution of Eq. (10) in Eq. (8) yields the relation

$$\mathcal{G}(k) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(h) g(x) e^{2\pi i(k-h)x}\, dh\, dx. \tag{11}$$

*If the factor 2π is not included in the exponents, its inverse will appear as a factor before either integral.

By reversing the order of integration in Eq. (11)

$$\mathcal{G}(k) = \int_{-\infty}^{\infty} F(h) \int_{-\infty}^{\infty} g(x) e^{2\pi i (k-h)x} \, \mathrm{d}x \, \mathrm{d}h \tag{12}$$

and it is apparent that the inner integral is just the Fourier transform $\mathcal{F} g(x) = G(k-h)$. Thus,

$$\mathcal{G}(k) = \int_{-\infty}^{\infty} F(h) G(k-h) \, \mathrm{d}h \equiv F(k) \bigstar G(k). \tag{13}$$

The star in Eq. (13) specifies the convolution operation. This operation arises in many branches of physics, chemistry and engineering. It is sometimes referred to as "scanning" or "smoothing". In general the convolution of one function with another is carried out by accumulating the result of successively displacing one function with respect to the other along the abscissa. Examples of the application of this principle are described later in this chapter. Numerical methods of evaluating the convolution operation are summarized in Chapter 13.

It is appropriate to note here that convolution is commutative, *viz.*

$$F(k) \bigstar G(k) = G(k) \bigstar F(k) \tag{14}$$

(problem 1). Furthermore, it is associative, as

$$F(k) \bigstar [G(k) \bigstar H(k)] = [F(k) \bigstar G(k)] \bigstar H(k) \tag{15}$$

and distributive under addition, with

$$F(k) \bigstar [G(k) + H(k)] = F(k) \bigstar G(k) + F(k) \bigstar H(k). \tag{16}$$

A particular case of convolution is that of a function with itself. From Eq. (13) this self-convolution can be expressed by

$$F(k) \bigstar F(k) = \int_{-\infty}^{\infty} F(h) F(k-h) \, \mathrm{d}h. \tag{17}$$

It can be considered to represent the cumulative effect of scanning the function $F(k)$ over itself.

11.1.2 Fourier transform pairs

In the following sections the most important, and relatively simple, transform pairs will be described. They have been chosen, as they represent those that are routinely applied in physical chemistry. Specifically, they are the functions that form the basis of the Fourier-transform techniques that are currently employed in virtually all areas of atomic and molecular spectroscopy. These functions are all even, or can be made so, thus their Fourier transforms are real.

The function "boxcar"

Consider the rectangular function shown in Fig. 1. It is a function that is equal to zero outside the region defined by the limits $-\ell$ and $+\ell$. However, within this region it has a constant value, determined by the condition that the integral over the function is equal to unity. That is to say, the function has been normalized. The rectangular function $\sqcap(x/2\ell)$ is often referred to as the "boxcar".

The Fourier transform of the normalized boxcar function can be obtained as follows. With $f(x) = (1/2\ell)\ \sqcap(x/2\ell)$, Eq. (2) can be written in the form

$$\mathscr{F}[(1/2\ell)\ \sqcap(x/2\ell)] = \frac{1}{2\ell}\int_{-\infty}^{\infty} \sqcap(x/2\ell)\, cos(2\pi kx)\, \mathrm{d}x \tag{18}$$

$$= \frac{1}{\ell}\int_{0}^{\ell} cos(2\pi kx)\, \mathrm{d}x, \tag{19}$$

as the integrand in Eq. (18) is an even function of x. The result given by Eq. (19) leads to

$$\mathscr{F}(1/2\ell)\ \sqcap(x/2\ell) = \frac{sin(2\pi k\ell)}{2\pi k\ell} \equiv sinc(2\pi k\ell) \tag{20}$$

(problem 2). This Fourier transform pair is illustrated in Fig. 1.

The sharp cutoff at the limits $-\ell$ and ℓ, as illustrated by the boxcar function, often occurs in the frequency domain. In this case the boxcar acts as a low-pass filter in applications in electronics. All frequencies below $|\ell|$ are unaltered, while in this ideal case all higher ones are suppressed.

