3

Fourier and Laplace Transforms

The complex exponentials $\exp(i2\pi nx/L)$ are orthonormal and easy to differentiate (and to integrate), but they are periodic with period L. If one wants to represent functions that are not periodic, a better choice is the complex exponentials $\exp(ikx)$, where k is an arbitrary real number. These orthonormal functions are the basis of the Fourier transform. The choice of complex k leads to the transforms of Laplace, Mellin, and Bromwich.

3.1 Fourier transforms

The interval $[-L/2, L/2]$ is arbitrary in the Fourier series pair (2.46)

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad \text{and} \quad f_n = \int_{-L/2}^{L/2} f(x) \frac{e^{-i2\pi nx/L}}{\sqrt{L}}\, dx. \tag{3.1}$$

What happens when we stretch this interval without limit, letting $L \to \infty$?

We may use the **nearest-integer function** $[y]$ to convert the coefficients f_n into a function of a continuous variable $\hat{f}(y) \equiv f_{[y]}$ such that $\hat{f}(y) = f_n$ when $|y - n| < 1/2$. In terms of this function $\hat{f}(y)$, the Fourier series (3.1) for the function $f(x)$ is

$$f(x) = \sum_{n=-\infty}^{\infty} \int_{n-1/2}^{n+1/2} \hat{f}(y) \frac{e^{i2\pi[y]x/L}}{\sqrt{L}}\, dy = \int_{-\infty}^{\infty} \hat{f}(y) \frac{e^{i2\pi[y]x/L}}{\sqrt{L}}\, dy. \tag{3.2}$$

Since $[y]$ and y differ by no more than $1/2$, the absolute value of the difference between $\exp(i\pi[y]x/L)$ and $\exp(i\pi yx/L)$ for fixed x is

$$\left| e^{i2\pi[y]x/L} - e^{i2\pi yx/L} \right| = \left| e^{i2\pi([y]-y)x/L} - 1 \right| \approx \frac{\pi|x|}{L} \tag{3.3}$$

which goes to zero as $L \to \infty$. So in this limit, we may replace $[y]$ by y and

express $f(x)$ as

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(y)\, \frac{e^{i2\pi yx/L}}{\sqrt{L}}\, dy. \tag{3.4}$$

We let $y = Lk/(2\pi)$ so $k = 2\pi y/L$ and find for $f(x)$ the integral

$$f(x) = \int_{-\infty}^{\infty} \hat{f}\left(\frac{Lk}{2\pi}\right) \frac{e^{ikx}}{\sqrt{L}}\, \frac{L}{2\pi}\, dk = \int_{-\infty}^{\infty} \sqrt{\frac{L}{2\pi}}\; \hat{f}\left(\frac{Lk}{2\pi}\right) e^{ikx}\, \frac{dk}{\sqrt{2\pi}}. \tag{3.5}$$

Now in terms of the Fourier transform $\tilde{f}(k)$ defined as

$$\tilde{f}(k) = \sqrt{\frac{L}{2\pi}}\, \hat{f}\left(\frac{Lk}{2\pi}\right) \tag{3.6}$$

the integral (3.5) for $f(x)$ is the inverse Fourier transform

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}}. \tag{3.7}$$

To find $\tilde{f}(k)$, we use its definition (3.6), the definition (3.1) of f_n, our formulas $\tilde{f}(k) = \sqrt{Lk/(2\pi)}\hat{f}(Lk/(2\pi))$ and $\hat{f}(y) = f_{[y]}$, and the inequality $|2\pi[Lk/2\pi]/L - k| \le \pi/2L$ to write

$$\tilde{f}(k) = \sqrt{\frac{L}{2\pi}} f_{\left[\frac{Lk}{2\pi}\right]} = \sqrt{\frac{L}{2\pi}} \int_{-L/2}^{L/2} f(x) \frac{e^{-i2\pi\left[\frac{Lk}{2\pi}\right]\frac{x}{L}}}{\sqrt{L}} dx \approx \int_{-L/2}^{L/2} f(x) e^{-ikx} \frac{dx}{\sqrt{2\pi}}.$$

This formula becomes exact in the limit $L \to \infty$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, \frac{dx}{\sqrt{2\pi}} \tag{3.8}$$

and so we have the Fourier transformations

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}} \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, \frac{dx}{\sqrt{2\pi}}. \tag{3.9}$$

The function $\tilde{f}(k)$ is the **Fourier transform** of $f(x)$, and $f(x)$ is the **inverse Fourier transform** of $\tilde{f}(k)$.

In these symmetrical relations (3.9), the distinction between a Fourier transform and an inverse Fourier transform is entirely a matter of convention. There is no rule for which sign, ikx or $-ikx$, goes with which transform or for where to put the 2π's. Thus one often sees

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{\pm ikx}\, dk \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x)\, e^{\mp ikx}\, \frac{dx}{2\pi} \tag{3.10}$$

as well as

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{\pm ikx}\, \frac{dk}{2\pi} \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x)\, e^{\mp ikx}\, dx. \tag{3.11}$$

One often needs to relate a function's Fourier series to its Fourier transform. So let's compare the Fourier series (3.1) for the function $f(x)$ on the interval $[-L/2, L/2]$ with its Fourier transform (3.9) in the limit of large L setting $k_n = 2\pi n/L = 2\pi y/L$

$$f(x) = \sum_{n=-\infty}^{\infty} f_n\, \frac{e^{i2\pi nx/L}}{\sqrt{L}} = \sum_{n=-\infty}^{\infty} f_n\, \frac{e^{ik_n x}}{\sqrt{L}} = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}}. \tag{3.12}$$

Since $f_n = \hat{f}(y) = f_{[y]}$, by using the definition (3.6) of $\tilde{f}(k)$, we have

$$f_n = f_{[n]} = f_{[y]} = \hat{f}(y) = \hat{f}\left(\frac{Lk}{2\pi}\right) = \sqrt{\frac{2\pi}{L}}\, \tilde{f}(k). \tag{3.13}$$

Thus, to get the Fourier series from the Fourier transform, we multiply the series by $2\pi/L$ and use the Fourier transform at k_n divided by $\sqrt{2\pi}$

$$f(x) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} f_n\, e^{ik_n x} = \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} \frac{\tilde{f}(k_n)}{\sqrt{2\pi}}\, e^{ik_n x}. \tag{3.14}$$

Going the other way, we set $\tilde{f}(k) = \sqrt{L/2\pi}\, f_n = \sqrt{L/2\pi}\, f_{[Lk/2\pi]}$ and find

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}} = \frac{L}{2\pi} \int_{-\infty}^{\infty} \frac{f_{[Lk/2\pi]}}{\sqrt{L}}\, e^{ikx} dk. \tag{3.15}$$

Example 3.1 (The Fourier Transform of a Gaussian Is a Gaussian)**.** The Fourier transform of the gaussian $f(x) = \exp(-m^2\, x^2)$ is

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx}\, e^{-m^2\, x^2}. \tag{3.16}$$

We complete the square in the exponent:

$$\tilde{f}(k) = e^{-k^2/4m^2} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-m^2\, (x+ik/2m^2)^2}. \tag{3.17}$$

As we'll see in Sec. 5.14 when we study analytic functions, we may replace x by $x - ik/2m^2$ without changing the value of this integral. So we can drop the term $ik/2m^2$ in the exponential and get

$$\tilde{f}(k) = e^{-k^2/4m^2} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-m^2\, x^2} = \frac{1}{\sqrt{2}\, m}\, e^{-k^2/4m^2}. \tag{3.18}$$

Thus the Fourier transform of a gaussian is another gaussian

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx}\, e^{-m^2 x^2} = \frac{1}{\sqrt{2}\, m}\, e^{-k^2/4m^2}. \tag{3.19}$$

But the two gaussians are very different: if the gaussian $f(x) = \exp(-m^2 x^2)$ decreases slowly as $x \to \infty$ because m is small (or quickly because m is big), then its gaussian Fourier transform $\tilde{f}(k) = \exp(-k^2/4m^2)/m\sqrt{2}$ decreases quickly as $k \to \infty$ because m is small (or slowly because m is big).

Can we invert $\tilde{f}(k)$ to get $f(x)$? The inverse Fourier transform (3.7) says

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, e^{ikx} = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \frac{1}{m\sqrt{2}}\, e^{ikx - k^2/4m^2}. \tag{3.20}$$

By again completing the square in the exponent

$$f(x) = e^{-m^2 x^2} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \frac{1}{m\sqrt{2}}\, e^{-(k - i2m^2 x)^2/4m^2} \tag{3.21}$$

and shifting the variable of integration k to $k + i2m^2 x$, we find

$$f(x) = e^{-m^2 x^2} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \frac{1}{m\sqrt{2}}\, e^{-k^2/(4m^2)} = e^{-m^2 x^2} \tag{3.22}$$

which is reassuring.

Using (3.18) for $\tilde{f}(k)$ and the connections (3.12–3.15) between Fourier series and transforms, we see that a Fourier series for this gaussian is in the limit of $L \gg x$

$$f(x) = e^{-m^2 x^2} = \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi}\, m}\, e^{-k_n^2/(4m^2)} e^{ik_n x} \tag{3.23}$$

in which $k_n = 2\pi n/L$. □

3.2 Fourier transforms of real functions

If a function $f(x)$ is real, then the complex conjugate of its Fourier transform (3.8)

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, f(x)\, e^{-ikx} \tag{3.24}$$

is its Fourier transform evaluated at $-k$

$$\tilde{f}^*(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, f(x)\, e^{ikx} = \tilde{f}(-k). \tag{3.25}$$

It follows (exercise 3.1) that a real function $f(x)$ satisfies the relation

$$f(x) = \frac{1}{\pi} \int_0^\infty dk \int_{-\infty}^\infty f(y)\, \cos k(y-x)\, dy. \tag{3.26}$$

If $f(x)$ is both real and even, then

$$f(x) = \frac{2}{\pi} \int_0^\infty \cos kx\, dk \int_0^\infty f(y)\, \cos ky\, dy \tag{3.27}$$

if it is even, and

$$f(x) = \frac{2}{\pi} \int_0^\infty \sin kx\, dk \int_0^\infty f(y)\, \sin ky\, dy \tag{3.28}$$

if it is odd (exercise 3.2).

