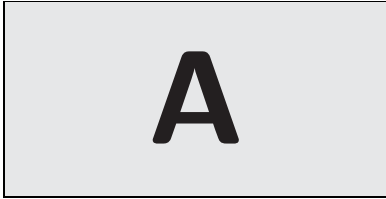


Appendix: Fourier methods



Why are Fourier methods important? Why is it so useful for us to transform functions of time and space $y(\mathbf{x}, t)$ into functions of frequency and wavevector $\tilde{y}(\mathbf{k}, \omega)$?

- *Humans hear frequencies.* The human ear analyzes pressure variations in the air into different frequencies. Large frequencies ω are perceived as high pitches; small frequencies are low pitches. The ear, very roughly, does a Fourier transform of the pressure $P(t)$ and transmits $|\tilde{P}(\omega)|^2$ to the brain.¹
- *Diffraction experiments measure Fourier components.* Many experimental methods diffract waves (light, X-rays, electrons, or neutrons) off of materials (Section 10.2). These experiments typically probe the absolute square of the Fourier amplitude of whatever is scattering the incoming beam.
- *Common mathematical operations become simpler in Fourier space.* Derivatives, correlation functions, and convolutions can be written as simple products when the functions are Fourier transformed. This has been important to us when calculating correlation functions (eqn 10.4), summing random variables (Exercises 1.2 and 12.11), and calculating susceptibilities (eqns 10.30, 10.39, and 10.53, and Exercise 10.9). In each case, we turn a calculus calculation into algebra.
- *Linear differential equations in translationally-invariant systems have solutions in Fourier space.*² We have used Fourier methods for solving the diffusion equation (Section 2.4.1), and more broadly to solve for correlation functions and susceptibilities (Chapter 10).

In Section A.1 we introduce the conventions typically used in physics for the Fourier series, Fourier transform, and fast Fourier transform. In Section A.2 we derive their integral and differential properties. In Section A.3, we interpret the Fourier transform as an orthonormal change-of-basis in function space. And finally, in Section A.4 we explain why Fourier methods are so useful for solving differential equations by exploring their connection to translational symmetry.

A.1 Fourier conventions

Here we define the Fourier series, the Fourier transform, and the fast Fourier transform, as they are commonly defined in physics and as they are used in this text.

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¹Actually, this is how the ear *seems* to work, but not how it *does* work. First, the signal to the brain is time dependent, with the tonal information changing as a word or tune progresses; it is more like a wavelet transform, giving the frequency content in various time slices. Second, the phase information in \tilde{P} is not completely lost; power and pitch are the primary signal, but the relative phases of different pitches are also perceptible. Third, experiments have shown that the human ear is very nonlinear in its mechanical response.

²Translation invariance in Hamiltonian systems implies momentum conservation. This is why in quantum mechanics Fourier transforms convert position-space wavefunctions into momentum-space wavefunctions—even for systems which are not translation invariant.

The Fourier series for functions of time, periodic with period T , is

$$\tilde{y}_m = \frac{1}{T} \int_0^T y(t) \exp(i\omega_m t) dt, \tag{A.1}$$

where $\omega_m = 2\pi m/T$, with integer m . The Fourier series can be re-summed to retrieve the original function using the *inverse Fourier series*:

$$y(t) = \sum_{m=-\infty}^{\infty} \tilde{y}_m \exp(-i\omega_m t). \tag{A.2}$$

Fourier series of functions in space are defined with the *opposite* sign convention³ in the complex exponentials. Thus in a three-dimensional box of volume $V = L \times L \times L$ with periodic boundary conditions, these formulæ become

$$\tilde{y}_{\mathbf{k}} = \frac{1}{V} \int y(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) dV, \tag{A.3}$$

and

$$y(\mathbf{x}) = \sum_{\mathbf{k}} \tilde{y}_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{x}), \tag{A.4}$$

where the \mathbf{k} run over a lattice of wavevectors

$$\mathbf{k}_{(m,n,o)} = [2\pi m/L, 2\pi n/L, 2\pi o/L] \tag{A.5}$$

in the box.

The Fourier transform is defined for functions on the entire infinite line:

$$\tilde{y}(\omega) = \int_{-\infty}^{\infty} y(t) \exp(i\omega t) dt, \tag{A.6}$$

where now ω takes on all values.⁴ We regain the original function by doing the inverse Fourier transform:

$$y(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{y}(\omega) \exp(-i\omega t) d\omega. \tag{A.7}$$

This is related to the inverse Fourier series by a continuum limit (Fig. A.1):

$$\frac{1}{2\pi} \int d\omega \approx \frac{1}{2\pi} \sum_{\omega} \Delta\omega = \frac{1}{2\pi} \sum_{\omega} \frac{2\pi}{T} = \frac{1}{T} \sum, \tag{A.8}$$

where the $1/T$ here compensates for the factor of T in the definitions of the forward Fourier series. In three dimensions the Fourier transform formula A.6 is largely unchanged,

$$\tilde{y}(\mathbf{k}) = \int y(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) dV, \tag{A.9}$$

while the inverse Fourier transform gets the cube of the prefactor:

$$y(\mathbf{x}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \tilde{y}(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{x}) d\mathbf{k}. \tag{A.10}$$

³This inconsistent convention allows waves of positive frequency to propagate forward rather than backward. A single component of the inverse transform, $e^{i\mathbf{k} \cdot \mathbf{x}} e^{-i\omega t} = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$ propagates in the $+\mathbf{k}$ direction with speed $\omega/|\mathbf{k}|$; had we used a $+i$ for Fourier transforms in both space and time $e^{i(\mathbf{k} \cdot \mathbf{x} + \omega t)}$ would move *backward* (along $-\mathbf{k}$) for $\omega > 0$.

⁴Why do we divide by T or L for the series and not for the transform? Imagine a system in an extremely large box. Fourier series are used for functions which extend over the entire box; hence we divide by the box size to keep them finite as $L \rightarrow \infty$. Fourier transforms are usually used for functions which vanish quickly, so they remain finite as the box size gets large.

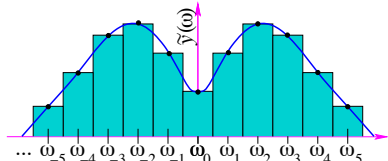


Fig. A.1 Approximating the integral as a sum. By approximating the integral $\int \tilde{y}(\omega) \exp(i\omega t) d\omega$ as a sum over the equally-spaced points ω_m , $\sum_m \tilde{y}(\omega) \exp(i\omega_m t) \Delta\omega$, we can connect the formula for the Fourier transform to the formula for the Fourier series, explaining the factor $1/2\pi$ in eqn A.7.

