

1

Linear Algebra

1.1 Numbers

The **natural** numbers are the positive integers and zero. **Rational** numbers are ratios of integers. **Irrational** numbers have decimal digits d_n

$$x = \sum_{n=m_x}^{\infty} \frac{d_n}{10^n} \quad (1.1)$$

that do not repeat. Thus the repeating decimals $1/2 = 0.50000\dots$ and $1/3 = 0.\bar{3} \equiv 0.33333\dots$ are rational, while $\pi = 3.141592654\dots$ is irrational. Decimal arithmetic was invented in India over 1500 years ago but was not widely adopted in Europe until the seventeenth century.

The **real** numbers \mathbb{R} include the rational numbers and the irrational numbers; they correspond to all the points on an infinite line called the **real line**.

The **complex** numbers \mathbb{C} are the real numbers with one new number i whose square is -1 . A complex number z is a linear combination of a real number x and a real multiple iy of i

$$z = x + iy. \quad (1.2)$$

Here $x = \operatorname{Re}z$ is the **real part** of z , and $y = \operatorname{Im}z$ is its **imaginary part**. One adds complex numbers by adding their real and imaginary parts

$$z_1 + z_2 = x_1 + iy_1 + x_2 + iy_2 = x_1 + x_2 + i(y_1 + y_2). \quad (1.3)$$

Since $i^2 = -1$, the product of two complex numbers is

$$z_1 z_2 = (x_1 + iy_1)(x_2 + iy_2) = x_1 x_2 - y_1 y_2 + i(x_1 y_2 + y_1 x_2). \quad (1.4)$$

The polar representation of $z = x + iy$ is

$$z = r e^{i\theta} = r(\cos \theta + i \sin \theta) \quad (1.5)$$

in which r is the **modulus** or **absolute value** of z

$$r = |z| = \sqrt{x^2 + y^2} \quad (1.6)$$

and θ is its **phase** or **argument**

$$\theta = \arctan(y/x). \quad (1.7)$$

Since $\exp(2\pi i) = 1$, there is an inevitable ambiguity in the definition of the phase of any complex number $z = re^{i\theta}$: for any integer n , the phase $\theta + 2\pi n$ gives the same z as θ . In various computer languages, the function $\text{atan2}(y, x)$ returns the angle θ in the interval $-\pi < \theta \leq \pi$ for which $(x, y) = r(\cos \theta, \sin \theta)$.

There are two common notations z^* and \bar{z} for the **complex conjugate** of a complex number $z = x + iy$

$$z^* = \bar{z} = x - iy. \quad (1.8)$$

The square of the modulus of a complex number $z = x + iy$ is

$$|z|^2 = x^2 + y^2 = (x + iy)(x - iy) = \bar{z}z = z^*z. \quad (1.9)$$

The inverse of a complex number $z = x + iy$ is

$$z^{-1} = (x + iy)^{-1} = \frac{x - iy}{(x - iy)(x + iy)} = \frac{x - iy}{x^2 + y^2} = \frac{z^*}{z^*z} = \frac{z^*}{|z|^2}. \quad (1.10)$$

Grassmann numbers θ_i are **anticommuting** numbers, that is, the **anticommutator** of any two Grassmann numbers vanishes

$$\{\theta_i, \theta_j\} \equiv [\theta_i, \theta_j]_+ \equiv \theta_i\theta_j + \theta_j\theta_i = 0. \quad (1.11)$$

So the square of any Grassmann number is zero, $\theta_i^2 = 0$. These numbers have amusing properties (used in chapter 20). For example, because $\theta_1\theta_2 = -\theta_2\theta_1$ and $\theta_1^2 = \theta_2^2 = 0$, the most general function of two Grassmann numbers is

$$f(\theta_1, \theta_2) = a + b\theta_1 + c\theta_2 + d\theta_1\theta_2 \quad (1.12)$$

and $1/(1 + a\theta_i) = 1 - a\theta_i$ in which a, b, c, d are complex numbers (Hermann Grassmann, 1809–1877).

1.2 Numerical Conventions

Physicists represent quantities that have been measured to within a certain **standard deviation** σ (section 15.2) either with \pm signs or with parentheses. For instance, the current value of the mass of the Higgs boson is written as $m_{H^0} = 125.25 \pm 0.17$ GeV or equivalently as $m_{H^0} = 125.25(17)$

GeV, and the mass of the Z boson as $m_Z = 91.1876 \pm 0.0021$ GeV or as $m_Z = 91.1876(21)$ GeV. Here factors of c^2 are suppressed as in **natural** units (chapter 23).

One uses n digits to represent a number that one knows to n digits. Thus $m_W = 80$ GeV means that the mass of the W boson is approximately 80 GeV, not that it is exactly 80 GeV. Its measured value is $m_W = 80.379 \pm 0.012$ GeV or $m_W = 80.379(12)$ GeV.

PEMDAS: the order in which arithmetic operations are carried out is determined first by parentheses, then by exponentiation, then by multiplication and division doing left before right, and finally addition and subtraction doing left before right. Thus $a + b/cde = a + (b/(cde))$. In this book, I have often inserted extra parentheses to avoid uncertainty and confusion.

1.3 Arrays

An **array** is an **ordered set** of numbers. Arrays play big roles in computer science, physics, and mathematics. They can be of any (integral) dimension.

A one-dimensional array (a_1, a_2, \dots, a_n) is variously called an **n -tuple**, a **row vector** when written horizontally, a **column vector** when written vertically, an **n -vector**, or simply a **vector**. The numbers a_k are its **entries** or **components**.

A two-dimensional array a_{ik} with i running from 1 to n and k from 1 to m is an $n \times m$ **matrix**. The numbers a_{ik} are its **entries**, **elements**, or **matrix elements**. One can think of a matrix as a stack of row vectors or as a queue of column vectors. The entry a_{ik} is in the i th row and the k th column.

One can add together arrays of the same dimension and shape by adding their entries. Two n -tuples add as

$$(a_1, \dots, a_n) + (b_1, \dots, b_n) = (a_1 + b_1, \dots, a_n + b_n) \quad (1.13)$$

and two $n \times m$ matrices a and b add as

$$(a + b)_{ik} = a_{ik} + b_{ik}. \quad (1.14)$$

One can multiply arrays by numbers: Thus z times the three-dimensional array a_{ijk} is the array with entries $z a_{ijk}$.

One can multiply an n -vector b_k by a matrix a_{ik} that has m rows and n columns and get an m -vector b'_i

$$b'_i = a_{i1}b_1 + a_{i2}b_2 + \dots + a_{in}b_n = \sum_{k=1}^n a_{ik}b_k \quad \text{for } i = 1, \dots, m. \quad (1.15)$$

Example 1.1 (Lorentz transformations) The spacetime coordinates x and x' in two inertial frames are related by matrix multiplication $x' = Lx$ or

$$x'^a = L^a_0 x^0 + L^a_1 x^1 + L^a_2 x^2 + L^a_3 x^3 \quad (1.16)$$

in which L is a 4×4 real matrix L^a_b . \square

One can multiply an $n \times n$ matrix a_{ik} by two n vectors b_k and c_i

$$c^T a b = \sum_{i=1}^n \sum_{k=1}^n c_i a_{ik} b_k. \quad (1.17)$$

Example 1.2 (Distance between points) The invariant squared distance between points whose coordinates differ by dx^i is given in terms of a 4×4 metric g_{ik} as

$$ds^2 = dx^T g dx = \sum_{i=1}^4 \sum_{k=1}^4 g_{ik} dx^i dx^k. \quad (1.18)$$

\square

One can multiply two arrays together no matter what their shapes and dimensions. The **outer product** of an n -tuple a and an m -tuple b is an $n \times m$ matrix with elements

$$(ab)_{ik} = a_i b_k \quad (1.19)$$

or an $m \times n$ matrix with entries $(ba)_{ki} = b_k a_i$. If a and b are complex, then one also can form the outer products $(\bar{a}b)_{ik} = \bar{a}_i b_k$, $(\bar{b}a)_{ki} = \bar{b}_k a_i$, and $(\bar{b}\bar{a})_{ki} = \bar{b}_k \bar{a}_i$. The outer product of a matrix a_{ik} and a three-dimensional array $b_{j\ell m}$ is a five-dimensional array

$$(ab)_{ikj\ell m} = a_{ik} b_{j\ell m}. \quad (1.20)$$

An **inner product** is possible when two arrays are of the same size in one of their dimensions. Thus the **inner product** $(a, b) \equiv \langle a|b \rangle$ or **dot product** $a \cdot b$ of two real n -tuples a and b is

$$(a, b) = \langle a|b \rangle = a \cdot b = (a_1, \dots, a_n) \cdot (b_1, \dots, b_n) = a_1 b_1 + \dots + a_n b_n. \quad (1.21)$$

The **hermitian inner product** of two complex n -tuples a and b is

$$(a, b) = \langle a|b \rangle = \bar{a} \cdot b = (\bar{a}_1, \dots, \bar{a}_n) \cdot (b_1, \dots, b_n) = \bar{a}_1 b_1 + \dots + \bar{a}_n b_n. \quad (1.22)$$

The inner product of a vector with itself is nonnegative $(a, a) \geq 0$.