Example 3.2 (Dirichlet's Discontinuous Factor)**.** Using (3.27), one may write the square wave

$$f(x) = \begin{cases} 1 & |x| < 1 \\ \frac{1}{2} & |x| = 1 \\ 0 & |x| > 1 \end{cases} \tag{3.29}$$

as Dirichlet's discontinuous factor

$$f(x) = \frac{2}{\pi} \int_0^\infty \frac{\sin k \cos kx}{k}\, dk \tag{3.30}$$

(exercise 3.3). □

Example 3.3 (Even and Odd Exponentials)**.** By using the Fourier-transform formulas (3.27 & 3.28), one may show that the Fourier transform of the even exponential $\exp(-\beta|x|)$ is

$$e^{-\beta|x|} = \frac{2}{\pi} \int_0^\infty \frac{\beta\, \cos kx}{\beta^2 + k^2}\, dk \tag{3.31}$$

while that of the odd exponential $x \exp(-\beta|x|)/|x|$ is

$$\frac{x}{|x|} e^{-\beta|x|} = \frac{2}{\pi} \int_0^\infty \frac{k\, \sin kx}{\beta^2 + k^2}\, dk \tag{3.32}$$

(exercise 3.4). □

3.3 Dirac, Parseval, and Poisson

Combining the basic equations (3.9) that define the Fourier transform, we may do something apparently useless: we may write the function $f(x)$ in terms of itself as

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, e^{ikx} = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}}\, e^{-iky}\, f(y). \tag{3.33}$$

Let's compare this equation

$$f(x) = \int_{-\infty}^{\infty} dy \left(\int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \exp[ik(x-y)] \right) f(y) \tag{3.34}$$

with one (2.116) that describes Dirac's delta function

$$f(x) = \int_{-\infty}^{\infty} dy\, \delta(x-y)\, f(y). \tag{3.35}$$

Thus for functions with sensible Fourier transforms, the delta function is

$$\delta(x-y) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \exp[ik(x-y)]. \tag{3.36}$$

The same integral from $-N$ to N

$$\delta_N(x-y) = \int_{-N}^{N} \frac{dk}{2\pi}\, \exp[ik(x-y)] = \frac{\sin(N(x-y))}{\pi(x-y)} \tag{3.37}$$

is plotted in Fig. 3.1 for the case $y = 0$ and $N = 10^6$.

The inner product (f, g) or $\langle f|g\rangle$ of two functions, $f(x)$ with Fourier transform $\tilde{f}(k)$ and $g(x)$ with Fourier transform $\tilde{g}(k)$, is

$$\langle f|g\rangle = (f, g) = \int_{-\infty}^{\infty} dx\, f^*(x)\, g(x). \tag{3.38}$$

Since $f(x)$ and $g(x)$ are related to $\tilde{f}(k)$ and to $\tilde{g}(k)$ by the Fourier transform (3.8), their inner product (f, g) is

$$\begin{aligned}
(f, g) &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \left(\tilde{f}(k)\, e^{ikx} \right)^* \int_{-\infty}^{\infty} \frac{dk'}{\sqrt{2\pi}}\, \tilde{g}(k')\, e^{ik'x} \\
&= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} \frac{dx}{2\pi}\, e^{ix(k'-k)}\, \tilde{f}^*(k)\, \tilde{g}(k') \\
&= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\, \delta(k'-k)\, \tilde{f}^*(k)\, \tilde{g}(k') = \int_{-\infty}^{\infty} dk\, \tilde{f}^*(k)\, \tilde{g}(k).
\end{aligned} \tag{3.39}$$

Thus we arrive at **Parseval's relation**

$$(f, g) = \int_{-\infty}^{\infty} dx\, f^*(x)\, g(x) = \int_{-\infty}^{\infty} dk\, \tilde{f}^*(k)\, \tilde{g}(k) = (\tilde{f}, \tilde{g}) \tag{3.40}$$

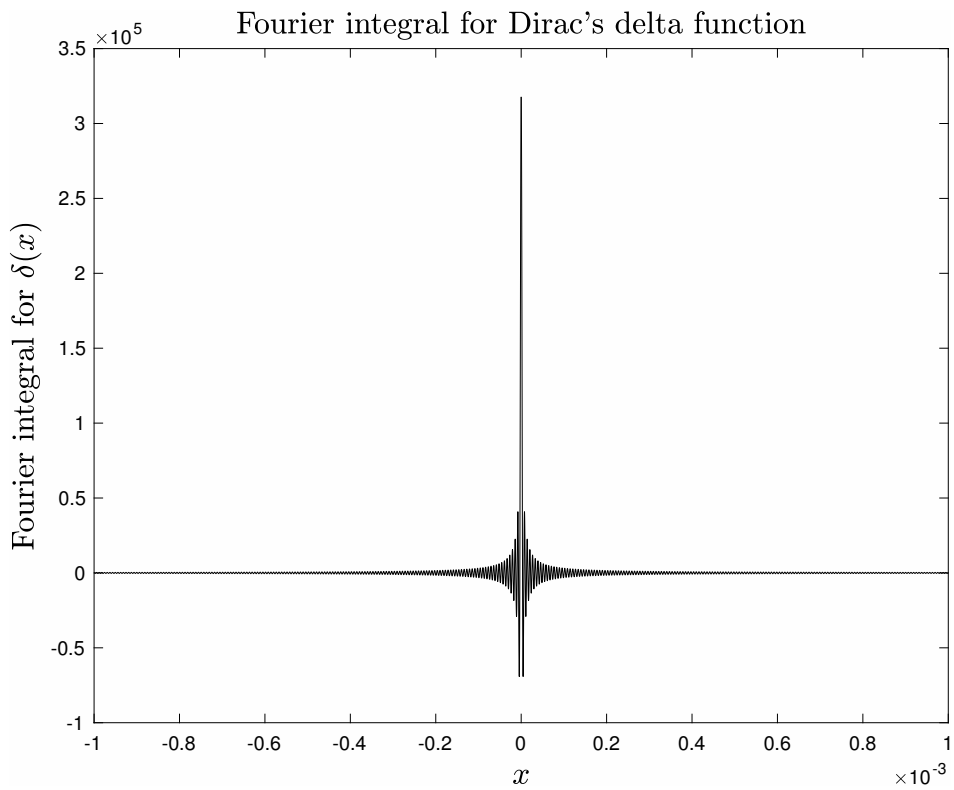

Figure 3.1 The integral (3.37) for $N = 10^6$ is plotted for $|x| \leq 0.001$.

which says that the inner product of two functions is the same as the inner product of their Fourier transforms The Fourier transform is a unitary transform. In particular, if $f = g$, then

$$\langle f|f\rangle = (f, f) = \int_{-\infty}^{\infty} dx\, |f(x)|^2 = \int_{-\infty}^{\infty} dk\, |\tilde{f}(k)|^2 \tag{3.41}$$

(Marc-Antoine Parseval des Chênes, 1755–1836).

In fact, one may show that the Fourier transform maps the space of (Lebesgue) square-integrable functions onto itself in a one-to-one manner. Thus the natural space for the Fourier transform is the space of square-integrable functions, and so the representation (3.36) of Dirac's delta function is suitable for continuous square-integrable functions.

This may be a good place to say a few words about how to evaluate integrals involving delta functions of more complicated arguments, such as

$$J = \int \delta(g(x))\, f(x)\, dx. \tag{3.42}$$

To see how this works, let's assume that $g(x)$ vanishes at a single point x_0 at which its derivative $g'(x_0) \neq 0$ isn't zero. Then the integral J involves f only at $f(x_0)$ which we can bring outside as a prefactor

$$J = f(x_0) \int \delta(g(x))\, dx. \tag{3.43}$$

Near x_0 the function $g(x)$ is approximately $g'(x_0)(x-x_0)$, and so the integral is

$$J = f(x_0) \int \delta(g'(x_0)(x - x_0))\, dx. \tag{3.44}$$

Since the delta function is nonnegative, we can write

$$\begin{aligned} J &= \frac{f(x_0)}{|g'(x_0)|} \int \delta(g'(x_0)(x - x_0))|g'(x_0)|\, dx \\ &= \frac{f(x_0)}{|g'(x_0)|} \int \delta(g - g_0)\, dg = \frac{f(x_0)}{|g'(x_0)|}. \end{aligned} \tag{3.45}$$

Thus for a function $g(x)$ that has a single zero, we have

$$\int \delta(g(x))\, f(x)\, dx = \frac{f(x_0)}{|g'(x_0)|} \quad \text{or} \quad \delta(g(x)) = \frac{\delta(x - x_0)}{|g'(x_0)|}. \tag{3.46}$$

If $g(x)$ has several zeros x_{0k}, then we must sum over them

$$\int \delta(g(x))\, f(x)\, dx = \sum_k \frac{f(x_{0k})}{|g'(x_{0k})|} \quad \text{or} \quad \delta(g(x)) = \sum_k \frac{\delta(x - x_{0k})}{|g'(x_{0k})|}. \tag{3.47}$$

Example 3.4 (Delta function of a function whose derivative vanishes)**.** The integral (3.42) for J is ill defined when $g(x_0) = g'(x_0) = 0$ unless $f(x_0) = 0$ in which case, with $y = (x - x_0)^2/2$, it is by (3.46)

$$\begin{aligned} J &= \int \delta(g(x))\, f(x)\, dx = \int \delta(\tfrac{1}{2}(x - x_0)^2\, g''(x_0))\, (x - x_0)\, f'(x_0)\, dx \\ &= \int \delta(y\, g''(x_0))\, f'(x_0)\, dy = \frac{f'(x_0)}{|g''(x_0)|}. \end{aligned} \tag{3.48}$$

So if x_0 is the only root of $g(x)$ and $g(x_0) = g'(x_0) = 0$, then

$$\delta(g(x)) = \frac{\delta(x - x_0)}{|g''(x_0)|\, (x - x_0)} \tag{3.49}$$

works in an integral like (3.42 or 3.48) if $f \in C^1$ and $f(x_0) = 0$. □

Our Dirac-comb formula (2.124) with $y = 0$ is

$$\sum_{n=-\infty}^{\infty} \frac{e^{-inx}}{2\pi} = \sum_{\ell=-\infty}^{\infty} \delta(x - 2\pi\ell). \tag{3.50}$$

Multiplying both sides of this comb by a function $f(x)$ and integrating over the real line, we have

$$\sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{-inx}}{2\pi} f(x)\, dx = \sum_{\ell=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x - 2\pi\ell)\, f(x)\, dx. \tag{3.51}$$

Our formula (3.9) for the Fourier transform $\tilde{f}(n)$ of a function $f(x)$ now gives us the **Poisson summation formula** relating a sum of a function $f(2\pi\ell)$ to a sum of its Fourier transform $\tilde{f}(n)$

$$\frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \tilde{f}(n) = \sum_{\ell=-\infty}^{\infty} f(2\pi\ell) \tag{3.52}$$

in which n and ℓ are summed over all the integers. The stretched version of the Poisson summation formula is

$$\frac{\sqrt{2\pi}}{L} \sum_{k=-\infty}^{\infty} \tilde{f}\,(2\pi k/L) = \sum_{\ell=-\infty}^{\infty} f(\ell L). \tag{3.53}$$

Both sides of these formulas make sense for continuous functions that are square integrable on the real line.