The fast Fourier transform (FFT) starts with N equally-spaced data points y_ℓ , and returns a new set of complex numbers \tilde{y}_m^{FFT} :

$$\tilde{y}_m^{\text{FFT}} = \sum_{\ell=0}^{N-1} y_\ell \exp(i2\pi m\ell/N), \tag{A.11}$$

with $m = 0, \dots, N - 1$. The inverse of the FFT is given by

$$y_\ell = \frac{1}{N} \sum_{m=0}^{N-1} \tilde{y}_m^{\text{FFT}} \exp(-i2\pi m\ell/N). \tag{A.12}$$

The FFT essentially samples the function $y(t)$ at equally-spaced points $t_\ell = \ell T/N$ for $\ell = 0, \dots, N - 1$:

$$\tilde{y}_m^{\text{FFT}} = \sum_{\ell=0}^{N-1} y_\ell \exp(i\omega_m t_\ell). \tag{A.13}$$

It is clear from eqn A.11 that $\tilde{y}_{m+N}^{\text{FFT}} = \tilde{y}_m^{\text{FFT}}$, so the fast Fourier transform is periodic with period $\omega_N = 2\pi N/T$. The inverse transform can also be written

$$y_\ell = \frac{1}{N} \sum_{m=-N/2+1}^{N/2} \tilde{y}_m^{\text{FFT}} \exp(-i\omega_m t_\ell), \tag{A.14}$$

where we have centered⁵ the sum ω_m at $\omega = 0$ by using the periodicity.⁶

Often the values $y(t)$ (or the data points y_ℓ) are real. In this case, eqns A.1 and A.6 show that the negative Fourier amplitudes are the complex conjugates of the positive ones: $\tilde{y}(\omega) = \tilde{y}^*(-\omega)$. Hence for real functions the real part of the Fourier amplitude will be even and the imaginary part will be odd.⁷

The reader may wonder why there are so many versions of roughly the same Fourier operation.

- (1) The function $y(t)$ can be defined on a finite interval with periodic boundary conditions on $(0, T)$ (series, FFT) or defined in all space (transform). In the periodic case, the Fourier coefficients are defined only at discrete wavevectors $\omega_m = 2\pi m/T$ consistent with the periodicity of the function; in the infinite system the coefficients are defined at all ω .
- (2) The function $y(t)$ can be defined at a discrete set of N points $t_n = n\Delta t = nT/N$ (FFT), or at all points t in the range (series, transform). If the function is defined only at discrete points, the Fourier coefficients are periodic with period $\omega_N = 2\pi/\Delta t = 2\pi N/T$.⁸

There are several arbitrary choices made in defining these Fourier methods, that vary from one field to another.

- Some use the notation $j = \sqrt{-1}$ instead of i .

⁵If N is odd, to center the FFT the sum should be taken over $-(N-1)/2 \leq m \leq (N-1)/2$.

⁶Notice that the FFT returns the negative ω Fourier coefficients as the last half of the array, $m = N/2 + 1, N/2 + 2, \dots$. (This works because $-N/2 + j$ and $N/2 + j$ differ by N , the periodicity of the FFT.) One must be careful about this when using Fourier transforms to solve calculus problems numerically. For example, to evolve a density $\rho(x)$ under the diffusion equation (Section 2.4.1) one must multiply the first half of the array $\tilde{\rho}_m$ by $\exp(-Dk_m^2 t) = \exp(-D[m(2\pi/L)]^2 t)$ but multiply the second half by $\exp(-D(K - k_m)^2 t) = \exp(-D[(N - m)(2\pi/L)]^2 t)$.

⁷This allows one to write slightly faster FFTs specialized for real functions. One pays for the higher speed by an extra programming step unpacking the resulting Fourier spectrum.

⁸There is one more logical possibility: a discrete set of points that fill all space; the atomic displacements in an infinite crystal is the classic example. In Fourier space, such a system has continuous k , but periodic boundary conditions at $\pm K/2 = \pm\pi/a$ (the edges of the Brillouin zone).

⁹The real world is invariant under the transformation $i \leftrightarrow -i$, but complex quantities will get conjugated. Swapping i for $-i$ in the time series formulæ, for example, would make $\chi''(\omega) = -\text{Im}[\chi(\omega)]$ in eqn 10.31 and would make χ analytic in the lower half-plane in Fig. 10.12.

- More substantively, some use the complex conjugate of our formulæ, substituting $-i$ for i in the time or space transform formulæ. This alternative convention makes no change for any real quantity.⁹
- Some use a $1/\sqrt{T}$ and $1/\sqrt{2\pi}$ factor symmetrically on the Fourier and inverse Fourier operations.
- Some use frequency and wavelength ($f = 2\pi\omega$ and $\lambda = 2\pi/k$) instead of angular frequency ω and wavevector k . This makes the transform and inverse transform more symmetric, and avoids some of the prefactors.

Our Fourier conventions are those most commonly used in physics.

A.2 Derivatives, convolutions, and correlations

The important differential and integral operations become multiplications in Fourier space. A calculus problem in t or x thus becomes an algebra exercise in ω or k .

Integrals and derivatives. Because $(d/dt)e^{-i\omega t} = -i\omega e^{i\omega t}$, the Fourier coefficient of the derivative of a function $y(t)$ is $-i\omega$ times the Fourier coefficient of the function:

$$dy/dt = \sum \tilde{y}_m (-i\omega_m \exp(-i\omega_m t)) = \sum (-i\omega_m \tilde{y}_m) \exp(-i\omega_m t), \tag{A.15}$$

so

$$\left. \frac{d\tilde{y}}{dt} \right|_{\omega} = -i\omega \tilde{y}_{\omega}. \tag{A.16}$$

This holds also for the Fourier transform and the fast Fourier transform. Since the derivative of the integral gives back the original function, the Fourier series for the indefinite integral of a function y is thus given by dividing by $-i\omega$:

$$\int \widetilde{y(t)} dt = \frac{\tilde{y}_{\omega}}{-i\omega} = i \frac{\tilde{y}_{\omega}}{\omega} \tag{A.17}$$

¹⁰Either the mean $\tilde{y}(\omega = 0)$ is zero or it is non-zero. If the mean of the function is zero, then $\tilde{y}(\omega)/\omega = 0/0$ is undefined at $\omega = 0$. This makes sense; the indefinite integral has an arbitrary integration constant, which gives its Fourier series an arbitrary value at $\omega = 0$. If the mean of the function \bar{y} is not zero, then the integral of the function will have a term $\bar{y}(t - t_0)$. Hence the integral is not periodic and has no Fourier series. (On the infinite interval the integral has no Fourier transform because it is not in \mathbb{L}^2 .)

except at $\omega = 0$.¹⁰

These relations are invaluable in the solution of many linear partial differential equations. For example, we saw in Section 2.4.1 that the diffusion equation