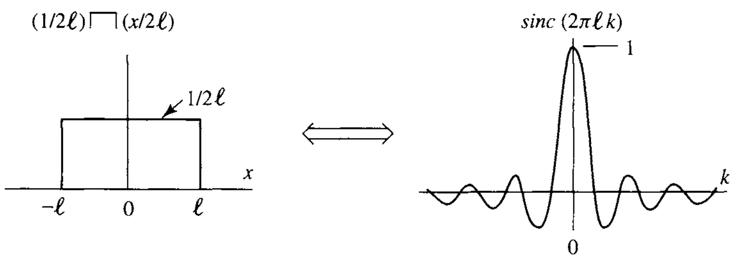

Fig. 1 The function boxcar and its Fourier transform, *sinc*.

The function triangle

This function can be defined by

$$\wedge(x/\ell) = \begin{cases} 0, & |x| > \ell \\ 1 - |x/\ell|, & |x| < \ell \end{cases}. \tag{21}$$

It is plotted with the appropriate normalizing factor in Fig. 2. The Fourier transform of this function can be evaluated as

$$\frac{1}{\ell}\int_{-\infty}^{\infty} \wedge(x/\ell)\, cos(2\pi kx)\,\mathrm{d}x = \frac{2}{\ell}\int_0^{\ell}\left(1 - \frac{x}{\ell}\right) cos(2\pi kx)\,\mathrm{d}x \tag{22}$$

$$= sinc^2(\pi k\ell) \tag{23}$$

(problem 3).

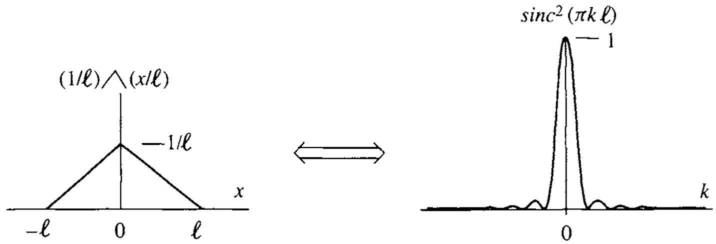

Fig. 2 The triangle function and its Fourier transform, $sinc^2$.

The Fourier transform of the triangle, as given by Eq. (23), is then

$$(1/\ell)\mathscr{F} \wedge (x/\ell) = sinc^2(\pi k\ell), \tag{24}$$

as shown in Fig. 2. From this result it is apparent that the triangle function is the result of the self-convolution of two boxcars. A well-known example in optics is provided by a monochromator in which the image of the rectangular entrance slit is scanned over a rectangular exit slit. The resulting triangle is referred to as the slit function (see problem 4).

Gauss's function

The Gaussian function was discussed in Section 3.4.5. When normalized it takes the form

$$f(x) = \sqrt{\frac{\alpha}{\pi}}\, e^{-\alpha x^2}. \tag{25}$$

The Fourier transform of the Gaussian is given by

$$F(k) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} cos(2\pi k x)\,\mathrm{d}x \tag{26}$$

$$= e^{-\pi^2 k^2/\alpha}. \tag{27}$$

Thus, the function of Gauss is its own Fourier transform, as shown in Fig. 3 (see problem 5).

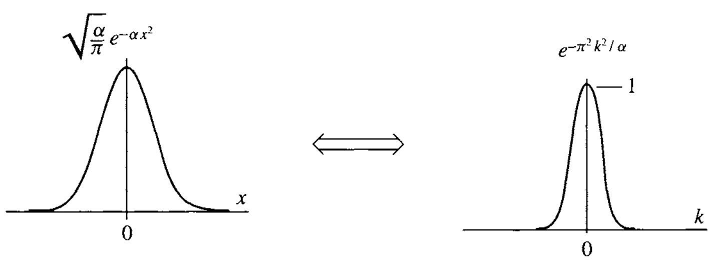

Fig. 3 The normalized Gaussian and its Fourier transform, a Gaussian in k space.