Example 3.5 (Poisson Summation Formula)**.** In example 3.1, we saw that the gaussian $f(x) = \exp(-m^2x^2)$ has $\tilde{f}(k) = \exp(-k^2/4m^2)/\sqrt{2}\, m$ as its Fourier transform. So in this case, the Poisson summation formula (3.52) gives

$$\frac{1}{2\sqrt{\pi}\, m} \sum_{k=-\infty}^{\infty} e^{-k^2/4m^2} = \sum_{\ell=-\infty}^{\infty} e^{-(2\pi\ell m)^2}. \tag{3.54}$$

For $m \gg 1$, the left-hand sum converges slowly, while the right-hand sum converges quickly. For $m \ll 1$, the right-hand sum converges slowly, while the left-hand sum converges quickly. □

A sum that converges slowly in space often converges quickly in momentum space. **Ewald summation** is a technique for summing electrostatic energies, which fall off only with a power of the distance, by summing their Fourier transforms (Darden et al., 1993).

3.4 Derivatives and integrals of Fourier transforms

By differentiating the inverse Fourier-transform relation (3.7)

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, e^{ikx} \tag{3.55}$$

we see that the Fourier transform of the derivative $f'(x)$ is $ik\tilde{f}(k)$

$$f'(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, ik\, \tilde{f}(k)\, e^{ikx}. \tag{3.56}$$

Differentiation with respect to x corresponds to multiplication by ik.

We may repeat the process and express the second derivative as

$$f''(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, (-k^2)\, \tilde{f}(k)\, e^{ikx} \tag{3.57}$$

and the nth derivative as

$$f^{(n)}(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, (ik)^n\, \tilde{f}(k)\, e^{ikx}. \tag{3.58}$$

The indefinite integral of the inverse Fourier transform (3.55) is

$$`f(x) \equiv \int^{x} dx_1\, f(x_1) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, \frac{e^{ikx}}{ik} \tag{3.59}$$

and the nth indefinite integral is

$$^{(n)}f(x) \equiv \int^{x} dx_1 \ldots \int^{x_{n-1}} dx_n\, f(x_n) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \tilde{f}(k)\, \frac{e^{ikx}}{(ik)^n}. \tag{3.60}$$

Whether these derivatives and integrals converge better or worse than $f(x)$ depends upon the behavior of $\tilde{f}(k)$ near $k = 0$ and as $|k| \to \infty$.

Example 3.6 (Momentum and Momentum Space)**.** Let's write the inverse Fourier transform (3.7) with ψ instead of f and with the wave number k replaced by $k = p/\hbar$

$$\psi(x) = \int_{-\infty}^{\infty} \tilde{\psi}(k)\, e^{ikx}\, \frac{dk}{\sqrt{2\pi}} = \int_{-\infty}^{\infty} \frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}}\, e^{ipx/\hbar} \frac{dp}{\sqrt{2\pi\hbar}}. \tag{3.61}$$

For a normalized wave function $\psi(x)$, Parseval's relation (3.41) implies

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2\, dk = \int_{-\infty}^{\infty} |\frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}}|^2\, dp. \tag{3.62}$$

or with $\psi(x) = \langle x|\psi\rangle$ and $\varphi(p) = \langle p|\psi\rangle = \tilde{\psi}(p/\hbar)/\sqrt{\hbar}$

$$\begin{aligned} 1 = \langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|\psi\rangle\, dx \\ &= \int_{-\infty}^{\infty} \langle\psi|p\rangle\langle p|\psi\rangle\, dp = \int_{-\infty}^{\infty} |\varphi(p)|^2\, dp. \end{aligned} \tag{3.63}$$

The inner product of any two states $|\psi\rangle$ and $|\phi\rangle$ is

$$\begin{aligned} \langle\psi|\phi\rangle &= \int_{-\infty}^{\infty} \psi^*(x)\phi(x)\, dx = \int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|\phi\rangle\, dx \\ &= \int_{-\infty}^{\infty} \psi^*(p)\phi(p)\, dp = \int_{-\infty}^{\infty} \langle\psi|p\rangle\langle p|\phi\rangle\, dp \end{aligned} \tag{3.64}$$

so the outer products $|x\rangle\langle x|$ and $|p\rangle\langle p|$ can represent the identity operator

$$I = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|. \tag{3.65}$$

The Fourier transform (3.61) relating the wave function in momentum space to that in position space is

$$\psi(x) = \int_{-\infty}^{\infty} e^{ipx/\hbar}\, \varphi(p)\, \frac{dp}{\sqrt{2\pi\hbar}} \tag{3.66}$$

and the inverse Fourier transform is

$$\varphi(p) = \int_{-\infty}^{\infty} e^{-ipx/\hbar}\, \psi(x)\, \frac{dx}{\sqrt{2\pi\hbar}}. \tag{3.67}$$

In Dirac notation, the first equation (3.66) of this pair is

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle\, dp = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\, \varphi(p)\, dp \tag{3.68}$$

so we identify $\langle x|p\rangle$ with

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.69}$$

which in turn is consistent with the delta-function relation (3.36)

$$\begin{aligned} \delta(x-y) = \langle x|y\rangle &= \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|y\rangle\, dp = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\, \frac{e^{-ipy/\hbar}}{\sqrt{2\pi\hbar}}\, dp \\ &= \int_{-\infty}^{\infty} \frac{e^{ip(x-y)/\hbar}}{2\pi\hbar}\, dp = \int_{-\infty}^{\infty} e^{ik(x-y)}\, \frac{dk}{2\pi}. \end{aligned} \tag{3.70}$$

If we differentiate $\psi(x)$ as given by (3.68), then we find as in (3.56)

$$\frac{\hbar}{i}\frac{d}{dx}\psi(x) = \int_{-\infty}^{\infty} p\,\varphi(p)\,e^{ipx/\hbar}\,\frac{dp}{\sqrt{2\pi\hbar}} \tag{3.71}$$

or

$$\frac{\hbar}{i}\frac{d}{dx}\psi(x) = \langle x|p|\psi\rangle = \int_{-\infty}^{\infty}\langle x|p|p'\rangle\,\langle p'|\psi\rangle\,dp' = \int_{-\infty}^{\infty} p'\,\varphi(p')\,e^{ip'x/\hbar}\,\frac{dp'}{\sqrt{2\pi\hbar}}$$

in Dirac notation. □

Example 3.7 (The Uncertainty Principle)**.** Let's first normalize the gaussian $\psi(x) = N\,\exp(-(x/a)^2)$ to unity over the real axis

$$1 = N^2\int_{-\infty}^{\infty} e^{-2(x/a)^2}\,dx = \sqrt{\frac{\pi}{2}}\,a\,N^2 \tag{3.72}$$

which gives $N^2 = \sqrt{2/\pi}/a$. So the normalized wave function is

$$\psi(x) \equiv \langle x|\psi\rangle = \left(\frac{2}{\pi}\right)^{1/4}\frac{1}{\sqrt{a}}\,e^{-(x/a)^2}. \tag{3.73}$$

The **mean value** $\langle A\rangle$ of an operator A in a state $|\psi\rangle$ is

$$\langle A\rangle \equiv \langle\psi|A|\psi\rangle. \tag{3.74}$$

More generally, the mean value of an operator A for a system described by a density operator ρ is the trace

$$\langle A\rangle \equiv \mathrm{Tr}\,(\rho A)\,. \tag{3.75}$$

Since the gaussian (3.73) is an even function of x (that is, $\psi(-x) = \psi(x)$), the mean value of the position operator x in the state (3.73) vanishes

$$\langle x\rangle = \langle\psi|x|\psi\rangle = \int_{-\infty}^{\infty} x\,|\psi(x)|^2\,dx = 0. \tag{3.76}$$

The **variance** of an operator A with mean value $\langle A\rangle$ in a state $|\psi\rangle$ is the mean value of the square of the difference $A - \langle A\rangle$

$$(\Delta A)^2 \equiv \langle\psi|\,(A - \langle A\rangle)^2\,|\psi\rangle. \tag{3.77}$$

For a system with density operator ρ, the variance of A is

$$(\Delta A)^2 \equiv \mathrm{Tr}\left[\rho\,(A - \langle A\rangle)^2\right]. \tag{3.78}$$

Since $\langle x \rangle = 0$, the variance of the position operator x is

$$(\Delta x)^2 = \langle \psi | (x - \langle x \rangle)^2 | \psi \rangle = \langle \psi | x^2 | \psi \rangle$$
$$= \int_{-\infty}^{\infty} x^2 \, |\psi(x)|^2 \, dx = \frac{a^2}{4}. \tag{3.79}$$

We can use the Fourier transform to find the variance of the momentum operator. By (3.67), the wave function $\varphi(p)$ in momentum space is

$$\varphi(p) = \langle p | \psi \rangle = \int_{-\infty}^{\infty} \langle p | x \rangle \langle x | \psi \rangle \, dx. \tag{3.80}$$

By (3.69), the inner product $\langle p | x \rangle = \langle x | p \rangle^*$ is $\langle p | x \rangle = e^{-ipx/\hbar}/\sqrt{2\pi\hbar}$, so

$$\varphi(p) = \langle p | \psi \rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \, e^{-ipx/\hbar} \langle x | \psi \rangle. \tag{3.81}$$

Thus by (3.72 & 3.73), $\varphi(p)$ is the Fourier transform

$$\varphi(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \, e^{-ipx/\hbar} \left(\frac{2}{\pi}\right)^{1/4} \frac{1}{\sqrt{a}} \, e^{-(x/a)^2}. \tag{3.82}$$

Using our formula (3.19) for the Fourier transform of a gaussian, we get

$$\varphi(p) = \sqrt{\frac{a}{2\hbar}} \left(\frac{2}{\pi}\right)^{1/4} e^{-(ap)^2/(2\hbar)^2}. \tag{3.83}$$

Since the gaussian $\varphi(p)$ is an even function of p, the mean value $\langle p \rangle$ of the momentum operator vanishes, like that of the position operator. So the variance of the momentum operator is

$$(\Delta p)^2 = \langle \psi | (p - \langle p \rangle)^2 | \psi \rangle = \langle \psi | p^2 \, | \psi \rangle = \int_{-\infty}^{\infty} p^2 \, |\varphi(p)|^2 \, dp$$
$$= \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} p^2 \, \frac{a}{2\hbar} \, e^{-(ap)^2/2\hbar^2} \, dp = \frac{\hbar^2}{a^2}. \tag{3.84}$$

Thus in this case, the product of the two variances is

$$(\Delta x)^2 \, (\Delta p)^2 = \frac{a^2}{4} \, \frac{\hbar^2}{a^2} = \frac{\hbar^2}{4} \tag{3.85}$$

which is the minimum value that the product of the variances can assume according to **Heisenberg's uncertainty principle**

$$\Delta x \, \Delta p \geq \frac{\hbar}{2} \tag{3.86}$$

which follows from the Fourier-transform relations between the conjugate variables x and p.