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \tag{A.18}$$

becomes manageable when we Fourier transform x to k :

$$\frac{\partial \tilde{\rho}_k}{\partial t} = -Dk^2 \tilde{\rho}, \tag{A.19}$$

$$\tilde{\rho}_k(t) = \rho_k(0) \exp(-Dk^2 t). \tag{A.20}$$

Correlation functions and convolutions. The absolute square of the Fourier transform¹¹ $|\tilde{y}(\omega)|^2$ is given by the Fourier transform of the

¹¹The absolute square of the Fourier transform of a time signal is called the *power spectrum*.

correlation function $C(\tau) = \langle y(t)y(t + \tau) \rangle$:

$$\begin{aligned} |\tilde{y}(\omega)|^2 &= \tilde{y}(\omega)^* \tilde{y}(\omega) = \int dt' e^{-i\omega t'} y(t') \int dt e^{i\omega t} y(t) \\ &= \int dt dt' e^{i\omega(t-t')} y(t') y(t) = \int d\tau e^{i\omega\tau} \int dt' y(t') y(t' + \tau) \\ &= \int d\tau e^{i\omega\tau} T \langle y(t)y(t + \tau) \rangle = T \int d\tau e^{i\omega\tau} C(\tau) \\ &= T \tilde{C}(\omega), \end{aligned} \tag{A.21}$$

where T is the total time t during which the Fourier spectrum is being measured. Thus diffraction experiments, by measuring the square of the \mathbf{k} -space Fourier transform, give us the spatial correlation function for the system (Section 10.2).

The convolution¹² $h(z)$ of two functions $f(x)$ and $g(y)$ is defined as

$$h(z) = \int f(x)g(z - x) dx. \tag{A.22}$$

The Fourier transform of the convolution is the product of the Fourier transforms. In three dimensions,¹³

$$\begin{aligned} \tilde{f}(\mathbf{k})\tilde{g}(\mathbf{k}) &= \int e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) d\mathbf{x} \int e^{-i\mathbf{k}\cdot\mathbf{y}} g(\mathbf{y}) d\mathbf{y} \\ &= \int e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{y})} f(\mathbf{x})g(\mathbf{y}) d\mathbf{x} d\mathbf{y} = \int e^{-i\mathbf{k}\cdot\mathbf{z}} d\mathbf{z} \int f(\mathbf{x})g(\mathbf{z} - \mathbf{x}) d\mathbf{x} \\ &= \int e^{-i\mathbf{k}\cdot\mathbf{z}} h(\mathbf{z}) d\mathbf{z} = \tilde{h}(\mathbf{k}). \end{aligned} \tag{A.23}$$

¹²Convolutions show up in sums and Green's functions. The sum $\mathbf{z} = \mathbf{x} + \mathbf{y}$ of two random vector quantities with probability distributions $f(\mathbf{x})$ and $g(\mathbf{y})$ has a probability distribution given by the convolution of f and g (Exercise 1.2). An initial condition $f(\mathbf{x}, t_0)$ propagated in time to $t_0 + \tau$ is given by convolving with a Green's function $g(\mathbf{y}, \tau)$ (Section 2.4.2).

¹³The convolution and correlation theorems are closely related; we do convolutions in time and correlations in space to illustrate both the one-dimensional and vector versions of the calculation.

A.3 Fourier methods and function space

There is a nice analogy between the space of vectors \mathbf{r} in three dimensions and the space of functions $y(t)$ periodic with period T , which provides a simple way of thinking about Fourier series. It is natural to define our function space to including all complex functions $y(t)$. (After all, we want the complex Fourier plane-waves $e^{-i\omega_m t}$ to be in our space.) Let us list the following common features of these two spaces.

- **Vector space.** A vector $\mathbf{r} = (r_1, r_2, r_3)$ in \mathbb{R}^3 can be thought of as a real-valued function on the set $\{1, 2, 3\}$. Conversely, the function $y(t)$ can be thought of as a vector with one complex component for each $t \in [0, T)$.

Mathematically, this is an evil analogy. Most functions which have independent random values for each point t are undefinable, unintegrable, and generally pathological. The space becomes well defined if we confine ourselves to functions $y(t)$ whose absolute squares $|y(t)|^2 = y(t)y^*(t)$ can be integrated. This vector space of functions is called \mathbb{L}^2 .¹⁴

¹⁴More specifically, the Fourier transform is usually defined on $\mathbb{L}^2[\mathbb{R}]$, and the Fourier series is defined on $\mathbb{L}^2[0, T]$.

- **Inner product.** The analogy to the dot product of two three-dimensional vectors $\mathbf{r} \cdot \mathbf{s} = r_1s_1 + r_2s_2 + r_3s_3$ is an inner product between two functions y and z :

$$y \cdot z = \frac{1}{T} \int_0^T y(t)z^*(t) dt. \tag{A.24}$$

You can think of this inner product as adding up all the products $y_t z_t^*$ over all points t , except that we weight each point by dt/T .

- **Norm.** The distance between two three-dimensional vectors \mathbf{r} and \mathbf{s} is given by the *norm* of the difference $|\mathbf{r} - \mathbf{s}|$. The norm of a vector is the square root of the dot product of the vector with itself, so $|\mathbf{r} - \mathbf{s}| = \sqrt{(\mathbf{r} - \mathbf{s}) \cdot (\mathbf{r} - \mathbf{s})}$. To make this inner product norm work in function space, we need to know that the inner product of a function with itself is never negative. This is why, in our definition A.24, we took the complex conjugate of $z(t)$. This norm on function space is called the L^2 norm:

$$\|y\|_2 = \sqrt{\frac{1}{T} \int_0^T |y(t)|^2 dt}. \tag{A.25}$$

Thus our restriction to square-integrable functions makes the norm of all functions in our space finite.¹⁵

¹⁵Another important property is that the only vector whose norm is zero is the zero vector. There are many functions whose absolute squares have integral zero, like the function which is zero except at $T/2$, where it is one, and the function which is zero on irrationals and one on rationals. Mathematicians finesse this difficulty by defining the vectors in L^2 not to be functions, but rather to be *equivalence classes* of functions whose relative distance is zero. Hence the zero vector in L^2 includes all functions with norm zero.

- **Basis.** A natural basis for \mathbb{R}^3 is given by the three unit vectors $\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \hat{\mathbf{x}}_3$. A natural basis for our space of functions is given by the functions $\hat{f}_m = e^{-i\omega_m t}$, with $\omega_m = 2\pi m/T$ to keep them periodic with period T .
- **Orthonormality.** The basis in \mathbb{R}^3 is orthonormal, with $\hat{\mathbf{x}}_i \cdot \hat{\mathbf{x}}_j$ equaling one if $i = j$ and zero otherwise. Is this also true of the vectors in our basis of plane waves? They are normalized:

$$\|\hat{f}_m\|_2^2 = \frac{1}{T} \int_0^T |e^{-i\omega_m t}|^2 dt = 1. \tag{A.26}$$

They are also orthogonal, with

$$\begin{aligned} \hat{f}_m \cdot \hat{f}_n &= \frac{1}{T} \int_0^T e^{-i\omega_m t} e^{i\omega_n t} dt = \frac{1}{T} \int_0^T e^{-i(\omega_m - \omega_n)t} dt \\ &= \frac{1}{-i(\omega_m - \omega_n)T} e^{-i(\omega_m - \omega_n)t} \Big|_0^T = 0 \end{aligned} \tag{A.27}$$

(unless $m = n$) since $e^{-i(\omega_m - \omega_n)T} = e^{-i2\pi(m-n)} = 1 = e^{-i0}$.