*Exponential decay: The Lorentz profile**

A phenomenon that exhibits an exponential decay – for example, in time – results in a Lorentian function in the frequency domain. The Fourier transform of the normalized function

$$f(x) = \frac{\beta}{2} e^{-\beta|x|} \tag{28}$$

is given by

$$F(k) = \frac{\beta}{2} \int_{-\infty}^{\infty} e^{-\beta|x|} cos(2\pi k x)\,\mathrm{d}x \tag{29}$$

$$= \frac{1}{1 + (4\pi^2 k^2/\beta^2)} \tag{30}$$

(see problem 6). This function, is sometimes referred to as the function of Cauchy. It is, along with the Gaussian [Eq. (25)], often used to describe the profile of an observed spectroscopic feature, *e.g.* the "bandshape".

There is a fundamental interest in the profiles of spectral bands. As they are functions of frequency, it should be clear from the arguments presented

*Hendrik Antoon Lorentz, Dutch physicist (1853–1928).

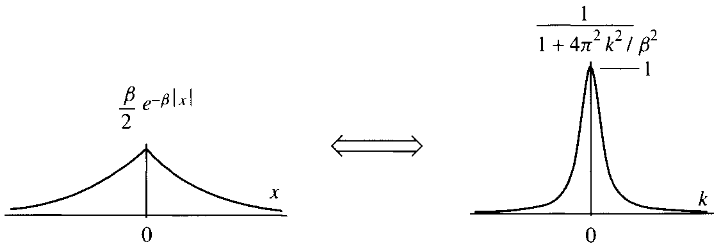

Fig. 4 The normalized exponential and its Fourier transform, the Lorentzian.

above that their Fourier transforms are functions of time. Thus the analyses of observed bandshapes provides molecular dynamic information, that is, quantitative descriptions of the time evolution of molecular interactions.

The delta function of Dirac and the "Shah"

The Dirac delta function represents an intense impulse of very short time duration. An example is the "hit" of a baseball by the bat. From a mathematical point of view this function can be defined by the relations

$$\delta(x) = 0, \quad \text{if } x \neq 0 \tag{31}$$

and

$$\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1. \tag{32}$$

Dirac's $\delta(x)$ cannot be considered to be a function in the usual sense. Although in principle it can only be written under an integral sign, Eq. (32) can be interpreted as a limit, *viz.* $\lim_{t \to 0} \int_{-\infty}^{\infty} 1/2\ell \;\sqcap(x/2\ell)\,\mathrm{d}x$. The integrand in this expression has unit area. Thus, as $\ell \to 0$ the function is limited to the region near the origin and, as it becomes narrower, its height increases to compensate. This property of the delta function is illustrated in Fig. 5.

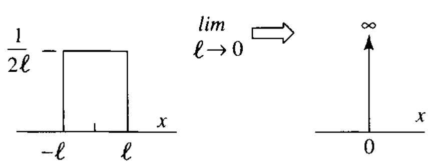

Fig. 5 The delta function as the limit of the boxcar.

The Fourier transform of the function $\delta(x - \ell)$ is given by

$$F(k) = \int_{-\infty}^{\infty} \delta(x - \ell)\, cos(2\pi k\ell)\, \mathrm{d}x. \tag{33}$$

Therefore, with $\ell = 0$ it is apparent that the Fourier transform of the delta function is equal to unity.

Two properties of the delta function are of particular interest:

(i) If it is multiplied by a function $f(x)$, its effect is to yield only the value of the function at the point where the delta function is nonzero. Thus,

$$f(x)\delta(x - \ell) = f(\ell) \tag{34}$$

and the function $f(x)$ has been "sampled" at the point $x = \ell$.

(ii) If it is convoluted with the function $f(x)$, it acts as a shifting operator. Then,

$$f(x)\bigstar\delta(x - \ell) = \int_{-\infty}^{\infty} f(x')\delta(x - x' - \ell)\, \mathrm{d}x' \tag{35}$$

$$= f(x - \ell) \tag{36}$$

and the function $f(x)$ has been shifted to $f(x - \ell)$.