The state $|\psi\rangle$ of a free particle at time $t = 0$

$$|\psi, 0\rangle = \int_{-\infty}^{\infty} |p\rangle\langle p|\psi\rangle \, dp = \int_{-\infty}^{\infty} |p\rangle \varphi(p) \, dp \tag{3.87}$$

evolves under the influence of the hamiltonian $H = p^2/(2m)$ to the state

$$e^{-iHt/\hbar}|\psi, 0\rangle = \int_{-\infty}^{\infty} e^{-iHt/\hbar}|p\rangle \, \varphi(p) \, dp = \int_{-\infty}^{\infty} e^{-ip^2t/(2\hbar m)}|p\rangle \, \varphi(p) \, dp \tag{3.88}$$

at time t. □

Example 3.8 (The Characteristic Function)**.** If $P(x)$ is a **probability distribution** normalized to unity over the range of x

$$\int P(x) \, dx = 1 \tag{3.89}$$

then its Fourier transform is the **characteristic function**

$$\chi(k) = \tilde{P}(k) = \int e^{ikx} P(x) \, dx. \tag{3.90}$$

The **expected value** of a function $f(x)$ is the integral

$$E[f(x)] = \int f(x) \, P(x) \, dx. \tag{3.91}$$

So the **characteristic function** $\chi(k) = E[\exp(ikx)]$ is the expected value of the exponential $\exp(ikx)$, and its derivatives at $k = 0$ are the **moments** $E[x^n] \equiv \mu_n$ of the probability distribution

$$E[x^n] = \int x^n \, P(x) \, dx = (-i)^n \frac{d^n \chi(k)}{dk^n}\bigg|_{k=0}. \tag{3.92}$$

We'll pick up this thread again in section 14.16. □

3.5 Fourier transforms of functions of several variables

If $f(x_1, x_2)$ is a function of two variables, then its double Fourier transform $\tilde{f}(k_1, k_2)$ is

$$\tilde{f}(k_1, k_2) = \int_{-\infty}^{\infty} \frac{dx_1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dx_2}{\sqrt{2\pi}} \, e^{-ik_1x_1 - ik_2x_2} \, f(x_1, x_2). \tag{3.93}$$

By twice using the Fourier representation (3.36) of Dirac's delta function, we may invert this double Fourier transformation

$$\begin{aligned}
&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi}\, e^{i(k_1x_1+k_2x_2)}\, \tilde{f}(k_1,k_2) \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dx_1' dx_2'}{2\pi}\, e^{ik_1(x_1-x_1')+ik_2(x_2-x_2')}\, f(x_1',x_2') \\
&= \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_1' dx_2'\, e^{ik_2(x_2-x_2')}\, \delta(x_1-x_1')\, f(x_1',x_2') \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_1' dx_2'\, \delta(x_1-x_1')\delta(x_2-x_2')\, f(x_1',x_2') = f(x_1,x_2). \qquad (3.94)
\end{aligned}$$

That is

$$f(x_1,x_2) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi}\, e^{i(k_1x_1+k_2x_2)}\, \tilde{f}(k_1,k_2). \qquad (3.95)$$

The Fourier transform of a function $f(x_1,\ldots,x_n)$ of n variables is

$$\tilde{f}(k_1,\ldots,k_n) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \frac{dx_1\ldots dx_n}{(2\pi)^{n/2}}\, e^{-i(k_1x_1+\ldots+k_nx_n)}\, f(x_1,\ldots,x_n) \qquad (3.96)$$

and its inverse is

$$f(x_1,\ldots,x_n) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \frac{dk_1\ldots dk_n}{(2\pi)^{n/2}}\, e^{i(k_1x_1+\ldots+k_nx_n)}\, \tilde{f}(k_1,\ldots,k_n) \qquad (3.97)$$

in which all the integrals run from $-\infty$ to ∞.

If we generalize the relations (3.12–3.15) between Fourier series and transforms from one to n dimensions, then we find that the Fourier series corresponding to the Fourier transform (3.97) is

$$f(x_1,\ldots,x_n) = \left(\frac{2\pi}{L}\right)^n \sum_{j_1=-\infty}^{\infty}\cdots\sum_{j_n=-\infty}^{\infty} e^{i(k_{j_1}x_1+\ldots+k_{j_n}x_n)}\, \frac{\tilde{f}(k_{j_1},\ldots,k_{j_n})}{(2\pi)^{n/2}} \qquad (3.98)$$

in which $k_{j_\ell} = 2\pi j_\ell/L$. Thus, for $n=3$ we have

$$f(\boldsymbol{x}) = \frac{(2\pi)^3}{V} \sum_{j_1=-\infty}^{\infty}\sum_{j_2=-\infty}^{\infty}\sum_{j_3=-\infty}^{\infty} e^{i\boldsymbol{k_j}\cdot\boldsymbol{x}}\, \frac{\tilde{f}(\boldsymbol{k_j})}{(2\pi)^{3/2}} \qquad (3.99)$$

in which $\boldsymbol{k_j} = (k_{j_1}, k_{j_2}, k_{j_3})$ and $V = L^3$ is the volume of the box.

Example 3.9 (The Feynman Propagator)**.** For a spinless quantum field of

mass m, Feynman's propagator is the four-dimensional Fourier transform

$$\triangle_F(x) = \int \frac{\exp(ik \cdot x)}{k^2 + m^2 - i\epsilon} \frac{d^4k}{(2\pi)^4} \tag{3.100}$$

where $k \cdot x = \boldsymbol{k} \cdot \boldsymbol{x} - k^0 x^0$, all physical quantities are in **natural units** ($c = \hbar = 1$), and $x^0 = ct = t$. The tiny imaginary term $-i\epsilon$ makes $\triangle_F(x-y)$ proportional to the mean value in the vacuum state $|0\rangle$ of the **time-ordered product** of the fields $\phi(x)$ and $\phi(y)$ (section 5.43)

$$\begin{aligned} -i \triangle_F (x-y) &= \langle 0 | \mathcal{T} [\phi(x)\phi(y)] | 0 \rangle \\ &\equiv \theta(x^0 - y^0) \langle 0 | \phi(x)\phi(y) | 0 \rangle + \theta(y^0 - x^0) \langle 0 | \phi(y)\phi(x) | 0 \rangle \end{aligned} \tag{3.101}$$

in which $\theta(a) = (a + |a|)/2|a|$ is the Heaviside function (2.174). □

3.6 Convolutions

The convolution of $f(x)$ with $g(x)$ is the integral

$$f * g(x) = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} f(x-y)\, g(y). \tag{3.102}$$

The convolution product is symmetric

$$f * g(x) = g * f(x) \tag{3.103}$$

because setting $z = x - y$, we have

$$\begin{aligned} f * g(x) &= \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} f(x-y)\, g(y) = -\int_{\infty}^{-\infty} \frac{dz}{\sqrt{2\pi}} f(z)\, g(x-z) \\ &= \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} g(x-z)\, f(z) = g * f(x). \end{aligned} \tag{3.104}$$

Convolutions may look strange at first, but they often occur in physics in the three-dimensional form

$$F(\boldsymbol{x}) = \int G(\boldsymbol{x} - \boldsymbol{x}')\, S(\boldsymbol{x}')\, d^3\boldsymbol{x}' \tag{3.105}$$

in which G is a Green's function and S is a source (George Green, 1793-1841).

Example 3.10 (Gauss's law and the potential for static electric fields)**.** The divergence of the electric field $\boldsymbol{E}$ is the microscopic charge density ρ divided by the electric permittivity of the vacuum $\epsilon_0 = 8.854 \times 10^{-12}$ F/m, that is, $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$. This constraint is known as Gauss's law. If the charges and fields are independent of time, then the electric field $\boldsymbol{E}$ is the gradient of a

scalar potential $\boldsymbol{E} = -\nabla\phi$. These last two equations imply that ϕ obeys Poisson's equation

$$-\nabla^2\phi = \frac{\rho}{\epsilon_0}. \tag{3.106}$$

We may solve this equation by using Fourier transforms as described in Sec. 3.13. If $\tilde{\phi}(\boldsymbol{k})$ and $\tilde{\rho}(\boldsymbol{k})$ respectively are the Fourier transforms of $\phi(\boldsymbol{x})$ and $\rho(\boldsymbol{x})$, then Poisson's differential equation (3.106) gives

$$\begin{aligned} -\nabla^2\phi(\boldsymbol{x}) &= -\nabla^2 \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\tilde{\phi}(\boldsymbol{k})\,d^3\boldsymbol{k} = \int \boldsymbol{k}^2\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\tilde{\phi}(\boldsymbol{k})\,d^3\boldsymbol{k} \\ &= \frac{\rho(\boldsymbol{x})}{\epsilon_0} = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\frac{\tilde{\rho}(\boldsymbol{k})}{\epsilon_0}\,d^3\boldsymbol{k} \end{aligned} \tag{3.107}$$

which implies the algebraic equation $\tilde{\phi}(\boldsymbol{k}) = \tilde{\rho}(\boldsymbol{k})/\epsilon_0\boldsymbol{k}^2$ which gives $\tilde{\phi}(\boldsymbol{k})$ as a product of the Fourier transforms $\tilde{\rho}(\boldsymbol{k})$ and $1/\boldsymbol{k}^2$ (and is an instance of (3.166)). The inverse Fourier transformation of $\tilde{\phi}(\boldsymbol{k})$ is the scalar potential

$$\begin{aligned} \phi(\boldsymbol{x}) &= \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\tilde{\phi}(\boldsymbol{k})\,d^3\boldsymbol{k} = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\frac{\tilde{\rho}(\boldsymbol{k})}{\epsilon_0\,\boldsymbol{k}^2}\,d^3\boldsymbol{k} \\ &= \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\frac{1}{\boldsymbol{k}^2}\int e^{-i\boldsymbol{k}\cdot\boldsymbol{x}'}\,\frac{\rho(\boldsymbol{x}')}{\epsilon_0}\,\frac{d^3\boldsymbol{x}'d^3\boldsymbol{k}}{(2\pi)^3} = \int G(\boldsymbol{x}-\boldsymbol{x}')\,\frac{\rho(\boldsymbol{x}')}{\epsilon_0}\,d^3\boldsymbol{x}' \end{aligned} \tag{3.108}$$

in which

$$G(\boldsymbol{x}-\boldsymbol{x}') = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\,\frac{1}{\boldsymbol{k}^2}\,e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}. \tag{3.109}$$