- **Coefficients.** The coefficients of a three-dimensional vector are given by taking dot products with the basis vectors: $r_n = \mathbf{r} \cdot \hat{\mathbf{x}}_n$. The analogy in function space gives us the definition of the Fourier coefficients, eqn A.1:

$$\tilde{y}_m = y \cdot \hat{f}_m = \frac{1}{T} \int_0^T y(t) \exp(i\omega_m t) dt. \tag{A.28}$$

- **Completeness.** We can write an arbitrary three-dimensional vector \mathbf{r} by summing the basis vectors weighted by the coefficients: $\mathbf{r} =$

$\sum r_n \hat{x}_n$. The analogy in function space gives us the formula A.2 for the inverse Fourier series:

$$y = \sum_{m=-\infty}^{\infty} \tilde{y}_m \hat{f}_m, \tag{A.29}$$

$$y(t) = \sum_{m=-\infty}^{\infty} \tilde{y}_m \exp(-i\omega_m t).$$

One says that a basis is *complete* if any vector can be expanded in that basis. Our functions \hat{f}_m are complete in \mathbb{L}^2 .¹⁶

Our coefficient eqn A.28 follows from our completeness eqn A.29 and orthonormality:

$$\begin{aligned} \tilde{y}_\ell &\stackrel{?}{=} y \cdot \hat{f}_\ell = \left(\sum_m \tilde{y}_m \hat{f}_m \right) \cdot \hat{f}_\ell \\ &= \sum_m \tilde{y}_m (\hat{f}_m \cdot \hat{f}_\ell) = \tilde{y}_\ell \end{aligned} \tag{A.30}$$

or, writing things out,

$$\begin{aligned} \tilde{y}_\ell &\stackrel{?}{=} \frac{1}{T} \int_0^T y(t) e^{i\omega_\ell t} dt \\ &= \frac{1}{T} \int_0^T \left(\sum_m \tilde{y}_m e^{-i\omega_m t} \right) e^{i\omega_\ell t} dt \\ &= \sum_m \tilde{y}_m \left(\frac{1}{T} \int_0^T e^{-i\omega_m t} e^{i\omega_\ell t} dt \right) = \tilde{y}_\ell. \end{aligned} \tag{A.31}$$

Our function space, together with our inner product (eqn A.24), is a *Hilbert space* (a complete inner product space).

A.4 Fourier and translational symmetry

Why are Fourier methods so useful? In particular, why are the solutions to linear differential equations so often given by plane waves: sines and cosines and e^{ikx} ?¹⁷ Most of our basic equations are derived for systems with a *translational symmetry*. Time-translational invariance holds for any system without an explicit external time-dependent force; invariance under spatial translations holds for all homogeneous systems.

Why are plane waves special for systems with translational invariance? *Plane waves are the eigenfunctions of the translation operator.* Define \mathcal{T}_Δ , an operator which takes function space into itself, and acts to shift the function a distance Δ to the right:¹⁸

$$\mathcal{T}_\Delta\{f\}(x) = f(x - \Delta). \tag{A.32}$$

Any solution $f(x, t)$ to a translation-invariant equation will be mapped by \mathcal{T}_Δ onto another solution. Moreover, \mathcal{T}_Δ is a linear operator (translating the sum is the sum of the translated functions). If we think of the

¹⁶You can imagine that proving they are complete would involve showing that there are no functions in \mathbb{L}^2 which are ‘perpendicular’ to all the Fourier modes. This is the type of tough question that motivates the mathematical field of real analysis.

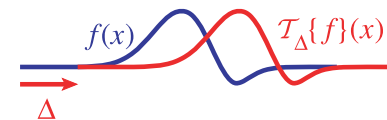


Fig. A.2 The mapping \mathcal{T}_Δ takes function space into function space, shifting the function to the right by a distance Δ . For a physical system that is translation invariant, a solution translated to the right is still a solution.

¹⁷It is true, we are making a big deal about what is usually called the separation of variables method. But why does separation of variables so often work, and why do the separated variables so often form sinusoids and exponentials?

¹⁸That is, if $g = \mathcal{T}_\Delta\{f\}$, then $g(x) = f(x - \Delta)$, so g is f shifted to the right by Δ .

¹⁹You are familiar with eigenvectors of 3×3 symmetric matrices M , which transform into multiples of themselves when multiplied by M , $M \cdot \mathbf{e}_n = \lambda_n \mathbf{e}_n$. The translation \mathcal{T}_Δ is a linear operator on function space just as M is a linear operator on \mathbb{R}^3 .

²⁰The real exponential e^{Ax} is also an eigenstate, with eigenvalue $e^{-A\Delta}$. This is also allowed. Indeed, the diffusion equation is time-translation invariant, and it has solutions which decay exponentially in time ($e^{-\omega_k t} e^{ikx}$, with $\omega_k = Dk^2$). Exponentially decaying solutions in space also arise in some translation-invariant problems, such as quantum tunneling and the penetration of electromagnetic radiation into metals.

²¹Written out in equations, this simple idea is even more obscure. Let \mathcal{U}_t be the time-evolution operator for a translationally-invariant equation (like the diffusion equation of Section 2.2). That is, $\mathcal{U}_t\{\rho\}$ evolves the function $\rho(x, \tau)$ into $\rho(x, \tau + t)$. (\mathcal{U}_t is not translation in time, but evolution in time.) Because our system is translation invariant, translated solutions are also solutions for translated initial conditions: $\mathcal{T}_\Delta\{\mathcal{U}_t\{\rho\}\} = \mathcal{U}_t\{\mathcal{T}_\Delta\{\rho\}\}$. Now, if $\rho_k(x, 0)$ is an eigenstate of \mathcal{T}_Δ with eigenvalue λ_k , is $\rho_k(x, t) = \mathcal{U}_t\{\rho_k\}(x)$ an eigenstate with the same eigenvalue? Yes indeed:

$$\begin{aligned} \mathcal{T}_\Delta\{\rho_k(x, t)\} &= \mathcal{T}_\Delta\{\mathcal{U}_t\{\rho_k(x, 0)\}\} \\ &= \mathcal{U}_t\{\mathcal{T}_\Delta\{\rho_k(x, 0)\}\} \\ &= \mathcal{U}_t\{\lambda_k \rho_k(x, 0)\} \\ &= \lambda_k \mathcal{U}_t\{\rho_k(x, 0)\} \\ &= \lambda_k \rho_k(x, t) \end{aligned} \tag{A.34}$$

because the evolution law \mathcal{U}_t is linear.