The principle of sampling suggested in the previous paragraph can be generalized in the form

$$(1/\ell)\ ш\ (x/\ell) = \sum_{n=-\infty}^{\infty} \delta(x - n\ell), \tag{37}$$

where n is an integer. The function ш (x/ℓ) (Hebrew: *shah*) has been introduced to represent the "sampling comb". Multiplication of a function $f(x)$ by ш (x/ℓ) selects its values at equal intervals, as the spacing ℓ between successive "teeth" in the comb is constant. Thus,

$$(1/\ell)\ ш\ (x/\ell) \times f(x) = \sum_{n=-\infty}^{\infty} f(n\ell). \tag{38}$$

The values of $f(x)$ are only retained at each particular point where $x = n\ell$. Furthermore, the convolution of a function $f(x)$ with the sampling comb results in a function

$$(1/\ell)\ ш\ (x/\ell)\bigstar f(x) = \sum_{n=-\infty}^{\infty} f(x - n\ell), \tag{39}$$

which represents the endless replication of the original function at equal intervals. This relation is the origin of what is known in Fourier-transform spectroscopy as "aliasing".

Like the Gaussian, discussed above, the function shah is its own Fourier transform. Thus,

$$F(k) = \frac{1}{\ell}\int_{-\infty}^{\infty} \text{Ш}\,(x/\ell)e^{2\pi ikx}\,\mathrm{d}x \tag{40}$$

$$= \frac{1}{\ell}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(x - n\ell)e^{2\pi ikx}\,\mathrm{d}x \tag{41}$$

$$= \frac{1}{\ell}\sum_{n=-\infty}^{\infty} \delta\left(k - \frac{n}{\ell}\right) = \text{Ш}\,(k\ell). \tag{42}$$

This relation is illustrated in Fig. 6.

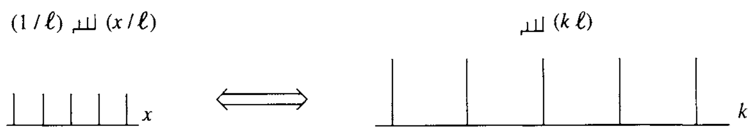

Fig. 6 The relation $\mathscr{F}(1/\ell)\ \text{Ш}\,(x/\ell) = \text{Ш}\,(k\ell)$.

11.2 THE LAPLACE TRANSFORM

The Laplace transform can be defined by

$$F(s) = \mathscr{L}f(t) = \int_0^{\infty} e^{-st} f(t)\,\mathrm{d}t. \tag{43}$$

As such, with integration limits from zero to infinity, it is referred to as a "one-sided" transform. For simplicity, it will be assumed here that the variable s is real and positive. Again, as in the case of the Fourier transform, the variables s and t have reciprocal dimensions and the operator $\mathscr{L}$ is linear (see Section 7.1).

11.2.1 Examples of simple Laplace transforms

(i) If $f(t) = 1$,

$$\mathscr{L}(1) = \int_0^{\infty} e^{-st}\,\mathrm{d}t = \frac{1}{s}\,. \quad t > 0 \tag{44}$$

(ii) If $f(t) = e^{kt}, \quad t > 0$ (45)

$$\mathcal{L}(e^{kt}) = \int_0^{\infty} e^{-st} e^{kt}\, dt = \frac{1}{s-k} \cdot \quad s > k \tag{46}$$

(iii) From (ii) the relations

$$\mathcal{L}(cosh\ kt) = \frac{s}{s^2 - k^2} \quad s > k \tag{47}$$

and

$$\mathcal{L}(sinh\ kt) = \frac{k}{s^2 - k^2} \quad s > k \tag{48}$$

can be easily derived [problem 7; see Eqs. (1-44) and (1-45)].

(iv) With the aid of Eqs. (1-46) and (1-47) the corresponding relations for the circular functions can be found, *viz.*

$$\mathcal{L}(cos\, kt) = \frac{s}{s^2 + k^2} \quad s > k \tag{49}$$

and

$$\mathcal{L}(sin\, kt) = \frac{k}{s^2 + k^2} \quad s > k \tag{50}$$

(problem 8).

(v) $\mathcal{L}(t^n) = \int_0^{\infty} e^{-st} t^n\, dt$ (51)

$$= \frac{n!}{s^{n+1}} = \frac{\Gamma(n+1)}{s^{n+1}}, \quad s > 0,\ n > -1 \tag{52}$$

where n is an integer (see Section 5.5.4 for the definition of the gamma function).