The product of an $m \times n$ matrix a_{ik} times an n -tuple b_k is an m -tuple b' whose i th component is

$$b'_i = a_{i1}b_1 + a_{i2}b_2 + \dots + a_{in}b_n = \sum_{k=1}^n a_{ik}b_k. \quad (1.23)$$

This product is $b' = ab$ in matrix notation.

If the size n of the second dimension of a matrix a matches that of the first dimension of a matrix b , then their product ab is a matrix with entries

$$(ab)_{i\ell} = a_{i1}b_{1\ell} + \dots + a_{in}b_{n\ell} = \sum_{k=1}^n a_{ik}b_{k\ell}. \quad (1.24)$$

1.4 Matrices

Matrices are two-dimensional arrays.

The **trace** of a square $n \times n$ matrix a is the sum of its diagonal elements

$$\text{Tr } a = \text{tr } a = a_{11} + a_{22} + \dots + a_{nn} = \sum_{i=1}^n a_{ii}. \quad (1.25)$$

The trace of the product of two matrices is independent of their order

$$\text{Tr}(ab) = \sum_{i=1}^n \sum_{k=1}^n a_{ik}b_{ki} = \sum_{k=1}^n \sum_{i=1}^n b_{ki}a_{ik} = \text{Tr}(ba) \quad (1.26)$$

as long as the matrix elements are numbers that commute with each other. It follows that the trace is **cyclic**

$$\text{Tr}(abc\dots z) = \text{Tr}(bc\dots za) = \text{Tr}(c\dots zab) = \dots \quad (1.27)$$

The **transpose** of an $n \times \ell$ matrix a is an $\ell \times n$ matrix a^\top with row and column indexes interchanged

$$(a^\top)_{ij} = a_{ji}. \quad (1.28)$$

Mathematicians often use a prime to mean transpose, as in $a' = a^\top$. By transposing indexes, you can sometimes write a sum of products of matrix elements more simply as the matrix element of a product of matrices

$$\sum_{i=1}^n a_{ik}b_{i\ell} = \sum_{i=1}^n a^\top_{ki}b_{i\ell} = (a^\top b)_{k\ell} = (b^\top a)_{\ell k}. \quad (1.29)$$

Transposition inverts the order of matrix multiplication

$$(ab)_{k\ell} = \sum_{i=1}^n a_{ki}b_{i\ell} = \sum_{i=1}^n b_{i\ell}a_{ki} = \sum_{i=1}^n b^{\top}_{\ell i}a^{\top}_{ik} = (b^{\top}a^{\top})_{\ell k} \quad (1.30)$$

which is $(ab)^{\top} = b^{\top}a^{\top}$ in matrix notation.

A matrix that is equal to its transpose

$$a = a^{\top} \quad (1.31)$$

is **symmetric**, $a_{ij} = a_{ji}$.

The (hermitian) **adjoint** of a matrix is the complex conjugate of its transpose. That is, the (hermitian) adjoint a^{\dagger} of an $N \times L$ complex matrix a is the $L \times N$ matrix with entries

$$(a^{\dagger})_{ij} = a^*_{ji}. \quad (1.32)$$

One may show that

$$(ab)^{\dagger} = b^{\dagger}a^{\dagger}. \quad (1.33)$$

A matrix that is equal to its adjoint

$$a_{ij} = (a^{\dagger})_{ij} = a^*_{ji} \quad (1.34)$$

(and which must be a square matrix) is **hermitian** or **self adjoint**

$$a = a^{\dagger} \quad (1.35)$$

(Charles Hermite 1822–1901).

Example 1.3 (The Pauli Matrices) All three of Pauli's matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.36)$$

are hermitian (Wolfgang Pauli 1900–1958). \square

A real hermitian matrix a is symmetric, $a_{ik} = a_{ki}$. If a matrix a is hermitian, then the double sum

$$\langle v|a|v \rangle = \sum_{i=1}^n \sum_{j=1}^n v_i^* a_{ij} v_j \in \mathbb{R} \quad (1.37)$$

is real for all complex n -tuples v .

The **Kronecker delta** δ_{ik} is defined to be unity if $i = k$ and zero if $i \neq k$

$$\delta_{ik} = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases} \quad (1.38)$$

(Leopold Kronecker 1823–1891). The **identity matrix** I has entries $I_{ik} = \delta_{ik}$.

The **inverse** a^{-1} of an $n \times n$ matrix a is a square matrix that satisfies

$$a^{-1}a = a a^{-1} = I \quad (1.39)$$

in which I is the $n \times n$ identity matrix.

So far we have been writing n -tuples and matrices and their elements with lower-case letters. It is equally common to use capital letters, and we will do so for the rest of this section.

A matrix U whose adjoint U^\dagger is its inverse

$$U^\dagger U = U U^\dagger = I \quad (1.40)$$

is **unitary**. Unitary matrices are square.

A real unitary matrix O is **orthogonal** and obeys the rule

$$O^\top O = O O^\top = I. \quad (1.41)$$

Orthogonal matrices are square.

An $n \times n$ hermitian matrix A is **nonnegative**

$$A \geq 0 \quad (1.42)$$

if for all complex vectors V the quadratic form

$$\langle V|A|V \rangle = \sum_{i=1}^n \sum_{j=1}^n V_i^* A_{ij} V_j \geq 0 \quad (1.43)$$

is nonnegative. It is **positive** or **positive definite** if

$$\langle V|A|V \rangle > 0 \quad (1.44)$$

for all nonzero vectors $|V\rangle$.

Example 1.4 (Kinds of Positivity) The nonsymmetric, nonhermitian 2×2 matrix

$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad (1.45)$$

is positive on the space of all real 2-vectors but not on the space of all complex 2-vectors. \square

Example 1.5 (Representations of Imaginary and Grassmann Numbers)
The 2×2 matrix

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (1.46)$$

can represent the number i since

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -I. \quad (1.47)$$

The 2×2 matrix

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (1.48)$$

can represent a Grassmann number since

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = 0. \quad (1.49)$$

To represent two Grassmann numbers, one needs 4×4 matrices, such as

$$\theta_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \theta_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (1.50)$$

The matrices that represent n Grassmann numbers are $2^n \times 2^n$ and have 2^n rows and 2^n columns. \square

Example 1.6 (Fermions) The matrices (1.50) also can represent lowering or annihilation operators for a system of two fermionic states. For $a_1 = \theta_1$ and $a_2 = \theta_2$ and their adjoints a_1^\dagger and a_2^\dagger , the creation operators, satisfy the anticommutation relations

$$\{a_i, a_k^\dagger\} = \delta_{ik} \quad \text{and} \quad \{a_i, a_k\} = \{a_i^\dagger, a_k^\dagger\} = 0 \quad (1.51)$$

where i and k take the values 1 or 2. In particular, the relation $(a_i^\dagger)^2 = 0$ implements **Pauli's exclusion principle**, the rule that no state of a fermion can be doubly occupied. \square

1.5 Vectors

Vectors are things that can be multiplied by numbers and added together to form other vectors in the same **vector space**. So if U and V are vectors

in a vector space S over a set F of numbers x and y and so forth, then

$$W = xU + yV \quad (1.52)$$

also is a vector in the vector space S .

A **basis** for a vector space S is a set B of vectors B_k for $k = 1 \dots n$ in terms of which every vector U in S can be expressed as a linear combination

$$U = u_1B_1 + u_2B_2 + \dots + u_nB_n \quad (1.53)$$

with numbers u_k in F . The numbers u_k are the **components** of the vector U in the basis B . If the **basis vectors** B_k are **orthonormal**, that is, if their inner products are $(B_k, B_\ell) = \langle B_k | B_\ell \rangle = \bar{B}_k \cdot B_\ell = \delta_{k\ell}$, then we might represent the vector U as the n -tuple (u_1, u_2, \dots, u_n) with $u_k = \langle B_k | U \rangle$ as the corresponding column vector.

Example 1.7 (Hardware Store) Suppose the vector W represents a certain kind of washer and the vector N represents a certain kind of nail. Then if n and m are natural numbers, the vector

$$H = nW + mN \quad (1.54)$$

would represent a possible inventory of a very simple hardware store. The vector space of all such vectors H would include all possible inventories of the store. That space is a two-dimensional vector space over the natural numbers, and the two vectors W and N form a basis for it. \square

Example 1.8 (Complex Numbers) The complex numbers are a vector space. Two of its vectors are the number 1 and the number i ; the vector space of complex numbers is then the set of all linear combinations

$$z = x1 + yi = x + iy. \quad (1.55)$$

The complex numbers are a two-dimensional vector space over the real numbers, and the vectors 1 and i are a basis for it.