$G(\boldsymbol{x}-\boldsymbol{x}')$ is the Green's function for the differential operator $-\nabla^2$ in the sense that

$$-\nabla^2 G(\boldsymbol{x}-\boldsymbol{x}') = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\,e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'). \tag{3.110}$$

We may think of G as the inverse of the operator $-\nabla^2$. The Green's function $G(\boldsymbol{x}-\boldsymbol{x}')$ ensures that $\phi(\boldsymbol{x})$ as given by (3.108) satisfies Poisson's equation (3.106). To integrate (3.109) and compute $G(\boldsymbol{x}-\boldsymbol{x}')$, we use spherical coordinates with the z-axis parallel to the vector $\boldsymbol{x}-\boldsymbol{x}'$

$$\begin{aligned} G(\boldsymbol{x}-\boldsymbol{x}') &= \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\,\frac{1}{\boldsymbol{k}^2}\,e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} = \int_0^\infty \frac{dk}{(2\pi)^2}\int_{-1}^{1} d\cos\theta\, e^{ik|\boldsymbol{x}-\boldsymbol{x}'|\cos\theta} \\ &= \int_0^\infty \frac{dk}{(2\pi)^2}\,\frac{e^{ik|\boldsymbol{x}-\boldsymbol{x}'|} - e^{-ik|\boldsymbol{x}-\boldsymbol{x}'|}}{ik|\boldsymbol{x}-\boldsymbol{x}'|} \\ &= \frac{1}{2\pi^2|\boldsymbol{x}-\boldsymbol{x}'|}\int_0^\infty \frac{\sin k|\boldsymbol{x}-\boldsymbol{x}'|\,dk}{k} = \frac{1}{2\pi^2|\boldsymbol{x}-\boldsymbol{x}'|}\int_0^\infty \frac{\sin k\,dk}{k}. \end{aligned} \tag{3.111}$$

In example 5.44 of section 5.43 on Cauchy's principal value, we'll show that

$$\int_0^\infty \frac{\sin k}{k}\, dk = \frac{\pi}{2}. \tag{3.112}$$

Using this result, we have

$$\int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\, \frac{1}{\boldsymbol{k}^2}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} = G(\boldsymbol{x}-\boldsymbol{x}') = \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{3.113}$$

Finally by substituting this formula for $G(\boldsymbol{x}-\boldsymbol{x}')$ into Eq. (3.108), we find that the Fourier transform $\phi(x)$ of the product $\tilde{\rho}(\boldsymbol{k})/\boldsymbol{k}^2$ of the functions $\tilde{\rho}(\boldsymbol{k})$ and $1/\boldsymbol{k}^2$ is the convolution

$$\phi(\boldsymbol{x}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|}\, d^3\boldsymbol{x}' \tag{3.114}$$

of their Fourier transforms $1/|\boldsymbol{x}-\boldsymbol{x}'|$ and $\rho(\boldsymbol{x}')$. The Fourier transform of the product of any two functions is the convolution of their Fourier transforms, as we'll see in the next section. (George Green 1793–1841) □

Example 3.11 (Static magnetic vector potential)**.** The magnetic induction $\boldsymbol{B}$ has zero divergence (as long as there are no magnetic monopoles) and so may be written as the curl $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ of a vector potential $\boldsymbol{A}$. For static currents, Ampère's law is $\nabla \times \boldsymbol{B} = \mu_0 \boldsymbol{J}$ in which $\mu_0 = 1/(\epsilon_0 c^2) = 4\pi \times 10^{-7}$ N A^{-2} is the permeability of the vacuum. It follows that in the Coulomb gauge $\nabla \cdot \boldsymbol{A} = 0$, the magnetostatic vector potential $\boldsymbol{A}$ satisfies the equation

$$\nabla \times \boldsymbol{B} = \nabla \times (\nabla \times \boldsymbol{A}) = \nabla\,(\nabla \cdot \boldsymbol{A}) - \nabla^2 \boldsymbol{A} = -\nabla^2 \boldsymbol{A} = \mu_0 \boldsymbol{J}. \tag{3.115}$$

Applying the Fourier-transform technique (3.106–3.114), we find that the Fourier transforms of $\boldsymbol{A}$ and $\boldsymbol{J}$ satisfy the algebraic equation

$$\tilde{\boldsymbol{A}}(\boldsymbol{k}) = \mu_0\, \frac{\tilde{\boldsymbol{J}}(\boldsymbol{k})}{\boldsymbol{k}^2} \tag{3.116}$$

which is an instance of (3.166). Performing the inverse Fourier transform, we see that $\boldsymbol{A}$ is the convolution

$$\boldsymbol{A}(\boldsymbol{x}) = \frac{\mu_0}{4\pi} \int d^3\boldsymbol{x}'\, \frac{\boldsymbol{J}(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{3.117}$$

If in the solution (3.114) of Poisson's equation, $\rho(\boldsymbol{x})$ is translated by $\boldsymbol{a}$, then so is $\phi(\boldsymbol{x})$. That is, if $\rho'(\boldsymbol{x}) = \rho(\boldsymbol{x}+\boldsymbol{a})$ then $\phi'(\boldsymbol{x}) = \phi(\boldsymbol{x}+\boldsymbol{a})$. Similarly, if the current $\boldsymbol{J}(\boldsymbol{x})$ in (3.117) is translated by $\boldsymbol{a}$, then so is the potential $\boldsymbol{A}(\boldsymbol{x})$.

Convolutions respect translational invariance. That's one reason why they occur so often in the formulas of physics. □

3.7 Fourier transform of a convolution

The Fourier transform of the convolution $f * g$ is the product of the Fourier transforms $\tilde{f}$ and $\tilde{g}$:

$$\widetilde{f * g}(k) = \tilde{f}(k)\,\tilde{g}(k). \tag{3.118}$$

To see why, we form the Fourier transform $\widetilde{f * g}(k)$ of the convolution $f*g(x)$

$$\begin{aligned}\widetilde{f * g}(k) &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx}\, f * g(x) \\ &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}}\, f(x-y)\, g(y).\end{aligned} \tag{3.119}$$

Now we write $f(x-y)$ and $g(y)$ in terms of their Fourier transforms $\tilde{f}(p)$ and $\tilde{g}(q)$

$$\widetilde{f * g}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, e^{-ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}}\, \tilde{f}(p)\, e^{ip(x-y)} \int_{-\infty}^{\infty} \frac{dq}{\sqrt{2\pi}}\, \tilde{g}(q)\, e^{iqy} \tag{3.120}$$

and use the representation (3.36) of Dirac's delta function twice to get

$$\begin{aligned}\widetilde{f * g}(k) &= \int_{-\infty}^{\infty} \frac{dy}{2\pi} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq\, \delta(p-k)\, \tilde{f}(p)\, \tilde{g}(q)\, e^{i(q-p)y} \\ &= \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq\, \delta(p-k)\, \delta(q-p)\, \tilde{f}(p)\, \tilde{g}(q) \\ &= \int_{-\infty}^{\infty} dp\, \delta(p-k)\, \tilde{f}(p)\, \tilde{g}(p) = \tilde{f}(k)\, \tilde{g}(k)\end{aligned} \tag{3.121}$$

which is (3.118). Examples 3.10 and 3.11 illustrate this result.

3.8 Fourier transforms and Green's functions

A Green's function $G(x)$ for a differential operator P turns into a delta function when acted upon by P, that is, $PG(x) = \delta(x)$. If the differential operator is a polynomial $P(\partial) \equiv P(\partial_1, \ldots, \partial_n)$ in the derivatives $\partial_1, \ldots, \partial_n$ with constant coefficients, then a suitable Green's function $G(x) \equiv G(x_1, \ldots, x_n)$ will satisfy

$$P(\partial)G(x) = \delta^{(n)}(x). \tag{3.122}$$

Expressing both $G(x)$ and $\delta^{(n)}(x)$ as Fourier transforms, we get

$$P(\partial)G(x) = \int d^n k\, P(ik)\, e^{ik\cdot x}\, \tilde{G}(k) = \delta^{(n)}(x) = \int \frac{d^n k}{(2\pi)^n}\, e^{ik\cdot x} \tag{3.123}$$

which gives us the algebraic equation

$$\tilde{G}(k) = \frac{1}{(2\pi)^n\, P(ik)}. \tag{3.124}$$

Thus the Green's function G_P for the differential operator $P(\partial)$ is

$$G_P(x) = \int \frac{d^n k}{(2\pi)^n}\, \frac{e^{ik\cdot x}}{P(ik)}. \tag{3.125}$$

Example 3.12 (Green and Yukawa)**.** In 1935, Hideki Yukawa (1907–1981) proposed the partial differential equation

$$P_Y(\partial)G_Y(\boldsymbol{x}) \equiv (-\triangle + m^2)G_Y(\boldsymbol{x}) = (-\nabla^2 + m^2)G_Y(\boldsymbol{x}) = \delta(\boldsymbol{x}). \tag{3.126}$$

Our (3.125) gives as the Green's function for $P_Y(\partial)$ the Yukawa potential

$$G_Y(x) = \int \frac{d^3 k}{(2\pi)^3}\, \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{P_Y(ik)} = \int \frac{d^3 k}{(2\pi)^3}\, \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{\boldsymbol{k}^2 + m^2} = \frac{e^{-mr}}{4\pi r} \tag{3.127}$$

an integration done in example 5.26. □

3.9 Laplace transforms

The Laplace transform $f(s)$ of a function $F(t)$ is the integral

$$f(s) = \int_0^\infty dt\, e^{-st}\, F(t). \tag{3.128}$$

Because the integration is over positive values of t, the exponential $\exp(-st)$ falls off rapidly with the real part of s. As $\operatorname{Re} s$ increases, the Laplace transform $f(s)$ becomes smoother and smaller. For $\operatorname{Re} s > 0$, the exponential $\exp(-st)$ lets many functions $F(t)$ that are not integrable over the half line $[0, \infty)$ have well-behaved Laplace transforms.

For instance, the function $F(t) = 1$ is not integrable over the half line $[0, \infty)$, but its Laplace transform

$$f(s) = \int_0^\infty dt\, e^{-st}\, F(t) = \int_0^\infty dt\, e^{-st} = \frac{1}{s} \tag{3.129}$$

is well defined for $\operatorname{Re} s > 0$ and square integrable for $\operatorname{Re} s > \epsilon$.