(vi) If s is replaced by $(s - a)$ in Eq. (43), the Laplace transform becomes

$$F(s-a) = \int_0^{\infty} e^{-(s-a)t} f(t)\, dt \tag{53}$$

$$= \mathcal{L}[e^{at} f(t)]. \tag{54}$$

This relation can be employed to obtain other Laplace transforms. For example, with the use of Eqs. (49) and (50),

$$\mathcal{L}(e^{at} \cos kt) = \frac{s-a}{(s-a)^2+k^2} \tag{55}$$

and

$$\mathcal{L}(e^{at} \sin kt) = \frac{k}{(s-a)^2+k^2}\,. \tag{56}$$

Many other Laplace transforms can be derived in this way. Extensive tables of Laplace transforms are available and are of routine use, particularly by electronics engineers.

11.2.2 The transform of derivatives

The Laplace transform of the derivative of a function $f(t)$ is given by

$$\mathcal{L}\left[\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right] = \int_0^\infty e^{-st}\frac{\mathrm{d}f(t)}{\mathrm{d}t}\,\mathrm{d}t. \tag{57}$$

Integration by parts yields the result

$$\mathcal{L}\left[\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right] = e^{-st}f(t)\Big|_0^\infty + s\int_0^\infty e^{-st}f(t)\,\mathrm{d}t \tag{58}$$

$$= -f(0) + s\mathcal{L}f(t). \tag{59}$$

The transforms of higher derivatives can be found by the same method, *e.g.*

$$\mathcal{L}\left[\frac{\mathrm{d}^2 f(t)}{\mathrm{d}t^2}\right] = s^2\mathcal{L}f(t) - sf(0) - \frac{\mathrm{d}f}{\mathrm{d}t}(0) \tag{60}$$

(problem 10).

A simple example of the application of Eq. (60) is provided by the function *sin kt*. As

$$\frac{\mathrm{d}^2 \sin kt}{\mathrm{d}t^2} = -k^2 \sin kt \tag{61}$$

and

$$\mathcal{L}\left[\frac{\mathrm{d}^2 \sin kt}{\mathrm{d}t^2}\right] = -k^2\mathcal{L} \sin kt \tag{62}$$

$$= s^2\mathcal{L} \sin kt - \sin(0) - \frac{\mathrm{d}\sin kt}{\mathrm{d}t}\Big|_{t=0}\,. \tag{63}$$

Then, as $(\mathrm{d}\,sin\,kt/\mathrm{d}t)|_{t=0} = k$ and $sin(0) = 0$,

$$\mathcal{L}\,sin\,kt = \frac{k}{s^2 + k^2}, \tag{64}$$

in agreement with Eq. (50).

11.2.3 Solution of differential equations

It should be evident that the expressions for the Laplace transforms of derivatives of functions can facilitate the solution of differential equations. A trivial example is that of the classical harmonic oscillator. Its equation of motion is given by Eq. (5-33), namely,

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \frac{\kappa}{m}x = 0. \tag{65}$$

By taking the Laplace transform, this equation becomes

$$\mathcal{L}\left[\frac{\mathrm{d}^2x}{\mathrm{d}t^2}\right] + \frac{\kappa}{m}\mathcal{L}(x) = 0. \tag{66}$$

Note that the use of Eq. (60) for the transform of the second derivative includes the initial conditions on the solution to the problem. The introduction of the initial conditions at this point is to be compared with the procedure employed earlier (see Section 5.2.2). If the conditions $x(0) = x_0$ and $\mathrm{d}x/\mathrm{d}t = 0$ are applied,

$$s^2X(s) - sx_0 + \frac{\kappa}{m}X(s) = 0 \tag{67}$$

and

$$X(s) = \frac{s}{s^2 + (\kappa/m)^2}x_0. \tag{68}$$

Thus, from Eq. (49) the solution is given by

$$x(t) = x_0\,cos\,\omega_0 t \tag{69}$$

where $\omega_0^2 = \kappa/m$.