The complex numbers also form a one-dimensional vector space over the complex numbers. Here any nonzero real or complex number, for instance the number 1 can be a basis consisting of the single vector 1. This one-dimensional vector space is the set of all $z = z1$ for arbitrary complex z . \square

Example 1.9 (2-space) Ordinary flat two-dimensional space is the set of all linear combinations

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} \quad (1.56)$$

in which x and y are real numbers and $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are perpendicular vectors of unit length (unit vectors with $\hat{x} \cdot \hat{x} = 1 = \hat{y} \cdot \hat{y}$ and $\hat{x} \cdot \hat{y} = 0$). This vector space, called \mathbb{R}^2 , is a 2-d space over the reals.

The vector \mathbf{r} can be described by the basis vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ and also by any other set of basis vectors, such as $-\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} = -y(-\hat{\mathbf{y}}) + x\hat{\mathbf{x}}. \quad (1.57)$$

The components of the vector \mathbf{r} are (x, y) in the $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ basis and $(-y, x)$ in the $\{-\hat{\mathbf{y}}, \hat{\mathbf{x}}\}$ basis. **Each vector is unique, but its components depend upon the basis.** \square

Example 1.10 (3-Space) Ordinary flat three-dimensional space is the set of all linear combinations

$$\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}} \quad (1.58)$$

in which x, y , and z are real numbers. It is a 3-d space over the reals. \square

Example 1.11 (Matrices) Arrays of a given dimension and size can be added and multiplied by numbers, and so they form a vector space. For instance, all complex three-dimensional arrays a_{ijk} in which $1 \leq i \leq 3$, $1 \leq j \leq 4$, and $1 \leq k \leq 5$ form a vector space over the complex numbers. \square

Example 1.12 (Partial Derivatives) Derivatives are vectors; so are partial derivatives. For instance, the linear combinations of x and y partial derivatives taken at $x = y = 0$

$$a \frac{\partial}{\partial x} + b \frac{\partial}{\partial y} \quad (1.59)$$

form a vector space. \square

Example 1.13 (Functions) The space of all linear combinations of a set of functions $f_i(x)$ defined on an interval $[a, b]$

$$f(x) = \sum_i z_i f_i(x) \quad (1.60)$$

is a vector space over the natural \mathbb{N} , real \mathbb{R} , or complex \mathbb{C} numbers $\{z_i\}$. \square

Example 1.14 (States in quantum mechanics) In quantum mechanics, if the properties of a system have been measured as completely as possible, then the system (or our knowledge of it) is said to be in a **state**, often called a **pure state**, and is represented by a vector ψ or $|\psi\rangle$ in Dirac's notation. If

the properties of a system have not been measured as completely as possible, then the system (or our knowledge of it) is said to be in a **mixture** or a **mixed state**, and is represented by a density operator (section 1.37).

If c_1 and c_2 are complex numbers, and $|\psi_1\rangle$ and $|\psi_2\rangle$ are any two states, then the linear combination

$$|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle \quad (1.61)$$

also is a possible state of the system.

A harmonic oscillator in its k th excited state is in a state described by a vector $|k\rangle$. A particle exactly at position q is in a state described by a vector $|q\rangle$. An electron moving with momentum \mathbf{p} and spin σ is in a state represented by a vector $|\mathbf{p}, \sigma\rangle$. A hydrogen atom at rest in its ground state is in a state $|E_0\rangle$. \square

Example 1.15 (Polarization of photons and gravitons) The general state of a photon of momentum \vec{k} is one of elliptical polarization

$$|\vec{k}, \theta, \phi\rangle = \cos\theta e^{i\phi}|\vec{k}, +\rangle + \sin\theta e^{-i\phi}|\vec{k}, -\rangle \quad (1.62)$$

in which the states of positive and negative helicity $|\vec{k}, \pm\rangle$ represent a photon whose angular momentum $\pm\hbar$ is parallel or antiparallel to its momentum \vec{k} . If $\theta = \pi/4 + n\pi$, the polarization is linear, and the electric field is parallel to an axis that depends upon ϕ and is perpendicular to \vec{k} .

The general state of a graviton of momentum \vec{k} also is one of elliptical polarization (1.62), but now the states of positive and negative helicity $|\vec{k}, \pm\rangle$ have angular momentum $\pm 2\hbar$ parallel or antiparallel to the momentum \vec{k} . Linear polarization again is $\theta = \pi/4 + n\pi$. The state $|\vec{k}, +\rangle$ represents space being stretched and squeezed along one axis while being squeezed and stretched along another axis, both axes perpendicular to each other and to \vec{k} . In the state $|\vec{k}, \times\rangle$, the stretching and squeezing axes are rotated by 45° about \vec{k} relative to those of $|\vec{k}, +\rangle$. \square

1.6 Linear operators

A **linear operator** A maps each vector V in its **domain** into a vector $V' = A(V) \equiv AV$ in its **range** in a way that is linear. So if V and W are two vectors in its domain and b and c are numbers, then

$$A(bV + cW) = bA(V) + cA(W) = bAV + cAW. \quad (1.63)$$

If the domain and the range are the same vector space S , then A maps each basis vector B_i of S into a linear combination of the basis vectors B_k

$$A B_i = a_{1i} B_1 + a_{2i} B_2 + \dots + a_{ni} B_n = \sum_{k=1}^n a_{ki} B_k \quad (1.64)$$

a formula that is clearer in Dirac's notation (section 1.13). The square matrix a_{ki} **represents** the linear operator A in the B_k basis. The effect of A on any vector $U = u_1 B_1 + u_2 B_2 + \dots + u_n B_n$ in S then is

$$A U = A \sum_{i=1}^n u_i B_i = \sum_{i=1}^n u_i A B_i = \sum_{i,k=1}^n u_i a_{ki} B_k = \sum_{i,k=1}^n a_{ki} u_i B_k. \quad (1.65)$$

So the k th component u'_k of the vector $U' = A U$ is

$$u'_k = a_{k1} u_1 + a_{k2} u_2 + \dots + a_{kn} u_n = \sum_{i=1}^n a_{ki} u_i. \quad (1.66)$$

Thus the column vector u' of the components u'_k of the vector $U' = A U$ is the product $u' = a u$ of the matrix with elements a_{ki} that represents the linear operator A in the B_k basis and the column vector with components u_i that represents the vector U in that basis. In each basis, vectors and linear operators are represented by column vectors and matrices.

Each linear operator is unique, but its matrix depends upon the basis. If we change from the B_k basis to another basis B'_i

$$B'_i = \sum_{k=1}^n u_{ki} B_k \quad (1.67)$$

in which the $n \times n$ matrix $u_{\ell k}$ has an inverse matrix u_{ki}^{-1} so that

$$\sum_{k=1}^n u_{ki}^{-1} B'_k = \sum_{k=1}^n u_{ki}^{-1} \sum_{\ell=1}^n u_{\ell k} B_\ell = \sum_{\ell=1}^n \left(\sum_{k=1}^n u_{\ell k} u_{ki}^{-1} \right) B_\ell = \sum_{\ell=1}^n \delta_{\ell i} B_\ell = B_i \quad (1.68)$$

then the old basis vectors B_i are given by

$$B_i = \sum_{k=1}^n u_{ki}^{-1} B'_k. \quad (1.69)$$

Thus (exercise 1.9) the linear operator A maps the basis vector B'_i to

$$A B'_i = \sum_{k=1}^n u_{ki} A B_k = \sum_{j,k=1}^n u_{ki} a_{jk} B_j = \sum_{j,k,\ell=1}^n u_{ki} a_{jk} u_{\ell j}^{-1} B'_\ell. \quad (1.70)$$

So the matrix a' that represents A in the B' basis is related to the matrix a that represents it in the B basis by a **similarity transformation**

$$a'_{\ell i} = \sum_{jk=1}^n u_{\ell j}^{-1} a_{jk} u_{ki} \quad \text{or} \quad a' = u^{-1} a u \quad (1.71)$$

in matrix notation. If the matrix u is **unitary**, then its inverse is its hermitian adjoint

$$u^{-1} = u^\dagger \quad (1.72)$$

and the similarity transformation (1.71) is

$$a'_{\ell i} = \sum_{jk=1}^n u_{\ell j}^\dagger a_{jk} u_{ki} = \sum_{jk=1}^n u_{j\ell}^* a_{jk} u_{ik} \quad \text{or} \quad a' = u^\dagger a u. \quad (1.73)$$

Because traces are cyclic, they are invariant under similarity transformations

$$\text{Tr}(a') = \text{Tr}(u^{-1} a u) = \text{Tr}(a u u^{-1}) = \text{Tr}(a). \quad (1.74)$$

Example 1.16 (Change of Basis) Let the action of the linear operator A on the basis vectors $\{B_1, B_2\}$ be $AB_1 = B_2$ and $AB_2 = 0$. If the column vectors

$$b_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad b_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (1.75)$$

represent the basis vectors B_1 and B_2 , then the matrix

$$a = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (1.76)$$

represents the linear operator A . But if we use the basis vectors

$$B'_1 = \frac{1}{\sqrt{2}}(B_1 + B_2) \quad \text{and} \quad B'_2 = \frac{1}{\sqrt{2}}(B_1 - B_2) \quad (1.77)$$

then the vectors

$$b'_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad b'_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (1.78)$$

would represent B_1 and B_2 , and the matrix

$$a' = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \quad (1.79)$$

would represent the linear operator A (exercise 1.10). \square

A linear operator A also may map a vector space S with basis B_k into a different vector space T with its own basis C_k .

$$A B_i = \sum_{k=1}^M a_{ki} C_k. \quad (1.80)$$

It then maps an arbitrary vector $V = u_1 B_1 + \dots + u_n B_n$ in S into the vector

$$A V = \sum_{k=1}^M \left(\sum_{i=1}^n a_{ki} u_i \right) C_k \quad (1.81)$$

in T .