translation operator as a big matrix acting on function space, we can ask for its eigenvalues¹⁹ and eigenvectors (or *eigenfunctions*) f_k :

$$\mathcal{T}_\Delta\{f_k\}(x) = f_k(x - \Delta) = \lambda_k f_k(x). \tag{A.33}$$

This equation is solved by our complex plane waves $f_k(x) = e^{ikx}$, with $\lambda_k = e^{-ik\Delta}$.²⁰

Why are these eigenfunctions useful? The time evolution of an eigenfunction must have the same eigenvalue λ ! The argument is something of a tongue-twister: translating the time-evolved eigenfunction gives the same answer as time evolving the translated eigenfunction, which is time evolving λ times the eigenfunction, which is λ times the time-evolved eigenfunction.²¹

The fact that the different eigenvalues do not mix under time evolution is precisely what made our calculation work; time evolving $A_0 e^{ikx}$ had to give a multiple $A(t) e^{ikx}$ since there is only one eigenfunction of translations with the given eigenvalue. Once we have reduced the partial differential equation to an ordinary differential equation for a few eigenstate amplitudes, the calculation becomes feasible.

Quantum physicists will recognize the tongue-twister above as a statement about simultaneously diagonalizing commuting operators: since translations commute with time evolution, one can find a complete set of translation eigenstates which are also time-evolution solutions. Mathematicians will recognize it from group representation theory: the solutions to a translation-invariant linear differential equation form a representation of the translation group, and hence they can be decomposed into irreducible representations of that group. These approaches are basically equivalent, and very powerful. One can also use these approaches for systems with other symmetries. For example, just as the invariance of homogeneous systems under translations leads to plane-wave solutions with definite wavevector k , it is true that:

- the invariance of isotropic systems (like the hydrogen atom) under the rotation group leads naturally to solutions involving spherical harmonics with definite angular momenta ℓ and m ;
- the invariance of the strong interaction under SU(3) leads naturally to the ‘8-fold way’ families of mesons and baryons; and
- the invariance of the Universe under the Poincaré group of space-time symmetries (translations, rotations, and Lorentz boosts) leads naturally to particles with definite mass and spin!

Exercises

We begin with three Fourier series exercises, *Sound wave*, *Fourier cosines* (numerical), and *Double sinusoids*. We then explore Fourier transforms with *Fourier Gaussians* (numerical) and *Uncertainty*, focusing on the effects of translating and scaling the width of the function to be transformed. *Fourier relationships* analyzes the normalization needed to go from the FFT to the Fourier series, and *Aliasing and windowing* explores two common numerical inaccuracies associated with the FFT. *White noise* explores the behavior of Fourier methods on random functions. *Fourier matching* is a quick, visual test of one's understanding of Fourier methods. Finally, *Gibbs phenomenon* explores what happens when you torture a Fourier series by insisting that smooth sinusoids add up to a function with a jump discontinuity.

(A.1) Sound wave. ①

A musical instrument playing a note of frequency ω_1 generates a pressure wave $P(t)$ periodic with period $2\pi/\omega_1$: $P(t) = P(t + 2\pi/\omega_1)$. The complex Fourier series of this wave (eqn A.2) is zero except for $m = \pm 1$ and ± 2 , corresponding to the fundamental ω_1 and the first overtone. At $m = 1$, the Fourier amplitude is $2 - i$, at $m = -1$ it is $2 + i$, and at $m = \pm 2$ it is 3. What is the pressure $P(t)$:

- (A) $\exp((2 + i)\omega_1 t) + 2 \exp(3\omega_1 t)$,
- (B) $\exp(2\omega_1 t) \exp(i\omega_1 t) \times 2 \exp(3\omega_1 t)$,
- (C) $\cos 2\omega_1 t - \sin \omega_1 t + 2 \cos 3\omega_1 t$,
- (D) $4 \cos \omega_1 t - 2 \sin \omega_1 t + 6 \cos 2\omega_1 t$,
- (E) $4 \cos \omega_1 t + 2 \sin \omega_1 t + 6 \cos 2\omega_1 t$?

(A.2) Fourier cosines. (Computation) ②

In this exercise, we will use the computer to illustrate features of Fourier series and discrete fast Fourier transforms using sinusoidal waves. Download the Fourier software, or the relevant hints files, from the computer exercises section of the book web site [129].²²

First, we will take the Fourier series of periodic functions $y(x) = y(x + L)$ with $L = 20$. We will sample the function at $N = 32$ points, and use a FFT to approximate the Fourier series. The Fourier series will be plotted as functions

of k , at $-k_{N/2}, \dots, k_{N/2-2}, k_{N/2-1}$. (Remember that the negative m points are given by the last half of the FFT.)

(a) Analytically (that is, with paper and pencil) derive the Fourier series \tilde{y}_m in this interval for $\cos(k_1 x)$ and $\sin(k_1 x)$. Hint: They are zero except at the two values $m = \pm 1$. Use the spatial transform (eqn A.3).

(b) What spacing δk between k -points k_m do you expect to find? What is $k_{N/2}$? Evaluate each analytically as a function of L and numerically for $L = 20$.

Numerically (on the computer) choose a cosine wave $A \cos(k(x - x_0))$, evaluated at 32 points from $x = 0$ to 20 as described above, with $k = k_1 = 2\pi/L$, $A = 1$, and $x_0 = 0$. Examine its Fourier series.

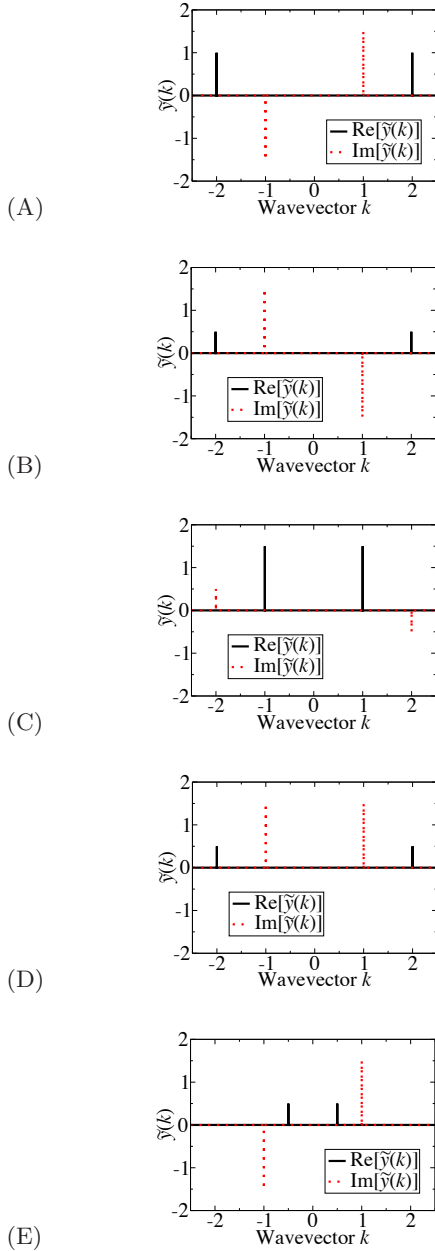
(c) Check your predictions from part (a) for the Fourier series for $\cos(k_1 x)$ and $\sin(k_1 x)$. Check your predictions from part (b) for δk and for $k_{N/2}$.