As a somewhat more complicated example, consider the electrical circuit of the damped oscillator shown in Fig. 5-3. The charge $q(t)$ is determined by Eq. (5-45), namely,

$$\frac{\mathrm{d}^2q(t)}{\mathrm{d}t^2} + \frac{R}{L}\frac{\mathrm{d}q(t)}{\mathrm{d}t} + \frac{1}{LC}q(t) = 0, \tag{70}$$

where R is the resistance, L the inductance and C the capacitance. The capacitance will be assumed to have an initial charge q_0, at which time there is no current flowing in the circuit. Thus, the initial conditions are $q(0) = q_0$ and $(\mathrm{d}q/\mathrm{d}t)(0) = 0$. The Laplace transform then yields the relation

$$s^2(X)(s) - sq_0 + \frac{R}{L}[sX(s) - q_0] + \frac{1}{LC}X(s) = 0. \tag{71}$$

Then,

$$X(s) = q_0 \frac{s + R/L}{s^2 + s(R/L) + 1/LC} \tag{72}$$

and the condition for oscillation is

$$\omega_1^2 = \frac{1}{LC} - \frac{R^2}{4L^2} > 0. \tag{73}$$

This result is equivalent to that derived in Section 5.2.3 for the mechanical analog (problem 11). Equation (72) can be written

$$X(s) = q_0 \frac{s + R/L}{(s + R/2L)^2 + \omega_1^2} = q_0 \frac{s + R/2L}{(s + R/2L)^2 + \omega_1^2} + q_0 \frac{R/2L}{(s + R/2L)^2 + \omega_1^2} \tag{74}$$

and, with the aid of Eqs. (49) and (50), the solution becomes

$$q(t) = q_0 e^{-Rt/2L}\left(\cos \omega_1 t + \frac{R}{2L\omega_1} \sin \omega_1 t\right), \tag{75}$$

in agreement with Eq. (5-43). Here again, the initial conditions are specified at the outset (problem 12).

11.2.4 Laplace transforms: Convolution and inversion

The convolution and general properties of the Fourier transform, as presented in Section 11.1, are equally applicable to the Laplace transform. Thus,

$$\int_{-\infty}^{\infty} F(h)G(k - h)\,\mathrm{d}h \equiv F(k)\bigstar G(k), \tag{76}$$

where $F(k)$ and $G(k)$ are the Laplace transforms of $f(x)$ and $g(x)$, respectively.

The inversion of the Laplace transform presents a more difficult problem. From a fundamental point of view the inverse of a given Laplace transform is known as the Bromwich integral.* Its evaluation is carried out by application

*Thomas John I'anson Bromwich, English mathematician (1875–1929).

of the theory of residues. As contour integration is not treated in this book, the reader is referred to more advanced texts for the explanation of this method.

In practice, the inverse Laplace transformations are obtained by reference to the rather extensive tables that are available. It is sometimes useful to develop the function in question in partial fractions, as employed in Section 3.3.3. The resulting sum of integrals can often be evaluated with the use of the tables.

In principle, numerical methods can be employed to evaluate inverse Laplace transforms. However, the procedure is subject to errors that are often very large–even catastrophic.

11.2.5 Green's functions*

The introduction of these somewhat mysterious functions allows certain differential equations to be converted into equivalent integral equations. Although the method is particularly useful in its application to partial differential equations, it will be illustrated here with the aid of a relatively simple example, the forced vibrations of a classical oscillator.

Consider first the inhomogeneous differential equation as given by Eq. (5-57). For simplicity, assume here that the oscillator is not damped; hence, $h = 0$. The problems to be treated are now represented by the differential equation

$$\frac{d^2x}{dt^2} + \omega_0^2 x = \phi(t). \tag{77}$$

The function $\phi(t)$, aside from a constant, expresses the time-dependent force acting on the harmonic oscillator and $\omega_0 = \sqrt{\kappa/m}$ is the angular frequency of the system (Section 5.3.3).