1.7 Inner products

Most of the vector spaces used by physicists have an inner product. A **positive-definite inner product** associates a number (f, g) with every ordered pair of vectors f and g in the vector space V and obeys, for every three vectors f, g, h and numbers z, w with $v = z g + w h$, the three rules

$$(f, g) = (g, f)^* \quad (1.82)$$

$$(f, v) = (f, z g + w h) = z (f, g) + w (f, h) \quad (1.83)$$

$$(f, f) \geq 0 \quad \text{and} \quad (f, f) = 0 \iff f = 0. \quad (1.84)$$

The first rule says that the inner product is **hermitian**. The second rule says that it is **linear** in the second vector $v = z g + w h$ of the pair. The third rule says that it is **positive definite**. The first two rules imply that (exercise 1.11) the inner product is **anti-linear** in the first vector of the pair

$$(z g + w h, f) = z^*(g, f) + w^*(h, f). \quad (1.85)$$

A **Schwarz inner product** obeys the first two rules (1.82, 1.83) for an inner product and the fourth (1.85) but only the first part of the third (1.84)

$$(f, f) \geq 0. \quad (1.86)$$

This condition of **nonnegativity** implies (exercise 1.15) that a vector f of zero length must be orthogonal to all vectors g in the vector space V

$$(f, f) = 0 \implies (g, f) = 0 \quad \text{for all } g \in V. \quad (1.87)$$

So a Schwarz inner product is *almost* positive definite.

Inner products of 4-vectors can be negative. To accommodate them we define an **indefinite** inner product without regard to positivity as one that satisfies the first two rules (1.82 & 1.83) and therefore also the fourth rule (1.85) and that instead of being positive definite is **nondegenerate**

$$(f, g) = 0 \text{ for all } f \in V \implies g = 0. \quad (1.88)$$

This rule says that only the zero vector is orthogonal to all the vectors of the space. The positive-definite condition (1.84) is stronger than and implies nondegeneracy (1.88) (exercise 1.14).

Apart from the indefinite inner products of 4-vectors in special and general relativity, most of the inner products physicists use are Schwarz inner products or positive-definite inner products. For such inner products, we can define the **norm** or **length** $|f| = \|f\|$ of a vector f as the square root of the nonnegative inner product (f, f)

$$\|f\| = \sqrt{(f, f)}. \quad (1.89)$$

A vector $\hat{f} = f / \|f\|$ has unit norm and is said to be **normalized**. Two measures of the distance between normalized vectors f and g are the **norm of their difference** and the **Bures distance**

$$D(f, g) = \|f - g\| \quad \text{and} \quad D_B(f, g) = \arccos(|(f, g)|) \quad (1.90)$$

which are bounded by $0 \leq \|f - g\| \leq 2$ and by $0 \leq \arccos(|(f, g)|) \leq \pi/2$.

Example 1.17 (Euclidian space) The space of real vectors U, V with n components U_i, V_i forms an n -dimensional vector space over the real numbers with an inner product

$$(U, V) = \sum_{i=1}^n U_i V_i \quad (1.91)$$

that is nonnegative when the two vectors are the same

$$(U, U) = \sum_{i=1}^n U_i U_i = \sum_{i=1}^n U_i^2 \geq 0 \quad (1.92)$$

and vanishes only if all the components U_i are zero, that is, if the vector $U = 0$. Thus the inner product (1.91) is positive definite. When (U, V) is zero, the vectors U and V are **orthogonal**. \square

Example 1.18 (Complex Euclidian Space) The space of complex vectors with n components U_i, V_i forms an n -dimensional vector space over the

complex numbers with inner product

$$(U, V) = \sum_{i=1}^n U_i^* V_i = (V, U)^*. \quad (1.93)$$

The inner product (U, U) is nonnegative and vanishes

$$(U, U) = \sum_{i=1}^n U_i^* U_i = \sum_{i=1}^n |U_i|^2 \geq 0 \quad (1.94)$$

only if $U = 0$. So the inner product (1.93) is positive definite. If (U, V) is zero, then U and V are orthogonal. \square

Example 1.19 (Complex Matrices) For the vector space of $n \times m$ complex matrices A, B, \dots , the trace of the adjoint (1.32) of A multiplied by B is an inner product

$$(A, B) = \text{Tr} A^\dagger B = \sum_{i=1}^n \sum_{j=1}^m (A^\dagger)_{ji} B_{ij} = \sum_{i=1}^n \sum_{j=1}^m A_{ij}^* B_{ij} \quad (1.95)$$

that is nonnegative when the matrices are the same

$$(A, A) = \text{Tr} A^\dagger A = \sum_{i=1}^n \sum_{j=1}^m A_{ij}^* A_{ij} = \sum_{i=1}^n \sum_{j=1}^m |A_{ij}|^2 \geq 0 \quad (1.96)$$

and zero only when $A = 0$. So this inner product is positive definite. \square

A vector space with a positive-definite inner product (1.82–1.85) is called an **inner-product space**, a **metric space**, or a **pre-Hilbert space**.

A sequence of vectors f_n is a **Cauchy sequence** if for every $\epsilon > 0$ there is an integer $N(\epsilon)$ such that $\|f_n - f_m\| < \epsilon$ whenever both n and m exceed $N(\epsilon)$. A sequence of vectors f_n **converges** to a vector f if for every $\epsilon > 0$ there is an integer $N(\epsilon)$ such that $\|f - f_n\| < \epsilon$ whenever n exceeds $N(\epsilon)$. An inner-product space with a norm defined as in (1.89) is **complete** if each of its Cauchy sequences converges to a vector in that space. A **Hilbert space** is a complete inner-product space. Every finite-dimensional inner-product space is complete and so is a Hilbert space. An infinite-dimensional complete inner-product space, such as the space of all square-integrable functions, also is a Hilbert space (David Hilbert, 1862–1943).

Example 1.20 (Hilbert Space of Square-Integrable Functions) For the vector space of functions (1.60), a natural inner product is

$$(f, g) = \int_a^b dx f^*(x) g(x). \quad (1.97)$$

The squared norm $\|f\|$ of a function $f(x)$ is

$$\|f\|^2 = \int_a^b dx |f(x)|^2. \quad (1.98)$$

A function is **square integrable** if its norm is finite. The space of all square-integrable functions is an inner-product space; it also is complete and so is a Hilbert space. \square

Example 1.21 (Minkowski inner product) The Minkowski or Lorentz inner product (p, x) of two 4-vectors $p = (E/c, p_1, p_2, p_3)$ and $x = (ct, x_1, x_2, x_3)$ is $\mathbf{p} \cdot \mathbf{x} - Et$. It is indefinite, nondegenerate (1.88), and invariant under Lorentz transformations, and often is written as $p \cdot x$ or as px . If p is the 4-momentum of a freely moving physical particle of mass m , then

$$p \cdot p = \mathbf{p} \cdot \mathbf{p} - E^2/c^2 = -c^2 m^2 \leq 0. \quad (1.99)$$

The Minkowski inner product satisfies the rules (1.82, 1.83, and 1.88), but it is **not positive definite**, and it does not satisfy the Schwarz inequality (Hermann Minkowski 1864–1909, Hendrik Lorentz 1853–1928). \square

Example 1.22 (Inner products in quantum mechanics) The probability $P(\phi|\psi)$ that a system in the state $|\psi\rangle$ will be measured to be in the state $|\phi\rangle$ is the absolute value squared of the inner product $\langle\phi|\psi\rangle$ divided by the squared norms of the two states

$$P(\phi|\psi) = \frac{|\langle\phi|\psi\rangle|^2}{\langle\phi|\phi\rangle\langle\psi|\psi\rangle}. \quad (1.100)$$