The function $F(t) = \exp(kt)$ diverges exponentially for $\operatorname{Re} k > 0$, but its Laplace transform

$$f(s) = \int_0^\infty dt\, e^{-st}\, F(t) = \int_0^\infty dt\, e^{-(s-k)t} = \frac{1}{s-k} \tag{3.130}$$

is well defined for $\operatorname{Re} s > k$ with a simple pole at $s = k$ (section 5.10) and is square integrable for $\operatorname{Re} s > k + \epsilon$.

The Laplace transforms of $\cosh kt$ and $\sinh kt$ are

$$f(s) = \int_0^\infty dt\, e^{-st}\, \cosh kt = \frac{1}{2} \int_0^\infty dt\, e^{-st} \left(e^{kt} + e^{-kt}\right) = \frac{s}{s^2 - k^2} \tag{3.131}$$

and

$$f(s) = \int_0^\infty dt\, e^{-st}\, \sinh kt = \frac{1}{2} \int_0^\infty dt\, e^{-st} \left(e^{kt} - e^{-kt}\right) = \frac{k}{s^2 - k^2}. \tag{3.132}$$

The Laplace transform of $\cos \omega t$ is

$$f(s) = \int_0^\infty dt\, e^{-st}\, \cos \omega t = \frac{1}{2} \int_0^\infty dt\, e^{-st} \left(e^{i\omega t} + e^{-i\omega t}\right) = \frac{s}{s^2 + \omega^2} \tag{3.133}$$

and that of $\sin \omega t$ is

$$f(s) = \int_0^\infty dt\, e^{-st}\, \sin \omega t = \frac{1}{2i} \int_0^\infty dt\, e^{-st} \left(e^{i\omega t} - e^{-i\omega t}\right) = \frac{\omega}{s^2 + \omega^2}. \tag{3.134}$$

Example 3.13 (Lifetime of a Fluorophore)**.** Fluorophores are molecules that emit visible light when excited by photons. The probability $P(t, t')$ that a fluorophore with a lifetime τ will emit a photon at time t if excited by a photon at time t' is

$$P(t, t') = \tau\, e^{-(t-t')/\tau}\, \theta(t - t') \tag{3.135}$$

in which $\theta(t - t') = (t - t' + |t - t'|)/2|t - t'|$ is the Heaviside function. One way to measure the lifetime τ of a fluorophore is to modulate the exciting laser beam at a frequency $\nu = 2\pi\omega$ of the order of 60 MHz and to detect the phase-shift ϕ in the light $L(t)$ emitted by the fluorophore. That light is the integral of $P(t, t')$ times the modulated beam $\sin \omega t$ or equivalently the convolution of $e^{-t/\tau}\theta(t)$ with $\sin \omega t$

$$\begin{aligned} L(t) &= \int_{-\infty}^\infty P(t, t')\, \sin(\omega t')\, dt' = \int_{-\infty}^\infty \tau\, e^{-(t-t')/\tau} \theta(t - t')\, \sin(\omega t')\, dt' \\ &= \int_{-\infty}^t \tau\, e^{-(t-t')/\tau} \sin(\omega t')\, dt'. \end{aligned} \tag{3.136}$$

Letting $u = t - t'$ and using the trigonometric formula

$$\sin(a - b) = \sin a \cos b - \cos a \sin b \tag{3.137}$$

we may relate this integral to the Laplace transforms of a sine (3.134) and a cosine (3.133)

$$\begin{aligned} L(t) &= -\tau \int_0^\infty e^{-u/\tau} \sin\omega(u - t)\, du \\ &= -\tau \int_0^\infty e^{-u/\tau} \left(\sin\omega u \cos\omega t - \cos\omega u \sin\omega t\right) du \\ &= \tau \left(\frac{\sin(\omega t)/\tau}{1/\tau^2 + \omega^2} - \frac{\omega \cos\omega t}{1/\tau^2 + \omega^2} \right). \end{aligned} \tag{3.138}$$

Setting $\cos\phi = (1/\tau)/\sqrt{1/\tau^2 + \omega^2}$ and $\sin\phi = \omega/\sqrt{1/\tau^2 + \omega^2}$, we have

$$L(t) = \frac{\tau}{\sqrt{1/\tau^2 + \omega^2}} \left(\sin\omega t \cos\phi - \cos\omega t \sin\phi\right) = \frac{\tau}{\sqrt{1/\tau^2 + \omega^2}} \sin(\omega t - \phi). \tag{3.139}$$

The phase-shift ϕ then is given by

$$\phi = \arcsin \frac{\omega}{\sqrt{1/\tau^2 + \omega^2}} \leq \frac{\pi}{2}. \tag{3.140}$$

So by inverting this formula, we get the lifetime of the fluorophore

$$\tau = (1/\omega) \tan\phi \tag{3.141}$$

in terms of the phase-shift ϕ which is much easier to measure. □

3.10 Derivatives and integrals of Laplace transforms

The derivatives of a Laplace transform $f(s)$ are by its definition (3.128)

$$\frac{d^n f(s)}{ds^n} = \int_0^\infty dt\, (-t)^n\, e^{-st}\, F(t). \tag{3.142}$$

They usually are well defined if $f(s)$ is well defined. For instance, if we differentiate the Laplace transform (3.129) of the function $F(t) = 1$ which is $f(s) = 1/s$, then we get

$$(-1)^n \frac{d^n s^{-1}}{ds^n} = \frac{n!}{s^{n+1}} = \int_0^\infty dt\, e^{-st}\, t^n \tag{3.143}$$

which tells us that the Laplace transform of t^n is $n!/s^{n+1}$.

The result of differentiating the function $F(t)$ also has a simple form. Integrating by parts, we find for the Laplace transform of $F'(t)$

$$\begin{aligned}\int_0^\infty dt\, e^{-st}\, F'(t) &= \int_0^\infty dt\, \left\{ \frac{d}{dt}\left[e^{-st}\, F(t)\right] - F(t)\frac{d}{dt}\, e^{-st} \right\} \\ &= -\, F(0) + \int_0^\infty dt\, F(t)\, s\, e^{-st} \\ &= -\, F(0) + s\, f(s) \end{aligned} \tag{3.144}$$

as long as $e^{-st}F(t) \to 0$ as $t \to \infty$.

The indefinite integral of the Laplace transform (3.128) is

$$`f(s) \equiv \int ds_1\, f(s_1) = \int_0^\infty dt\, \frac{e^{-st}}{(-t)}\, F(t) \tag{3.145}$$

and its nth indefinite integral is

$$^{(n)}f(s) \equiv \int ds_n \ldots \int ds_1\, f(s_1) = \int_0^\infty dt\, \frac{e^{-st}}{(-t)^n}\, F(t). \tag{3.146}$$

If $f(s)$ is a well-behaved function, then these indefinite integrals usually are well defined for $s > 0$ as long as $F(t) \to 0$ suitably as $t \to 0$.

3.11 Laplace transforms and differential equations

Suppose we wish to solve the differential equation

$$P(d/ds)\, f(s) = j(s). \tag{3.147}$$

By writing $f(s)$ and $j(s)$ as Laplace transforms

$$f(s) = \int_0^\infty e^{-st}\, F(t)\, dt \quad \text{and} \quad j(s) = \int_0^\infty e^{-st}\, J(t)\, dt. \tag{3.148}$$

and using the formula (3.142) for the nth derivative of a Laplace transform, we see that the differential equation (3.147) amounts to

$$P(d/ds)\, f(s) = \int_0^\infty e^{-st}\, P(-t)\, F(t)\, dt = \int_0^\infty e^{-st}\, J(t)\, dt. \tag{3.149}$$

which is equivalent to the algebraic equation

$$F(t) = \frac{J(t)}{P(-t)}. \tag{3.150}$$

A particular solution to the inhomogeneous differential equation (3.147) is then the Laplace transform of this ratio

$$f(s) = \int_0^\infty e^{-st}\, \frac{J(t)}{P(-t)}\, dt. \tag{3.151}$$

A fairly general solution of the associated homogeneous equation

$$P(d/ds)\, f(s) = 0 \tag{3.152}$$

is the Laplace transform

$$f(s) = \int_0^\infty e^{-st}\, \delta(P(-t))\, H(t)\, dt \tag{3.153}$$

because

$$P(d/ds)\, f(s) = \int_0^\infty e^{-st}\, P(-t)\, \delta(P(-t))\, H(t)\, dt = 0 \tag{3.154}$$

as long as the function $H(t)$ is suitably smooth but otherwise arbitrary. Thus our solution of the inhomogeneous equation (3.147) is the sum of the two

$$f(s) = \int_0^\infty e^{-st}\, \frac{J(t)}{P(-t)}\, dt + \int_0^\infty e^{-st}\, \delta(P(-t))\, H(t)\, dt. \tag{3.155}$$

One may generalize this method to differential equations in n variables. But to carry out this procedure, one must be able to find the inverse Laplace transform $J(t)$ of the source function $j(s)$ as outlined in the next section.

3.12 Inversion of Laplace transforms

How do we invert the Laplace transform

$$f(s) = \int_0^\infty dt\, e^{-st}\, F(t)? \tag{3.156}$$

First we extend the Laplace transform from real s to $s + iu$

$$f(s + iu) = \int_0^\infty dt\, e^{-(s+iu)t}\, F(t) \tag{3.157}$$

and choose s to be sufficiently positive that $f(s+iu)$ is suitably smooth and bounded. Then we apply the delta-function formula (3.36) to the integral

$$\begin{aligned} \int_{-\infty}^\infty \frac{du}{2\pi}\, e^{iut}\, f(s + iu) &= \int_{-\infty}^\infty \frac{du}{2\pi} \int_0^\infty dt'\, e^{iut}\, e^{-(s+iu)t'}\, F(t') \\ &= \int_0^\infty dt'\, e^{-st'}\, F(t') \int_{-\infty}^\infty \frac{du}{2\pi}\, e^{iu(t-t')} \\ &= \int_0^\infty dt'\, e^{-st'}\, F(t')\, \delta(t - t') = e^{-st}\, F(t). \end{aligned} \tag{3.158}$$

So our inversion formula is

$$F(t) = e^{st} \int_{-\infty}^\infty \frac{du}{2\pi}\, e^{iut}\, f(s + iu) \tag{3.159}$$

for sufficiently large s. Some call this inversion formula a Bromwich integral, others a Fourier-Mellin integral.