Now consider the external force acting on the system to be composed of a series of instantaneous impacts, each of which can be expressed mathematically by a delta function. The response of the system can then be represented by a function $G(t)$. The differential equation to be solved then takes on the form

$$\frac{d^2}{dt^2}G(t,t') + \omega_0^2 G(t,t') = \delta(t-t'). \tag{78}$$

The function $\delta(t-t')$ corresponds to an impact on the system at the instant $t = t'$. The function $G(t,t')$ is known as a Green's function. It has been implied here that the forcing function $\phi(t)$ can be represented by a sum of such delta functions, as given by

$$\phi(t) = \int_0^\infty \phi(t')\delta(t-t')\,dt' \qquad t > t' > 0 \tag{79}$$

*George Green, English mathematician (1793–1841).

[See Eq. (35) and Eq. (36) with $x - \ell$ replaced by t]. In effect, the delta function samples the forcing function at each point in time. The proof of Eq. (79) constitutes problem 13.

The solution of Eq. (78) can be obtained with the use of the Laplace transform. However, it is first necessary to develop the expression for the Laplace transform of the delta function, as given on the right-hand side of Eq. (78). With the use of the definition of the Laplace transform [Eq. (43)] and $f(t) = \delta(t - t')$, the desired result becomes

$$\mathcal{L}\delta(t - t') = e^{-st'}. \tag{80}$$

The Laplace transform of Eq. (78) can then be written as

$$(s^2 + \omega_0^2)\mathcal{L}G(t, t') = \mathcal{L}\delta(t - t') = e^{-st}, \tag{81}$$

where Eq. (60) has been employed with the initial conditions $G(0, 0) = G'(0, 0) = 0$. Thus, with the use of Eqs. (50) and (54) to obtain the inverse Laplace transforms, the solution is given by

$$G(t, t') = \mathcal{L}^{-1}\left[\frac{e^{-st}}{s^2 + \omega_0^2}\right] = \frac{1}{\omega_0} sin[\omega_0(t - t')] \tag{82}$$

(see problem 14). This result is easily verified by substitution in Eq. (78). Once the Green's function has been found for this type of problem, the solution of Eq. (77) for a specific forcing function $\phi(t')$ can, at least in principle, be obtained by direct integration, namely,

$$x(t) = \int_0^\infty G(t, t')\phi(t')\,dt' \tag{83}$$

(problem 15). Note that Eq. (83) is an integral equation with $G(t, t')$ the kernel.

As a simple example of the general method outlined above, consider the vibrations of the harmonic oscillator under the forcing function $\phi(t') = F_0 \, sin\, \omega t'$, as in Eq. (5-58). Thus, Eq. (83) becomes

$$x(t) = \frac{F_0}{\omega_0}\int_0^\infty sin[\omega_0(t - t')]\, sin\, \omega t'\,dt'. \tag{84}$$

This integral can be evaluated with the aid of the appropriate trigonometric relations. Furthermore, the upper limit can be replaced by t, as $t' < t$. The result,

$$x(t) = F_0 \frac{sin\, \omega_0 t}{\omega^2 - \omega_0^2} \tag{85}$$

is (aside from the factor F_0) the same as Eq. (5-59) for the special case where $h = 0$. This solution to the inhomogeneous differential equation is referred to as the "steady-state" solution, as contrasted to the transient one [Eq. (5-34)] that becomes negligible with increasing time. The catastrophic behavior of the forced oscillator if ω is close to ω_0 was discussed in Section 5-33.

PROBLEMS

1. Show that $F(k)\bigstar G(k) = G(k)\bigstar F(k)$.
2. Derive the expression for the Fourier transform of the boxcar [Eq. (20)].
3. Verify Eq. (23).
4. To illustrate the self-convolution operation, draw two identical boxcars and evaluate the area in common as a function of their relative separation along the abscissa.
5. Show that the Fourier transform of a Gaussian is also a Gaussian.
6. Verify Eq. (30).
7. Verify Eqs. (44) to (48).
8. Verify Eqs. (49) and (50).
9. Derive Eqs. (52) to (56).
10. Derive Eq. (60).
11. Compare Eq. (73) with the corresponding result for the damped mechanical oscillator.
12. Verify Eq. (75).
13. Derive Eq. (79).
14. Substitute Eq. (82) to show that it is a solution to Eq. (78).
15. Demonstrate that Eq. (73) is a solution to Eq. (77).
16. Carry out the integration indicated in Eq. (84) to obtain Eq. (85).