If the two states are normalized, then the probability is just the absolute value squared of their inner product, $P(\phi|\psi) = |\langle\phi|\psi\rangle|^2$. \square

1.8 Cauchy–Schwarz inequalities

For any two vectors f and g , the Schwarz inequality

$$(f, f)(g, g) \geq |(f, g)|^2 \quad (1.101)$$

holds for any Schwarz inner product (and so for any positive-definite inner product). The condition (1.86) of **nonnegativity** ensures that for any complex number λ the inner product of the vector $f - \lambda g$ with itself is nonnegative

$$(f - \lambda g, f - \lambda g) = (f, f) - \lambda^*(g, f) - \lambda(f, g) + |\lambda|^2(g, g) \geq 0. \quad (1.102)$$

Now if $(g, g) = 0$, then for $(f - \lambda g, f - \lambda g)$ to remain nonnegative for all complex values of λ it is necessary that $(f, g) = 0$ also vanish (exercise 1.15). Thus if $(g, g) = 0$, then the Schwarz inequality (1.101) is trivially true because both sides of it vanish. So we assume that $(g, g) > 0$ and set $\lambda = (g, f)/(g, g)$. The inequality (1.102) then gives us

$$(f - \lambda g, f - \lambda g) = \left(f - \frac{(g, f)}{(g, g)} g, f - \frac{(g, f)}{(g, g)} g \right) = (f, f) - \frac{(f, g)(g, f)}{(g, g)} \geq 0$$

which is the Schwarz inequality (1.101)

$$(f, f)(g, g) \geq |(f, g)|^2. \quad (1.103)$$

Taking the square root of each side, we have

$$\|f\| \|g\| \geq |(f, g)| \quad (1.104)$$

(Hermann Schwarz 1843–1921).

Example 1.23 (Triangle inequality) The square of $\|f + g\|$ is

$$\begin{aligned} \|f + g\|^2 &= (f + g, f + g) = (f, f) + (f, g) + (g, f) + (g, g) \\ &= \|f\|^2 + (f, g) + (g, f) + \|g\|^2 \leq \|f\|^2 + 2|(f, g)| + \|g\|^2. \end{aligned} \quad (1.105)$$

The Schwarz inequality (1.101) says that $|(f, g)| \leq \|f\| \|g\|$. So we have

$$\|f + g\|^2 \leq \|f\|^2 + 2\|f\| \|g\| + \|g\|^2 = (\|f\| + \|g\|)^2 \quad (1.106)$$

whose square root is the triangle inequality

$$\|f + g\| \leq \|f\| + \|g\|. \quad (1.107)$$

Equivalently with $f = a - c$ and $g = c - b$, this is $\|a - b\| \leq \|a - c\| + \|c - b\|$. \square

Example 1.24 (Some Schwarz Inequalities) For the dot product of two real 3-vectors \mathbf{r} & \mathbf{R} , the Cauchy-Schwarz inequality is

$$(\mathbf{r} \cdot \mathbf{r})(\mathbf{R} \cdot \mathbf{R}) \geq (\mathbf{r} \cdot \mathbf{R})^2 = (\mathbf{r} \cdot \mathbf{r})(\mathbf{R} \cdot \mathbf{R}) \cos^2 \theta \quad (1.108)$$

where θ is the angle between \mathbf{r} and \mathbf{R} .

The Schwarz inequality for two real n -vectors \mathbf{x} is

$$(\mathbf{x} \cdot \mathbf{x})(\mathbf{y} \cdot \mathbf{y}) \geq (\mathbf{x} \cdot \mathbf{y})^2 = (\mathbf{x} \cdot \mathbf{x})(\mathbf{y} \cdot \mathbf{y}) \cos^2 \theta \quad (1.109)$$

and it implies (exercise 1.16) that

$$\|\mathbf{x}\| + \|\mathbf{y}\| \geq \|\mathbf{x} + \mathbf{y}\|. \quad (1.110)$$

For two complex n -vectors \mathbf{u} and \mathbf{v} , the Schwarz inequality is

$$(\mathbf{u}^* \cdot \mathbf{u})(\mathbf{v}^* \cdot \mathbf{v}) \geq |\mathbf{u}^* \cdot \mathbf{v}|^2 = (\mathbf{u}^* \cdot \mathbf{u})(\mathbf{v}^* \cdot \mathbf{v}) \cos^2 \theta \quad (1.111)$$

and it implies (exercise 1.17) that

$$\|\mathbf{u}\| + \|\mathbf{v}\| \geq \|\mathbf{u} + \mathbf{v}\|. \quad (1.112)$$

The inner product (1.97) of two complex functions f and g provides another example

$$\int_a^b dx |f(x)|^2 \int_a^b dx |g(x)|^2 \geq \left| \int_a^b dx f^*(x) g(x) \right|^2 \quad (1.113)$$

of the Schwarz inequality. \square

1.9 Linear independence and completeness

A set of n vectors V_1, V_2, \dots, V_n is **linearly dependent** over the real (complex) numbers if there exist real (complex) numbers c_i , *not all zero*, such that the linear combination

$$c_1 V_1 + \dots + c_n V_n = 0 \quad (1.114)$$

vanishes. A set of vectors is **linearly independent** if it is not linearly dependent.

A set $\{V_i\}$ of linearly independent vectors is **maximal** in a vector space S if the addition of any other vector U in S to the set $\{V_i\}$ makes the enlarged set $\{U, V_i\}$ linearly dependent.

A set of n linearly independent vectors V_1, V_2, \dots, V_n that is maximal in a vector space S can represent any vector U in the space S as a linear combination of its vectors, $U = u_1 V_1 + \dots + u_n V_n$. For if we enlarge the maximal set $\{V_i\}$ by including in it any vector U not already in it, then the bigger set $\{U, V_i\}$ will be linearly dependent. Thus there will be numbers c_0, c_1, \dots, c_n , not all zero, that make the sum

$$c_0 U + c_1 V_1 + \dots + c_n V_n = 0 \quad (1.115)$$

vanish. Now if c_0 were 0, then the set $\{V_i\}$ would be linearly dependent. Thus $c_0 \neq 0$, and so we may divide by c_0 and express the arbitrary vector U as a linear combination of the vectors V_i

$$U = -\frac{1}{c_0} (c_1 V_1 + \dots + c_n V_n) = u_1 V_1 + \dots + u_n V_n \quad (1.116)$$

with $u_k = -c_k/c_0$. Thus a set of linearly independent vectors $\{V_i\}$ that is maximal in a space S can represent every vector U in S as a linear combination $U = u_1 V_1 + \dots + u_n V_n$ of its vectors. Such a set $\{V_i\}$ of linearly

independent vectors that is maximal in a space S is called a **basis** for S ; it **spans** S ; it is a **complete** set of vectors in S .

The maximum number of linearly independent vectors in a space is the **dimension** of the space.

1.10 Dimension of a vector space

If V_1, \dots, V_n and W_1, \dots, W_m are any two bases for a vector space S , then $n = m$.

To see why, suppose that the n vectors C_1, C_2, \dots, C_n are complete in a vector space S , and that the m vectors L_1, L_2, \dots, L_m in S are linearly independent (Halmos, 1958, sec. 1.8). Since the C 's are complete, the set of vectors L_m, C_1, \dots, C_n is linearly dependent. So we can omit one of the C 's and the remaining set $L_m, C_1, \dots, C_{i-1}, C_{i+1}, \dots, C_n$ still spans S . Repeating this argument, we find that the vectors

$$L_{m-1}, L_m, C_1, \dots, C_{i-1}, C_{i+1}, \dots, C_n \quad (1.117)$$

are linearly dependent, and that the vectors

$$L_{m-1}, L_m, C_1, \dots, C_{i-1}, C_{i+1}, \dots, C_{j-1}, C_{j+1}, \dots, C_n \quad (1.118)$$

still span S . We continue to repeat these steps until we run out of L 's or C 's. If n were less than m , then we'd end up with a set of vectors L_k, \dots, L_m that would be complete and therefore each of the vectors L_1, \dots, L_{k-1} would have to be linear combinations of the vectors L_k, \dots, L_m . But the L 's by assumption are linearly independent. So $n \geq m$. Thus if both the C 's and the L 's are bases for the same space S , and so are both complete and linearly independent in it, then both $n \geq m$ and $m \geq n$. So all the bases of a vector space consist of the same number of vectors. This number is the **dimension** of the space.

The steps of the above demonstration stop for $n = m$ when the m linearly independent L 's have replaced the n complete C 's leaving us with $n = m$ linearly independent L 's that are complete. Thus in a vector space of n dimensions, every set of n linearly independent vectors is complete and so forms a basis for the space.