3.13 Application to differential equations

Let us consider a linear partial differential equation in n variables

$$P(\partial_1, \ldots, \partial_n) f(x_1, \ldots, x_n) = g(x_1, \ldots, x_n) \tag{3.160}$$

in which P is a polynomial in the derivatives

$$\partial_j \equiv \frac{\partial}{\partial x_j} \tag{3.161}$$

with constant coefficients. If $g = 0$, the equation is homogeneous; otherwise it is inhomogeneous. We expand the solution and source as integral transforms

$$\begin{aligned} f(x_1, \ldots, x_n) &= \int \tilde{f}(k_1, \ldots, k_n)\, e^{i(k_1 x_1 + \ldots + k_n x_n)} d^n k \\ g(x_1, \ldots, x_n) &= \int \tilde{g}(k_1, \ldots, k_n)\, e^{i(k_1 x_1 + \ldots + k_n x_n)} d^n k \end{aligned} \tag{3.162}$$

in which the k integrals may run from $-\infty$ to ∞ as in a Fourier transform or up the imaginary axis from 0 to ∞ as in a Laplace transform.

The correspondence (3.58) between differentiation with respect to x_j and multiplication by ik_j tells us that ∂_j^m acting on f gives

$$\partial_j^m f(x_1, \ldots, x_n) = \int \tilde{f}(k_1, \ldots, k_n)\, (ik_j)^m\, e^{i(k_1 x_1 + \ldots + k_n x_n)}\, d^n k. \tag{3.163}$$

If we abbreviate $f(x_1, \ldots, x_n)$ by $f(x)$ and do the same for g, then we may write our partial differential equation (3.160) as

$$\begin{aligned} P(\partial_1, \ldots, \partial_n) f(x) &= \int \tilde{f}(k)\, P(ik_1, \ldots, ik_n)\, e^{i(k_1 x_1 + \ldots + k_n x_n)}\, d^n k \\ &= \int \tilde{g}(k)\, e^{i(k_1 x_1 + \ldots + k_n x_n)}\, d^n k. \end{aligned} \tag{3.164}$$

Thus the inhomogeneous partial differential equation

$$P(\partial_1, \ldots, \partial_n) f_i(x_1, \ldots, x_n) = g(x_1, \ldots, x_n) \tag{3.165}$$

becomes an algebraic equation in k-space

$$P(ik_1, \ldots, ik_n)\, \tilde{f}_i(k_1, \ldots, k_n) = \tilde{g}(k_1, \ldots, k_n) \tag{3.166}$$

where $\tilde{g}(k_1, \ldots, k_n)$ is the mixed Fourier-Laplace transform of $g(x_1, \ldots, x_n)$. So one solution of the inhomogeneous differential equation (3.160) is

$$f_i(x_1, \ldots, x_n) = \int e^{i(k_1 x_1 + \ldots + k_n x_n)} \frac{\tilde{g}(k_1, \ldots, k_n)}{P(ik_1, \ldots, ik_n)} \, d^n k. \tag{3.167}$$

The space of solutions to the **homogeneous** form of equation (3.160)

$$P(\partial_1, \ldots, \partial_n) f_h(x_1, \ldots, x_n) = 0 \tag{3.168}$$

is vast. We will focus on those that satisfy the algebraic equation

$$P(ik_1, \ldots, ik_n) \tilde{f}_h(k_1, \ldots, k_n) = 0 \tag{3.169}$$

and that we can write in terms of Dirac's delta function as

$$\tilde{f}_h(k_1, \ldots, k_n) = \delta(P(ik_1, \ldots, ik_n)) \, h(k_1, \ldots, k_n) \tag{3.170}$$

in which the function $h(k)$ is arbitrary. That is

$$f_h(x) = \int e^{i(k_1 x_1 + \ldots + k_n x_n)} \delta(P(ik_1, \ldots, ik_n)) \, h(k) \, d^n k. \tag{3.171}$$

Our solution to the differential equation (3.160) then is a sum of a particular solution (3.167) of the inhomogeneous equation (3.166) and our solution (3.171) of the associated homogeneous equation (3.168)

$$\begin{aligned} f(x_1, \ldots, x_n) = \int e^{i(k_1 x_1 + \ldots + k_n x_n)} \Bigg[& \frac{\tilde{g}(k_1, \ldots, k_n)}{P(ik_1, \ldots, ik_n)} \\ & + \delta(P(ik_1, \ldots, ik_n)) \, h(k_1, \ldots, k_n) \Bigg] d^n k \end{aligned} \tag{3.172}$$

in which $h(k_1, \ldots, k_n)$ is an arbitrary function. The wave equation and the diffusion equation will provide examples of this formula

$$f(x) = \int e^{ik \cdot x} \left[\frac{\tilde{g}(k)}{P(ik)} + \delta(P(ik)) h(k) \right] d^n k. \tag{3.173}$$

Example 3.14 (Wave Equation for a Scalar Field)**.** A free scalar field $\phi(x)$ of mass m in flat spacetime obeys the wave equation

$$\left(\nabla^2 - \partial_t^2 - m^2 \right) \phi(x) = 0 \tag{3.174}$$

in natural units ($\hbar = c = 1$). We may use a four-dimensional Fourier transform to represent the field $\phi(x)$ as

$$\phi(x) = \int e^{ik \cdot x} \, \tilde{\phi}(k) \, \frac{d^4 k}{(2\pi)^2} \tag{3.175}$$

in which $k \cdot x = \boldsymbol{k} \cdot \boldsymbol{x} - k^0 t$ is the Lorentz-invariant inner product.

The homogeneous wave equation (3.174) then says

$$\left(\nabla^2 - \partial_t^2 - m^2\right) \phi(x) = \int \left(-\boldsymbol{k}^2 + (k^0)^2 - m^2\right) e^{ik\cdot x}\, \tilde{\phi}(k)\, \frac{d^4k}{(2\pi)^2} = 0 \quad (3.176)$$

which implies the algebraic equation

$$\left(-\boldsymbol{k}^2 + (k^0)^2 - m^2\right) \tilde{\phi}(k) = 0 \quad (3.177)$$

an instance of (3.169). Our solution (3.171) is

$$\phi(x) = \int \delta\left(-\boldsymbol{k}^2 + (k^0)^2 - m^2\right)\, e^{ik\cdot x}\, h(k)\, \frac{d^4k}{(2\pi)^2} \quad (3.178)$$

in which $h(k)$ is an arbitrary function. The argument of the delta function

$$P(ik) = (k^0)^2 - \boldsymbol{k}^2 - m^2 = \left(k^0 - \sqrt{\boldsymbol{k}^2 + m^2}\right)\left(k^0 + \sqrt{\boldsymbol{k}^2 + m^2}\right) \quad (3.179)$$

has zeros at $k^0 = \pm\sqrt{\boldsymbol{k}^2 + m^2} \equiv \pm\omega_k$ with

$$\left|\frac{dP(\pm\omega_k)}{dk^0}\right| = 2\omega_k. \quad (3.180)$$

So using our formula (3.47) for integrals involving delta functions of functions, we have

$$\phi(x) = \int \left[e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, h_+(\boldsymbol{k}) + e^{i(\boldsymbol{k}\cdot\boldsymbol{x} + \omega_k t)}\, h_-(\boldsymbol{k})\right] \frac{d^3k}{(2\pi)^2 2\omega_k} \quad (3.181)$$

where $h_\pm(\boldsymbol{k}) \equiv h(\pm\omega_k, \boldsymbol{k})$. Since ω_k is an even function of $\boldsymbol{k}$, we can write

$$\phi(x) = \int \left[e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, h_+(\boldsymbol{k}) + e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, h_-(-\boldsymbol{k})\right] \frac{d^3k}{(2\pi)^2 2\omega_k}. \quad (3.182)$$

If $\phi(x) = \phi(\boldsymbol{x}, t)$ is a real-valued classical field, then its Fourier transform $h(\boldsymbol{k})$ must obey the relation (3.25) which says that $h_-(-\boldsymbol{k}) = h_+(\boldsymbol{k})^*$. If ϕ is a hermitian quantum field, then $h_-(-\boldsymbol{k}) = h_+^\dagger(\boldsymbol{k})$. In terms of the **annihilation** operator $a(\boldsymbol{k}) \equiv h_+(\boldsymbol{k})/\sqrt{4\pi\omega_k}$ and its adjoint $a^\dagger(\boldsymbol{k})$, a creation operator, the field $\phi(x)$ is the integral

$$\phi(x) = \int \left[e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, a(\boldsymbol{k}) + e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, a^\dagger(\boldsymbol{k})\right] \frac{d^3k}{\sqrt{(2\pi)^3 2\omega_k}}. \quad (3.183)$$

The momentum π canonically conjugate to the field is its time derivative

$$\pi(x) = -i \int \left[e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, a(\boldsymbol{k}) - e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\, a^\dagger(\boldsymbol{k})\right] \sqrt{\frac{\omega_k}{2(2\pi)^3}}\, d^3k. \quad (3.184)$$

If the operators a and $a^\dagger$ obey the commutation relations

$$[a(\boldsymbol{k}), a^\dagger(\boldsymbol{k'})] = \delta(\boldsymbol{k} - \boldsymbol{k'}) \quad \text{and} \quad [a(\boldsymbol{k}), a(\boldsymbol{k'})] = [a^\dagger(\boldsymbol{k}), a^\dagger(\boldsymbol{k'})] = 0 \tag{3.185}$$

then the field $\phi(\boldsymbol{x}, t)$ and its conjugate momentum $\pi(\boldsymbol{y}, t)$ satisfy (exercise 3.17) the equal-time commutation relations

$$[\phi(\boldsymbol{x}, t), \pi(\boldsymbol{y}, t)] = i\delta(\boldsymbol{x} - \boldsymbol{y}) \quad \text{and} \quad [\phi(\boldsymbol{x}, t), \phi(\boldsymbol{y}, t)] = [\pi(\boldsymbol{x}, t), \pi(\boldsymbol{y}, t)] = 0 \tag{3.186}$$

which generalize the commutation relations of quantum mechanics

$$[q_j, p_\ell] = i\hbar\delta_{j,\ell} \quad \text{and} \quad [q_j, q_\ell] = [p_j, p_\ell] = 0 \tag{3.187}$$

for a set of coordinates q_j and conjugate momenta p_ℓ. □

Example 3.15 (Fourier Series for a Scalar Field)**.** For a field defined in a cube of volume $V = L^3$, one often imposes periodic boundary conditions (section 2.14) in which a displacement of any spatial coordinate by $\pm L$ does not change the value of the field. A Fourier series can represent a periodic field. Using the relationship (3.99) between Fourier-transform and Fourier-series representations in 3 dimensions, we expect the Fourier series representation for the field (3.183) to be

$$\begin{aligned}\phi(x) &= \frac{(2\pi)^3}{V} \sum_{\boldsymbol{k}} \frac{1}{\sqrt{(2\pi)^3 2\omega_k}} \left[a(\boldsymbol{k}) e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)} + a^\dagger(\boldsymbol{k}) e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\right] \\ &= \sum_{\boldsymbol{k}} \frac{1}{\sqrt{2\omega_k V}} \sqrt{\frac{(2\pi)^3}{V}} \left[a(\boldsymbol{k}) e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)} + a^\dagger(\boldsymbol{k}) e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\right]\end{aligned} \tag{3.188}$$

in which the sum over $\boldsymbol{k} = (2\pi/L)(\ell, n, m)$ is over all (positive and negative) integers ℓ, n, and m. One can set

$$a_{\boldsymbol{k}} \equiv \sqrt{\frac{(2\pi)^3}{V}}\, a(\boldsymbol{k}) \tag{3.189}$$

and write the field as

$$\phi(x) = \sum_{\boldsymbol{k}} \frac{1}{\sqrt{2\omega_k V}} \left[a_{\boldsymbol{k}}\, e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)} + a^\dagger_{\boldsymbol{k}}\, e^{-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_k t)}\right]. \tag{3.190}$$