Decrease k to increase the number of wavelengths, keeping the number of data points fixed. Notice that the Fourier series looks fine, but that the real-space curves quickly begin to vary in amplitude, much like the patterns formed by beating (superimposing two waves of different frequencies). By increasing the number of data points, you can see that the beating effect is due to the small number of points we sample. Even for large numbers of sampled points N , though, beating will still happen at very small wavelengths (when we get close to $k_{N/2}$). Try various numbers of waves m up to and past $m = N/2$.

(A.3) Double sinusoid. ②

Which picture represents the spatial Fourier series (eqn A.4) associated with the function $f(x) = 3 \sin(x) + \cos(2x)$? (The solid line is the real part, the dashed line is the imaginary part.)

²²If this exercise is part of a computer lab, one could assign the analytical portions as a pre-lab exercise.



(A.4) **Fourier Gaussians.** (Computation) ②

In this exercise, we will use the computer to illustrate features of Fourier transforms, focusing on the particular case of Gaussian functions, but illustrating general properties. Download the Fourier software or the relevant hints files from the computer exercises portion of the text web site [129].²³

The Gaussian distribution (also known as the normal distribution) has the form

$$G(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right), \quad (\text{A.35})$$

where σ is the standard deviation and x_0 is the center. Let

$$G_0(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2) \quad (\text{A.36})$$

be the Gaussian of mean zero and $\sigma = 1$. The Fourier transform of G_0 is another Gaussian, of standard deviation one, but no normalization factor.²⁴

$$\tilde{G}_0(k) = \exp(-k^2/2). \quad (\text{A.38})$$

In this exercise, we study how the Fourier transform of $G(x)$ varies as we change σ and x_0 .

Widths. As we make the Gaussian narrower (smaller σ), it becomes more pointy. Shorter lengths mean higher wavevectors, so we expect that its Fourier transform will get wider.

(a) *Starting with the Gaussian with $\sigma = 1$, numerically measure the width of its Fourier transform at some convenient height. (The full width at half maximum, FWHM, is a sensible choice.) Change σ to 2 and to 0.1, and measure the widths, to verify that the Fourier space width goes inversely with the real width.*

(b) *Analytically show that this rule is true in general. Change variables in eqn A.6 to show that if $z(x) = y(Ax)$ then $\tilde{z}(k) = \tilde{y}(k/A)/A$. Using eqn A.36 and this general rule, write a formula for the Fourier transform of a Gaussian centered at zero with arbitrary width σ .*

²³If this exercise is taught as a computer lab, one could assign the analytical portions as a pre-lab exercise.

²⁴Here is an elementary-looking derivation. We complete the square inside the exponent, and change from x to $y = x + ik$:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \exp(-x^2/2) dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-(x+ik)^2/2) dx \exp((ik)^2/2) = \left[\int_{-\infty+ik}^{\infty+ik} \frac{1}{\sqrt{2\pi}} \exp(-y^2/2) dy \right] \exp(-k^2/2). \quad (\text{A.37})$$

The term in brackets is one (giving us $e^{-k^2/2}$) but to show it we need to shift the integration contour from $\text{Im}[y] = k$ to $\text{Im}[y] = 0$, which demands Cauchy's theorem (Fig. 10.11).

(c) Analytically compute the product $\Delta x \Delta k$ of the FWHM of the Gaussians in real and Fourier space. (Your answer should be independent of the width σ .) This is related to the Heisenberg uncertainty principle, $\Delta x \Delta p \sim \hbar$, which you learn about in quantum mechanics.

Translations. Notice that a narrow Gaussian centered at some large distance x_0 is a reasonable approximation to a δ -function. We thus expect that its Fourier transform will be similar to the plane wave $\tilde{G}(k) \sim \exp(-ikx_0)$ we would get from $\delta(x - x_0)$.

(d) Numerically change the center of the Gaussian. How does the Fourier transform change? Convince yourself that it is being multiplied by the factor $\exp(-ikx_0)$. How does the power spectrum $|\tilde{G}(\omega)|^2$ change as we change x_0 ?

(e) Analytically show that this rule is also true in general. Change variables in eqn A.6 to show that if $z(x) = y(x - x_0)$ then $\tilde{z}(k) = \exp(-ikx_0)\tilde{y}(k)$. Using this general rule, extend your answer from part (b) to write the formula for the Fourier transform of a Gaussian of width σ and center x_0 .

(A.5) **Uncertainty.** ②

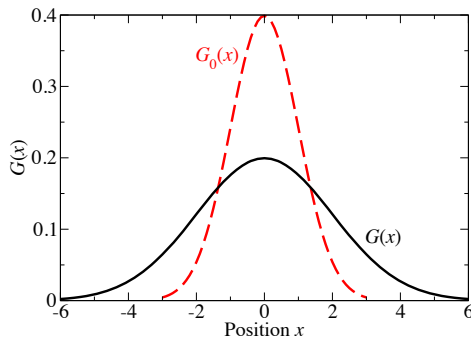
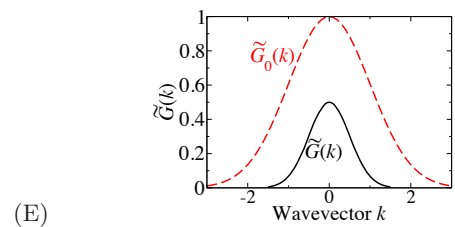
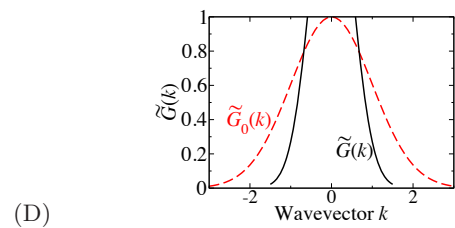
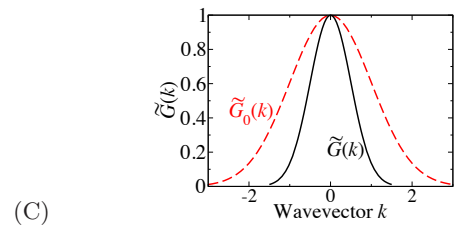
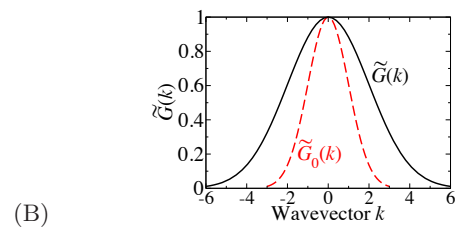
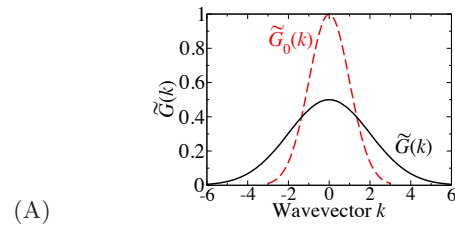