1.11 Orthonormal vectors

Suppose the vectors V_1, V_2, \dots, V_n are linearly independent. Then we can make out of them a set of n vectors U_i that are orthonormal

$$(U_i, U_j) = \delta_{ij}. \quad (1.119)$$

There are many ways to do this because there are many such sets of orthonormal vectors. We will use the Gram-Schmidt method. We set

$$U_1 = \frac{V_1}{\sqrt{(V_1, V_1)}} \quad (1.120)$$

so the first vector U_1 is normalized. Next we set $u_2 = V_2 + c_{12}U_1$ and require that u_2 be orthogonal to U_1

$$0 = (U_1, u_2) = (U_1, c_{12}U_1 + V_2) = c_{12} + (U_1, V_2). \quad (1.121)$$

Thus $c_{12} = -(U_1, V_2)$, and so

$$u_2 = V_2 - (U_1, V_2)U_1. \quad (1.122)$$

The normalized vector U_2 then is

$$U_2 = \frac{u_2}{\sqrt{(u_2, u_2)}}. \quad (1.123)$$

We next set $u_3 = V_3 + c_{13}U_1 + c_{23}U_2$ and ask that u_3 be orthogonal to U_1

$$0 = (U_1, u_3) = (U_1, c_{13}U_1 + c_{23}U_2 + V_3) = c_{13} + (U_1, V_3) \quad (1.124)$$

and also to U_2

$$0 = (U_2, u_3) = (U_2, c_{13}U_1 + c_{23}U_2 + V_3) = c_{23} + (U_2, V_3). \quad (1.125)$$

So $c_{13} = -(U_1, V_3)$ and $c_{23} = -(U_2, V_3)$, and we have

$$u_3 = V_3 - (U_1, V_3)U_1 - (U_2, V_3)U_2. \quad (1.126)$$

The normalized vector U_3 then is

$$U_3 = \frac{u_3}{\sqrt{(u_3, u_3)}}. \quad (1.127)$$

We may continue in this way until we reach the last of the n linearly independent vectors. We require the k th unnormalized vector u_k

$$u_k = V_k + \sum_{i=1}^{k-1} c_{ik}U_i \quad (1.128)$$

to be orthogonal to the $k-1$ vectors U_i and find that $c_{ik} = -(U_i, V_k)$ so that

$$u_k = V_k - \sum_{i=1}^{k-1} (U_i, V_k)U_i. \quad (1.129)$$

The normalized vector then is

$$U_k = \frac{u_k}{\sqrt{(u_k, u_k)}}. \quad (1.130)$$

If we were to renumber the original vectors V_1, \dots, V_n and repeat the Gram-Schmidt process, we would get a different set of orthonormal vectors U'_i in general.

A basis is more useful if its vectors are orthonormal.

1.12 Outer products

From any two vectors f and g , we may make an **outer-product** operator A that maps any vector h into the vector f multiplied by the inner product (g, h)

$$Ah = f(g, h) = (g, h) f. \quad (1.131)$$

The operator A is linear because for any vectors e, h and numbers z, w

$$A(zh + we) = (g, zh + we) f = z(g, h) f + w(g, e) f = zAh + wAe. \quad (1.132)$$

If f, g , and h are vectors with components f_i, g_i , and h_i in some basis, then the linear transformation (1.131) is

$$(Ah)_i = \sum_{j=1}^n A_{ij} h_j = f_i \sum_{j=1}^n g_j^* h_j \quad (1.133)$$

and in that basis A is the matrix with entries

$$A_{ij} = f_i g_j^*. \quad (1.134)$$

A is the **outer product** of the column vector f and the row vector g^* .

Example 1.25 (Outer Product) If in some basis the vectors f and g are

$$f = \begin{pmatrix} 2 \\ 3i \end{pmatrix} \quad \text{and} \quad g = \begin{pmatrix} i \\ 1 \\ 3i \end{pmatrix} \quad (1.135)$$

then their outer products are the matrices

$$\begin{pmatrix} 2 \\ 3i \end{pmatrix} (-i \quad 1 \quad -3i) = \begin{pmatrix} -2i & 2 & -6i \\ 3 & 3i & 9 \end{pmatrix} \quad (1.136)$$

and

$$\begin{pmatrix} i \\ 1 \\ 3i \end{pmatrix} \begin{pmatrix} 2 & -3i \end{pmatrix} = \begin{pmatrix} 2i & 3 \\ 2 & -3i \\ 6i & 9 \end{pmatrix}. \quad (1.137)$$

□

Example 1.26 (Dirac's outer products) Dirac's notation for outer products is neat. If the vectors $f = |f\rangle$ and $g = |g\rangle$ are

$$|f\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \text{and} \quad |g\rangle = \begin{pmatrix} z \\ w \end{pmatrix} \quad (1.138)$$

then $\langle f| = (a^* \ b^* \ c^*)$ and $\langle g| = (z^* \ w^*)$, and the outer products are

$$|f\rangle\langle g| = \begin{pmatrix} az^* & aw^* \\ bz^* & bw^* \\ cz^* & cw^* \end{pmatrix} \quad \text{and} \quad |g\rangle\langle f| = \begin{pmatrix} za^* & zb^* & zc^* \\ wa^* & wb^* & wc^* \end{pmatrix} \quad (1.139)$$

as well as

$$|f\rangle\langle f| = \begin{pmatrix} aa^* & ab^* & ac^* \\ ba^* & bb^* & bc^* \\ ca^* & cb^* & cc^* \end{pmatrix} \quad \text{and} \quad |g\rangle\langle g| = \begin{pmatrix} zz^* & zw^* \\ wz^* & ww^* \end{pmatrix}. \quad (1.140)$$

□

1.13 Dirac notation

Outer products are important in quantum mechanics, and so Dirac invented a notation for linear algebra that makes them easy to write. In his notation, a vector f is a **ket** $f = |f\rangle$. The new thing in his notation is the **bra** $\langle g|$. The inner product of two vectors (g, f) is the **bracket** $(g, f) = \langle g|f\rangle$. A matrix element (g, cf) of an operator c then is $(g, cf) = \langle g|c|f\rangle$ in which the bra and ket **bracket** the operator c .

In Dirac notation, an outer product like (1.131) $Ah = (g, h)f = f(g, h)$ reads $A|h\rangle = |f\rangle\langle g|h\rangle$, and the outer product A itself is $A = |f\rangle\langle g|$.

The bra $\langle g|$ is the **adjoint** (also called the **hermitian adjoint**, the **conjugate transpose**, and the **hermitian transpose**) of the ket $|g\rangle$, and the ket $|f\rangle$ is the adjoint of the bra $\langle f|$

$$\langle g| = (|g\rangle)^\dagger \quad \text{and} \quad |f\rangle = (\langle f|)^\dagger, \quad \text{so} \quad \langle g|^{\dagger\dagger} = \langle g| \quad \text{and} \quad |f\rangle^{\dagger\dagger} = |f\rangle. \quad (1.141)$$

The adjoint of an outer product is

$$(z|f\rangle\langle g|)^\dagger = z^*|g\rangle\langle f|. \quad (1.142)$$

In Dirac's notation, the most general linear operator is an arbitrary linear combination of outer products

$$A = \sum_{k\ell} z_{k\ell} |k\rangle\langle\ell|. \quad (1.143)$$

Its adjoint is

$$A^\dagger = \sum_{k\ell} z_{k\ell}^* |\ell\rangle\langle k|. \quad (1.144)$$

The adjoint of a ket $|h\rangle = A|f\rangle$ is

$$(|h\rangle)^\dagger = (A|f\rangle)^\dagger = \left(\sum_{k\ell} z_{k\ell} |k\rangle\langle\ell|f\rangle \right)^\dagger = \sum_{k\ell} z_{k\ell}^* \langle f|\ell\rangle\langle k| = \langle f|A^\dagger. \quad (1.145)$$

Before Dirac, bras were implicit in the definition of the inner product, but they did not appear explicitly; there was no simple way to write the bra $\langle g|$ or the outer product $|f\rangle\langle g|$.