The commutator of Fourier-series annihilation and creation operators is by (3.36, 3.185 & 3.189)

$$\begin{aligned}[a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k'}}] &= \frac{(2\pi)^3}{V} [a(\boldsymbol{k}), a^\dagger(\boldsymbol{k'})] = \frac{(2\pi)^3}{V} \delta(\boldsymbol{k} - \boldsymbol{k'}) \\ &= \frac{(2\pi)^3}{V} \int e^{i(\boldsymbol{k} - \boldsymbol{k'})\cdot\boldsymbol{x}} \frac{d^3x}{(2\pi)^3} = \frac{(2\pi)^3}{V} \frac{V}{(2\pi)^3} \delta_{\boldsymbol{k},\boldsymbol{k'}} = \delta_{\boldsymbol{k},\boldsymbol{k'}}\end{aligned} \tag{3.191}$$

in which the Kronecker delta $\delta_{\boldsymbol{k},\boldsymbol{k}'}$ is $\delta_{\ell,\ell'}\delta_{n,n'}\delta_{m,m'}$. □

Example 3.16 (Diffusion)**.** The flow rate $\boldsymbol{J}$ (per unit area, per unit time) of a fixed number of randomly moving particles, such as molecules of a gas or a liquid, is proportional to the negative gradient of their density $\rho(\boldsymbol{x},t)$

$$\boldsymbol{J}(\boldsymbol{x},t) = -D\,\nabla\rho(\boldsymbol{x},t) \tag{3.192}$$

where D is the **diffusion constant**, an equation known as **Fick's law** (Adolf Fick 1829–1901). Since the number of particles is conserved, the 4-vector $J = (\rho, \boldsymbol{J})$ obeys the conservation law

$$\frac{\partial}{\partial t}\int \rho(\boldsymbol{x},t)\,d^3\boldsymbol{x} = -\oint \boldsymbol{J}(\boldsymbol{x},t)\cdot d\boldsymbol{a} = -\int \nabla\cdot\boldsymbol{J}(\boldsymbol{x},t)d^3\boldsymbol{x} \tag{3.193}$$

which with Fick's law (3.192) gives the **diffusion equation**

$$\dot\rho(\boldsymbol{x},t) = -\nabla\cdot\boldsymbol{J}(\boldsymbol{x},t) = D\,\nabla^2\rho(\boldsymbol{x},t) \quad \text{or} \quad \left(D\,\nabla^2 - \partial_t\right)\rho(\boldsymbol{x},t) = 0. \tag{3.194}$$

Fourier had in mind such equations when he invented his transform.

If we write the density $\rho(\boldsymbol{x},t)$ as the transform

$$\rho(\boldsymbol{x},t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\omega t}\,\tilde\rho(\boldsymbol{k},\omega)\,d^3\boldsymbol{k}d\omega \tag{3.195}$$

then the diffusion equation becomes

$$\left(D\,\nabla^2 - \partial_t\right)\rho(\boldsymbol{x},t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\omega t}\left(-D\,\boldsymbol{k}^2 - i\omega\right)\tilde\rho(\boldsymbol{k},\omega)\,d^3\boldsymbol{k}\,d\omega = 0 \tag{3.196}$$

which implies the algebraic equation

$$\left(D\,\boldsymbol{k}^2 + i\omega\right)\tilde\rho(\boldsymbol{k},\omega) = 0. \tag{3.197}$$

Our solution (3.171) of this homogeneous equation is

$$\rho(\boldsymbol{x},t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\omega t}\,\delta\left(-D\,\boldsymbol{k}^2 - i\omega\right)h(\boldsymbol{k},\omega)\,d^3\boldsymbol{k}\,d\omega \tag{3.198}$$

in which $h(\boldsymbol{k},\omega)$ is an arbitrary function. Dirac's delta function requires ω to be imaginary $\omega = iD\boldsymbol{k}^2$, with $D\boldsymbol{k}^2 > 0$. So the ω-integration is up the imaginary axis. It is a Laplace transform, and we have

$$\rho(\boldsymbol{x},t) = \int_{-\infty}^{\infty} e^{i\boldsymbol{k}\cdot\boldsymbol{x}-D\boldsymbol{k}^2 t}\,\tilde\rho(\boldsymbol{k})\,d^3\boldsymbol{k} \tag{3.199}$$

in which $\tilde\rho(\boldsymbol{k}) \equiv h(\boldsymbol{k}, iD\boldsymbol{k}^2)$. Thus the function $\tilde\rho(\boldsymbol{k})$ is the Fourier transform of the initial density $\rho(\boldsymbol{x},0)$

$$\rho(\boldsymbol{x},0) = \int_{-\infty}^{\infty} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\,\tilde\rho(\boldsymbol{k})\,d^3\boldsymbol{k}. \tag{3.200}$$

So if the initial density $\rho(\boldsymbol{x}, 0)$ is concentrated at $\boldsymbol{y}$

$$\rho(\boldsymbol{x}, 0) = \delta(\boldsymbol{x} - \boldsymbol{y}) = \int_{-\infty}^{\infty} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \frac{d^3\boldsymbol{k}}{(2\pi)^3} \tag{3.201}$$

then its Fourier transform $\tilde{\rho}(\boldsymbol{k})$ is

$$\tilde{\rho}(\boldsymbol{k}) = \frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{y}}}{(2\pi)^3} \tag{3.202}$$

and at later times the density $\rho(\boldsymbol{x}, t)$ is given by (3.199) as

$$\rho(\boldsymbol{x}, t) = \int_{-\infty}^{\infty} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y}) - D\boldsymbol{k}^2 t} \frac{d^3\boldsymbol{k}}{(2\pi)^3}. \tag{3.203}$$

Using our formula (3.19) for the Fourier transform of a gaussian, we find

$$\rho(\boldsymbol{x}, t) = \frac{1}{(4\pi D t)^{3/2}} \, e^{-(\boldsymbol{x}-\boldsymbol{y})^2/(4Dt)}. \tag{3.204}$$

Since the diffusion equation is linear, it follows (exercise 3.18) that an arbitrary initial distribution $\rho(\boldsymbol{y}, 0)$ evolves to the convolution (section 3.6)

$$\rho(\boldsymbol{x}, t) = \frac{1}{(4\pi D t)^{3/2}} \int e^{-(\boldsymbol{x}-\boldsymbol{y})^2/(4Dt)} \, \rho(\boldsymbol{y}, 0) \, d^3\boldsymbol{y}. \tag{3.205}$$

□

Exercises

3.1 Show that the Fourier integral formula (3.26) for real functions follows from (3.9) and (3.25).

3.2 Show that the Fourier integral formula (3.26) for real functions implies (3.27) if f is even and (3.28) if it is odd.

3.3 Derive the formula (3.30) for the square wave (3.29).

3.4 By using the Fourier-transform formulas (3.27 & 3.28), derive the formulas (3.31) and (3.32) for the even and odd extensions of the exponential $\exp(-\beta|x|)$.

3.5 For the state $|\psi, t\rangle$ given by Eqs. (3.83 & 3.88), find the wave function $\psi(x, t) = \langle x|\psi, t\rangle$ at time t. Then find the variance of the position operator at that time. Does it grow as time goes by? How?

3.6 At time $t = 0$, a particle of mass m is in a gaussian superposition of momentum eigenstates centered at $p = \hbar K$

$$\psi(x, 0) = N \int_{-\infty}^{\infty} e^{ikx} e^{-L^2(k-K)^2}\, dk. \tag{3.206}$$

(a) Shift k by K and do the integral. Where is the particle most likely to be found? (b) At time t, the wave function $\psi(x, t)$ is $\psi(x, 0)$ but with ikx replaced by $ikx - i\hbar k^2 t/2m$. Shift k by K and do the integral. Where is the particle most likely to be found? (c) Does the wave packet spreads out like t or like $\sqrt{t}$ as in classical diffusion?

3.7 Express the characteristic function (3.90) of a probability distribution $P(x)$ as its Fourier transform.

3.8 Express the characteristic function (3.90) of a probability distribution as a power series in its moments (3.92).

3.9 Find the characteristic function (3.90) of the gaussian probability distribution

$$P_G(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \tag{3.207}$$

3.10 Find the moments $\mu_n = E[x^n]$ for $n = 0, \ldots, 3$ of the gaussian probability distribution $P_G(x, \mu, \sigma)$.

3.11 Derive (3.115) from $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ and Ampère's law $\boldsymbol{\nabla} \times \boldsymbol{B} = \mu_0 \boldsymbol{J}$.

3.12 Derive (3.116) from (3.115).

3.13 Derive (3.117) from (3.116).

3.14 Use the Green's function relations (3.110) and (3.111) to show that (3.117) satisfies (3.115).

3.15 Show that the Laplace transform of t^{z-1} is the gamma function (4.58) divided by s^z

$$f(s) = \int_0^{\infty} e^{-st}\, t^{z-1}\, dt = s^{-z}\, \Gamma(z). \tag{3.208}$$

3.16 Compute the Laplace transform of $1/\sqrt{t}$. Hint: let $t = u^2$.

3.17 Show that the commutation relations (3.185) of the annihilation and creation operators imply the equal-time commutation relations (3.186) for the field ϕ and its conjugate momentum π.

3.18 Use the linearity of the diffusion equation and equations (3.201–3.204) to derive the general solution (3.205) of the diffusion equation.