Fig. A.3 Real-space Gaussians.

The dashed line in Fig. A.3 shows

$$G_0(x) = 1/\sqrt{2\pi} \exp(-x^2/2). \quad (\text{A.39})$$

The dark line shows another function $G(x)$. The areas under the two curves $G(x)$ and $G_0(x)$ are the same. The dashed lines in the choices below represent the Fourier transform $\tilde{G}_0(k) = \exp(-k^2/2)$. Which has a solid curve that represents the Fourier transform of G ?



(A.6) **Fourier relationships.** ②

In this exercise, we explore the relationships between the Fourier series and the fast Fourier transform. The first is continuous and periodic

in real space, and discrete and unbounded in Fourier space; the second is discrete and periodic both in real and in Fourier space. Thus, we must again convert integrals into sums (as in Fig. A.1).

As we take the number of points N in our FFT to ∞ the spacing between the points gets smaller and smaller, and the approximation of the integral as a sum gets better and better.

Let $y_\ell = y(t_\ell)$ where $t_\ell = \ell(T/N) = \ell(\Delta t)$. Approximate the Fourier series integral A.1 above as a sum over y_ℓ , $(1/T) \sum_{\ell=0}^{N-1} y(t_\ell) \exp(-i\omega_m t_\ell) \Delta t$. For small positive m , give the constant relating \tilde{y}_m^{FFT} to the Fourier series coefficient \tilde{y}_m .

(A.7) **Aliasing and windowing.** (Computation) ③

In this exercise, we will use the computer to illustrate numerical challenges in using the fast Fourier transform. Download the Fourier software, or the relevant hints files, from the computer exercises section of the book web site [129].²⁵

The Fourier series \tilde{y}_m runs over all integers m . The fast Fourier transform runs only over $0 \leq m < N$. There are three ways to understand this difference: function-space dimension, wavelengths, and aliasing.

Function-space dimension. The space of periodic functions $y(x)$ on $0 \leq x < L$ is infinite, but we are sampling them only at $N = 32$ points. The space of possible fast Fourier series must also have N dimensions. Now, each coefficient of the FFT is complex (two dimensions), but the negative frequencies are complex conjugate to their positive partners (giving two net dimensions for the two wavevectors k_m and $k_{-m} \equiv k_{N-m}$). If you are fussy, \tilde{y}_0 has no partner, but is real (only one dimension), and if N is even $\tilde{y}_{-N/2}$ also is partnerless, but is real. So N k -points are generated by N real points.

Wavelength. The points at which we sample the function are spaced $\delta x = L/N$ apart. It makes sense that the fast Fourier transform would stop when the wavelength becomes close to δx ; we cannot resolve wiggles shorter than our sample spacing.

(a) Analytically derive the formula for y_ℓ for a cosine wave at k_N , the first wavelength not calculated by our FFT. It should simplify to a

constant. Give the simplified formula for y_ℓ at $k_{N/2}$ (the first missing wavevector after we have shifted the large m s to $N - m$ to get the negative frequencies). Numerically check your prediction for what y_ℓ looks like for $\cos(k_N x)$ and $\cos(k_{N/2} x)$.

So, the FFT returns Fourier components only until $k_{N/2}$ when there is one point per bump (half-period) in the cosine wave.

Aliasing. Suppose our function really does have wiggles with shorter distances than our sampling distance δx . Then its fast Fourier transform will have contributions to the long-wavelength coefficients \tilde{y}_m^{FFT} from these shorter wavelength wiggles; specifically $\tilde{y}_{m \pm N}$, $\tilde{y}_{m \pm 2N}$, etc. Let us work out a particular case of this: a short-wavelength cosine wave.

(b) On our sampled points x_ℓ , analytically show that $\exp(ik_{m \pm N} x_\ell) = \exp(ik_m x_\ell)$. Show that the short-wavelength wave $\cos(k_{m+N} x_\ell) = \cos(k_m x_\ell)$, and hence that its fast Fourier transform for small m will be a bogus peak at the long wavelength k_m . Numerically check your prediction for the transforms of $\cos(kx)$ for $k > k_{N/2}$.

If you sample a function at N points with Fourier components beyond $k_{N/2}$, their contributions get added to Fourier components at smaller wavevectors. This is called *aliasing*, and is an important source of error in Fourier methods. We always strive to sample enough points to avoid it.

You should see at least once how aliasing affects the FFT of functions that are not sines and cosines. Form a 32-point wave packet $y(x) = 1/(\sqrt{2\pi}\sigma) \exp(-x^2/2\sigma^2)$. Change the width σ of the packet to make it thinner. Notice that when the packet begins to look ratty (roughly as thin as the spacing between the sampled points x_ℓ) the Fourier series hits the edges and overlaps; high-frequency components are ‘folded over’ or *aliased* into the lower frequencies.

Windowing. One often needs to take Fourier series of functions which are not periodic in the interval. Set the number of data points N to 256 (powers of two are faster) and compare $y(x) = \cos k_m x$ for $m = 20$ with an ‘illegal’ non-integer value $m = 20.5$. Notice that the plot of the real-space function $y(x)$ is not periodic in the interval $[0, L)$ for $m = 20.5$. Notice that its Fourier series looks pretty complicated. Each

²⁵If this exercise is taught as a computer lab, one could assign the analytical portions as a pre-lab exercise.

of the two peaks has broadened into a whole staircase. Try looking at the power spectrum (which is proportional to $|\tilde{y}|^2$), and again compare $m = 20$ with $m = 20.5$. This is a numerical problem known as *windowing*, and there are various schemes to minimize its effects as well.

(A.8) **White noise.** (Computation) ②

White light is a mixture of light of all frequencies. White noise is a mixture of all sound frequencies, with constant average power per unit frequency. The hissing noise you hear on radio and TV between stations is approximately white noise; there are a lot more high frequencies than low ones, so it sounds high-pitched.