If the kets $|k\rangle$ form an orthonormal basis in an n -dimensional vector space, then we can expand an arbitrary ket in the space as

$$|f\rangle = \sum_{k=1}^n c_k |k\rangle. \quad (1.146)$$

Since the basis vectors are orthonormal $\langle\ell|k\rangle = \delta_{\ell k}$, we can identify the coefficients c_k by forming the inner product

$$\langle\ell|f\rangle = \sum_{k=1}^n c_k \langle\ell|k\rangle = \sum_{k=1}^n c_k \delta_{\ell,k} = c_\ell. \quad (1.147)$$

The original expansion (1.146) then must be

$$|f\rangle = \sum_{k=1}^n c_k |k\rangle = \sum_{k=1}^n \langle k|f\rangle |k\rangle = \sum_{k=1}^n |k\rangle \langle k|f\rangle = \left(\sum_{k=1}^n |k\rangle \langle k| \right) |f\rangle. \quad (1.148)$$

Since this equation must hold for every vector $|f\rangle$ in the space, it follows that the sum of outer products within the parentheses is the identity operator for the space

$$I = \sum_{k=1}^n |k\rangle \langle k|. \quad (1.149)$$

Every set of kets $|\alpha_j\rangle$ that forms an orthonormal basis $\langle\alpha_j|\alpha_\ell\rangle = \delta_{j\ell}$ for the space gives us an equivalent representation of the identity operator

$$I = \sum_{j=1}^n |\alpha_j\rangle \langle\alpha_j| = \sum_{k=1}^n |k\rangle \langle k|. \quad (1.150)$$

These resolutions of the identity operator give for every vector $|f\rangle$ in the space the expansions

$$|f\rangle = \sum_{j=1}^n |\alpha_j\rangle \langle\alpha_j|f\rangle = \sum_{k=1}^n |k\rangle \langle k|f\rangle. \quad (1.151)$$

Example 1.27 (Linear operators represented as matrices) The equations (1.64–1.71) that relate linear operators to the matrices that represent them are much clearer in Dirac's notation. If the kets $|B_k\rangle$ are n orthonormal basis vectors, that is, if $\langle B_k|B_\ell\rangle = \delta_{k\ell}$, for a vector space S , then a linear operator A acting on S maps the basis vector $|B_i\rangle$ into (1.64)

$$A|B_i\rangle = \sum_{k=1}^n |B_k\rangle \langle B_k|A|B_i\rangle = \sum_{k=1}^n a_{ki} |B_k\rangle, \quad (1.152)$$

and the matrix that represents the linear operator A in the $|B_k\rangle$ basis is $a_{ki} = \langle B_k|A|B_i\rangle$. If a unitary operator U maps these basis vectors into $|B'_k\rangle = U|B_k\rangle$, then in this new basis the matrix that represents A as in (1.145) is

$$\begin{aligned} a'_{\ell i} &= \langle B'_\ell|A|B'_i\rangle = \langle B_\ell|U^\dagger A U|B_i\rangle \\ &= \sum_{j=1}^n \sum_{k=1}^n \langle B_\ell|U^\dagger|B_j\rangle \langle B_j|A|B_k\rangle \langle B_k|U|B_i\rangle = \sum_{j=1}^n \sum_{k=1}^n u_{\ell j}^\dagger a_{jk} u_{ki} \end{aligned} \quad (1.153)$$

or $a' = u^\dagger a u$ in matrix notation. \square

Example 1.28 (Inner-product rules) In Dirac's notation, the rules (1.82–1.85), of a positive-definite inner product are

$$\begin{aligned} \langle f|g\rangle &= \langle g|f\rangle^* \\ \langle f|z_1 g_1 + z_2 g_2\rangle &= z_1 \langle f|g_1\rangle + z_2 \langle f|g_2\rangle \\ \langle z_1 f_1 + z_2 f_2|g\rangle &= z_1^* \langle f_1|g\rangle + z_2^* \langle f_2|g\rangle \\ \langle f|f\rangle &\geq 0 \quad \text{and} \quad \langle f|f\rangle = 0 \iff f = 0. \end{aligned} \quad (1.154)$$

States in Dirac notation often are labeled $|\psi\rangle$ or by their quantum numbers $|n, l, m\rangle$, and one rarely sees plus signs or complex numbers or operators inside bras or kets. But one should. \square

Example 1.29 (Gram Schmidt) In Dirac notation, the formula (1.129) for the k th orthogonal linear combination of the vectors $|V_\ell\rangle$ is

$$|u_k\rangle = |V_k\rangle - \sum_{i=1}^{k-1} |U_i\rangle \langle U_i|V_k\rangle = \left(I - \sum_{i=1}^{k-1} |U_i\rangle \langle U_i| \right) |V_k\rangle \quad (1.155)$$

and the formula (1.130) for the k th orthonormal linear combination of the vectors $|V_\ell\rangle$ is

$$|U_k\rangle = \frac{|u_k\rangle}{\sqrt{\langle u_k|u_k\rangle}}. \quad (1.156)$$

The vectors $|U_k\rangle$ are not unique; they vary with the order of the $|V_k\rangle$. \square

Vectors and linear operators are abstract. The numbers we compute with are inner products like $\langle g|f\rangle$ and $\langle g|A|f\rangle$. In terms of n orthonormal basis vectors $|j\rangle$ with $f_j = \langle j|f\rangle$ and $g_j^* = \langle g|j\rangle$, we can use the expansion (1.149) of the identity operator to write these inner products as

$$\begin{aligned} \langle g|f\rangle &= \langle g|I|f\rangle = \sum_{j=1}^n \langle g|j\rangle \langle j|f\rangle = \sum_{j=1}^n g_j^* f_j \\ \langle g|A|f\rangle &= \langle g|IAI|f\rangle = \sum_{j,\ell=1}^n \langle g|j\rangle \langle j|A|\ell\rangle \langle \ell|f\rangle = \sum_{j,\ell=1}^n g_j^* A_{j\ell} f_\ell \end{aligned} \quad (1.157)$$

in which $A_{j\ell} = \langle j|A|\ell\rangle$. We often gather the inner products $f_\ell = \langle \ell|f\rangle$ into a column vector f with components $f_\ell = \langle \ell|f\rangle$

$$f = \begin{pmatrix} \langle 1|f\rangle \\ \langle 2|f\rangle \\ \vdots \\ \langle n|f\rangle \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix} \quad (1.158)$$

and the $\langle j|A|\ell\rangle$ into a matrix A with matrix elements $A_{j\ell} = \langle j|A|\ell\rangle$. If we also line up the inner products $\langle g|j\rangle = \langle j|g\rangle^*$ in a row vector that is the transpose of the complex conjugate of the column vector g

$$g^\dagger = (\langle 1|g\rangle^*, \langle 2|g\rangle^*, \dots, \langle n|g\rangle^*) = (g_1^*, g_2^*, \dots, g_n^*), \quad (1.159)$$

then we can write inner products in matrix notation as $\langle g|f\rangle = g^\dagger f$ and as $\langle g|A|f\rangle = g^\dagger A f$.

One can compute the inner product $\langle g|f\rangle$ of two vectors f and g by doing the sum (1.157) of $g_j^* f_j$ over the index j only if one knows their components f_j and g_j which are their inner products $f_j = \langle j|f\rangle$ and $g_j = \langle j|g\rangle$ with the orthonormal states $|j\rangle$ of some basis. Thus an inner product implies

the existence of an orthonormal basis and a representation of the identity operator

$$I = \sum_{j=1}^n |j\rangle\langle j|. \quad (1.160)$$

If we switch to a different basis, say from $|k\rangle$'s to $|\alpha_k\rangle$'s, then the components of the column vectors change from $f_k = \langle k|f\rangle$ to $f'_k = \langle \alpha_k|f\rangle$, and similarly those of the row vectors g^\dagger and of the matrix A change, but the bras, the kets, the linear operators, and the inner products $\langle g|f\rangle$ and $\langle g|A|f\rangle$ do not change because the identity operator is basis independent (1.150)

$$\begin{aligned} \langle g|f\rangle &= \sum_{k=1}^n \langle g|k\rangle\langle k|f\rangle = \sum_{k=1}^n \langle g|\alpha_k\rangle\langle \alpha_k|f\rangle \\ \langle g|A|f\rangle &= \sum_{k,\ell=1}^n \langle g|k\rangle\langle k|A|\ell\rangle\langle \ell|f\rangle = \sum_{k,\ell=1}^n \langle g|\alpha_k\rangle\langle \alpha_k|A|\alpha_\ell\rangle\langle \alpha_\ell|f\rangle. \end{aligned} \quad (1.161)$$

Dirac's outer products show how to change from one basis to another. The sum of outer products $|\alpha_k\rangle\langle k|$ is a unitary operator (Section 1.17)

$$U = \sum_{k=1}^n |\alpha_k\rangle\langle k| \quad (1.162)$$

that maps the ket $|\ell\rangle$ of one orthonormal basis into that $|\alpha_\ell\rangle$ of another

$$U|\ell\rangle = \sum_{k=1}^n |\alpha_k\rangle\langle k|\ell\rangle = \sum_{k=1}^n |\alpha_k\rangle\delta_{k\ell} = |\alpha_\ell\rangle. \quad (1.163)$$

Example 1.30 (Simple change of basis) If the ket $|\alpha_k\rangle$ of the new basis is simply $|\alpha_k\rangle = |k+1\rangle$ with $|\alpha_n\rangle = |n+1\rangle \equiv |1\rangle$, then the operator that maps the n kets $|k\rangle$ into the kets $|\alpha_k\rangle$ is

$$U = \sum_{k=1}^n |\alpha_k\rangle\langle k| = \sum_{k=1}^n |k+1\rangle\langle k|. \quad (1.164)$$