Download the Fourier software or the relevant hints files from the computer exercises portion of the text web site [129].

What kind of time signal would generate white noise? Select *White Noise*, or generate independent random numbers $y_\ell = y(\ell L/N)$ chosen from a Gaussian²⁶ distribution $\rho(y) = (1/\sqrt{2\pi}) \exp(-y^2/2\sigma)$. You should see a jagged, random function. Set the number of data points to, say, 1024.

Examine the Fourier transform of the noise signal. The Fourier transform of the white noise looks amazingly similar to the original signal. It is different, however, in two important ways. First, it is complex: there is a real part and an imaginary part. The second is for you to discover.

Examine the region near $k = 0$ on the Fourier plot, and describe how the Fourier transform of the noisy signal is different from a random function. In particular, what symmetry do the real and imaginary parts have? Can you show that this is true for any real function $y(x)$?

Now examine the power spectrum $|\tilde{y}|^2$.²⁷ Check that the power is noisy, but on average is crudely independent of frequency. (You can check this best by varying the random number seed.) White noise is usually due to random, uncorrelated fluctuations in time.

(A.9) **Fourier matching.** ②

The top three plots (a)–(c) in Fig. A.4 are functions $y(x)$ of position. For each, pick out which of the six plots (1)–(6) are the corresponding function \tilde{y} in Fourier space? (Dark line is real part, lighter dotted line is imaginary part.) (This exercise should be fairly straightforward after doing Exercises A.2, A.4, and A.8.)

(A.10) **Gibbs phenomenon.** (Mathematics) ③

In this exercise, we will look at the Fourier series for the step function and the triangle function. They are challenging because of the sharp corners, which are hard for sine waves to mimic.

Consider a function $y(x)$ which is A in the range $0 < x < L/2$ and $-A$ in the range $L/2 < x < L$ (shown above). It is a kind of step function, since it takes a step downward at $L/2$ (Fig. A.5).²⁸

(a) *As a crude approximation, the step function looks a bit like a chunky version of a sine wave, $A \sin(2\pi x/L)$. In this crude approximation, what would the complex Fourier series be (eqn A.4)?*

(b) *Show that the odd coefficients for the complex Fourier series of the step function are $\tilde{y}_m = -2\text{Ai}/(m\pi)$ (m odd). What are the even ones? Check that the coefficients \tilde{y}_m with $m = \pm 1$ are close to those you guessed in part (a).*

(c) *Setting $A = 2$ and $L = 10$, plot the partial sum of the Fourier series (eqn A.1) for $m = -n, -n + 1, \dots, n$ with $n = 1, 3,$ and 5 . (You are likely to need to combine the coefficients \tilde{y}_m and \tilde{y}_{-m} into sines or cosines, unless your plotting package knows about complex exponentials.) Does it converge to the step function? If it is not too inconvenient, plot the partial sum up to $n = 100$, and concentrate especially on the overshoot near the jumps in the function at $0, L/2,$ and L . This overshoot is called the Gibbs phenomenon, and occurs when you try to approximate functions $y(x)$ which have discontinuities.*

One of the great features of Fourier series is that it makes taking derivatives and integrals easier. What does the integral of our step function look

²⁶We choose the numbers with probability given by the Gaussian distribution, but it would look about the same if we took numbers with a uniform probability in, say, the range $(-1, 1)$.

²⁷For a time signal $f(t)$, the average power at a certain frequency is proportional to $|\tilde{f}(\omega)|^2$; ignoring the proportionality constant, the latter is often termed the power spectrum. This name is sometimes also used for the square of the amplitude of spatial Fourier transforms as well.

²⁸It can be written in terms of the standard Heaviside step function $\Theta(x) = 0$ for $x < 0$ and $\Theta(x) = 1$ for $x > 0$, as $y(x) = A(1 - 2\Theta(x - L/2))$.

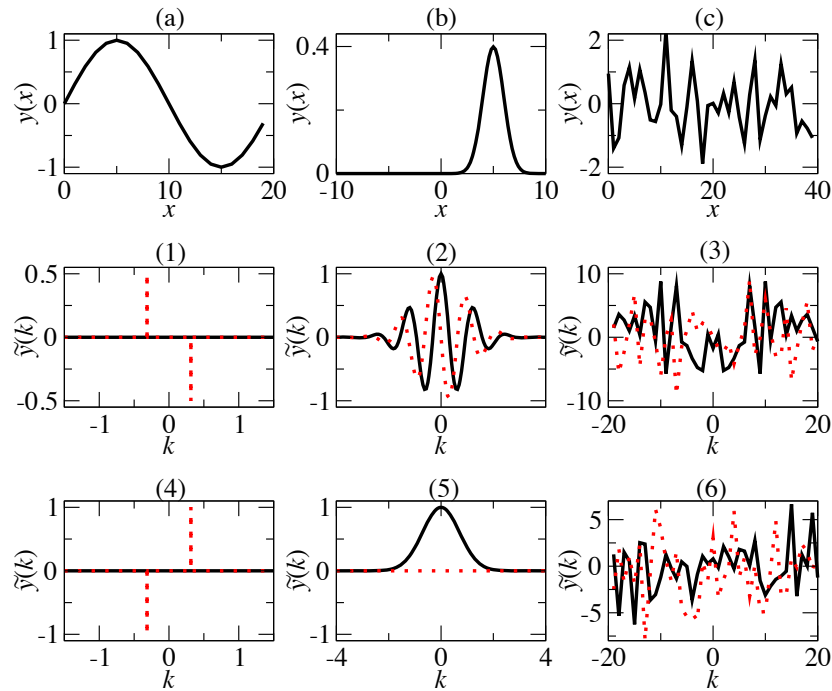


Fig. A.4 Fourier matching.

like? Let us sum the Fourier series for it!
 (d) Calculate the Fourier series of the integral of the step function, using your complex Fourier series from part (b) and the formula A.17 for the Fourier series of the integral. Plot your results, doing partial sums up to $\pm m = n$, with $n = 1, 3, \text{ and } 5$, again with $A = 2$ and $L = 10$. Would the derivative of this function look like the step function? If it is convenient, do $n = 100$, and notice there are no overshoots.

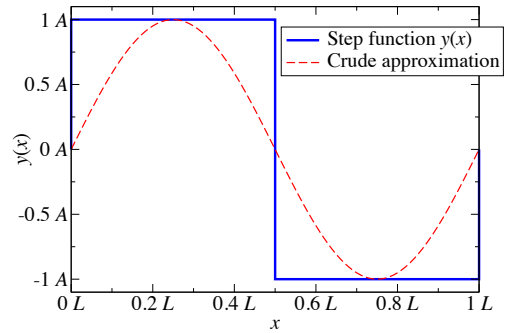


Fig. A.5 Step function.