The square U^2 of U also changes the basis; it sends $|k\rangle$ to $|k+2\rangle$. The set of operators U^ℓ for $\ell = 1, 2, \dots, n$ forms a group known as Z_n . \square

1.14 Adjoins of operators

The most general linear operator (1.143) on an n -dimensional vector space is a sum of outer products $z|k\rangle\langle\ell|$ in which z is a complex number and the kets $|k\rangle$ and $|\ell\rangle$ are two of the n orthonormal kets that make up a basis for the space. The **adjoint** (1.142) of this basic linear operator is

$$(z|k\rangle\langle\ell|)^\dagger = z^*|\ell\rangle\langle k|. \quad (1.165)$$

Thus with $z = \langle k|A|\ell\rangle$, the most general linear operator on the space is

$$A = IAI = \sum_{k,\ell=1}^n |k\rangle\langle k|A|\ell\rangle\langle\ell| \quad (1.166)$$

and its adjoint A^\dagger is the operator $IA^\dagger I$

$$A^\dagger = \sum_{k,\ell=1}^n |\ell\rangle\langle\ell|A^\dagger|k\rangle\langle k| = \sum_{k,\ell=1}^n |\ell\rangle\langle k|A|\ell\rangle^*\langle k|. \quad (1.167)$$

It follows that $\langle\ell|A^\dagger|k\rangle = \langle k|A|\ell\rangle^*$ so that the matrix $A_{k\ell}^\dagger$ that represents A^\dagger in this basis is

$$A_{\ell k}^\dagger = \langle\ell|A^\dagger|k\rangle = \langle k|A|\ell\rangle^* = A_{k\ell}^* = (A^{*\top})_{\ell k} \quad (1.168)$$

in agreement with our definition (1.32) of the adjoint of a matrix as the transpose of its complex conjugate, $A^\dagger = A^{*\top}$. We also have

$$\langle g|A^\dagger f\rangle = \langle g|A^\dagger|f\rangle = \langle f|A|g\rangle^* = \langle f|Ag\rangle^* = \langle Ag|f\rangle. \quad (1.169)$$

The adjoint of an adjoint is by (1.165)

$$\left[(z|k\rangle\langle\ell|)^\dagger\right]^\dagger = [z^*|\ell\rangle\langle k|]^\dagger = z|k\rangle\langle\ell| \quad (1.170)$$

no change at all. This also follows from the matrix formula (1.168) because both $(A^*)^* = A$ and $(A^\top)^\top = A$, and so

$$\left(A^\dagger\right)^\dagger = (A^{*\top})^{*\top} = A \quad (1.171)$$

the adjoint of the adjoint of a matrix is the original matrix.

Before Dirac, the adjoint A^\dagger of a linear operator A was defined by

$$(g, A^\dagger f) = (Ag, f) = (f, Ag)^*. \quad (1.172)$$

This definition also implies that $A^{\dagger\dagger} = A$ since

$$(g, A^{\dagger\dagger} f) = (A^\dagger g, f) = (f, A^\dagger g)^* = (Af, g)^* = (g, Af). \quad (1.173)$$

We also have $(g, Af) = (g, A^{\dagger\dagger} f) = (A^\dagger g, f)$.

1.15 Self-adjoint or hermitian linear operators

An operator A that is equal to its adjoint $A^\dagger = A$ is **self adjoint** or **hermitian**. In view of (1.168), the matrix elements of a self-adjoint linear operator A satisfy $\langle k|A^\dagger|\ell\rangle = \langle \ell|A|k\rangle^* = \langle k|A|\ell\rangle$ in any orthonormal basis. So a matrix that represents a hermitian operator is equal to the transpose of its complex conjugate

$$A_{k\ell} = \langle k|A|\ell\rangle = \langle k|A^\dagger|\ell\rangle = \langle \ell|A|k\rangle^* = A_{k\ell}^{*\Gamma} = A_{k\ell}^\dagger. \quad (1.174)$$

We also have

$$\langle g|Af\rangle = \langle g|A|f\rangle = \langle Ag|f\rangle = \langle f|Ag\rangle^* = \langle f|A|g\rangle^* = \langle Af|g\rangle^* \quad (1.175)$$

and in pre-Dirac notation

$$(g, Af) = (Ag, f) = (f, Ag)^* = (Af, g)^*. \quad (1.176)$$

A matrix A_{ij} that is **real and symmetric** or **imaginary and antisymmetric** is hermitian. But a self-adjoint linear operator A that is represented by a matrix A_{ij} that is real and symmetric (or imaginary and antisymmetric) in one orthonormal basis will not in general be represented by a matrix that is real and symmetric (or imaginary and antisymmetric) in a different orthonormal basis, but it will be represented by a hermitian matrix in every orthonormal basis.

A ket $|a'\rangle$ is an **eigenvector** of a linear operator A with **eigenvalue** a' if $A|a'\rangle = a'|a'\rangle$. As we'll see in section 1.31, hermitian matrices have real eigenvalues and complete sets of orthonormal eigenvectors. Hermitian operators and matrices represent physical variables in quantum mechanics.

Example 1.31 (Fierz identities for $n \times n$ hermitian matrices) The n^2 $n \times n$ hermitian matrices t^a form a vector space with an inner product $\langle a|b\rangle$ (section 1.7) defined by the trace (1.25) $\langle a|b\rangle = \text{Tr}(t^a t^b)$. One can use the Gram-Schmidt method (section 1.11) to make them orthonormal, so that

$$\langle a|b\rangle = \text{Tr}(t^a t^b) = \sum_{i,k=1}^n t_{ik}^a t_{ki}^b = \delta_{ab}. \quad (1.177)$$

Then the sum of their n^2 outer products (1.25) is the identity matrix of the n^2 -dimensional vector space

$$\left(\sum_{a=1}^{n^2} |a\rangle\langle a| \right)_{ij,kl} = \sum_{a=1}^{n^2} t_{ij}^a t_{kl}^a = I_{ik,lj} = \delta_{il} \delta_{kj} \quad (1.178)$$

because

$$t_{ij}^b = (|b\rangle)_{ij} = \sum_{a=1}^{n^2} (|a\rangle)_{ij} \langle a|b\rangle = \sum_{a=1}^{n^2} t_{ij}^a \text{Tr}(t^a t^b) = \sum_{a=1}^{n^2} \sum_{k,\ell=1}^n t_{ij}^a t_{k\ell}^a t_{\ell k}^b. \quad (1.179)$$

(Markus Fierz, 1912–2006) □

1.16 Real, symmetric linear operators

In quantum mechanics, we usually consider complex vector spaces, that is, spaces in which the vectors $|f\rangle$ are complex linear combinations

$$|f\rangle = \sum_{k=1}^n z_k |k\rangle \quad (1.180)$$

of complex orthonormal basis vectors $|i\rangle$.

But real vector spaces also are of interest. A real vector space is a vector space in which the vectors $|f\rangle$ are real linear combinations

$$|f\rangle = \sum_{k=1}^n x_k |k\rangle \quad (1.181)$$

of real orthonormal basis vectors, $x_k^* = x_k$ and $|k\rangle^* = |k\rangle$.

A real linear operator A on a real vector space

$$A = \sum_{k,\ell=1}^n |k\rangle \langle k| A |\ell\rangle \langle \ell| = \sum_{k,\ell=1}^n |k\rangle A_{k\ell} \langle \ell| \quad (1.182)$$

is represented by a real matrix $A_{k\ell}^* = A_{k\ell}$. A real linear operator A that is self adjoint on a real vector space satisfies the condition (1.176) of hermiticity but with the understanding that complex conjugation has no effect

$$(g, A f) = (A g, f) = (f, A g)^* = (f, A g). \quad (1.183)$$

Thus its matrix elements are symmetric, $\langle g|A|f\rangle = \langle f|A|g\rangle$. Since A is hermitian as well as real, the matrix $A_{k\ell}$ that represents it (in a real basis) is real and hermitian, and so is symmetric $A_{k\ell} = A_{\ell k}^* = A_{\ell k}$.

1.17 Unitary operators

A **unitary operator** U is one whose adjoint is its inverse

$$U U^\dagger = U^\dagger U = I. \quad (1.184)$$

Any operator that changes from one orthonormal basis $|k\rangle$ to another $|\alpha_k\rangle$

$$U = \sum_{k=1}^n |\alpha_k\rangle\langle k| \quad (1.185)$$

is unitary since

$$\begin{aligned} UU^\dagger &= \sum_{k=1}^n |\alpha_k\rangle\langle k| \sum_{\ell=1}^n |\ell\rangle\langle\alpha_\ell| = \sum_{k,\ell=1}^n |\alpha_k\rangle\langle k|\ell\rangle\langle\alpha_\ell| \\ &= \sum_{k,\ell=1}^n |\alpha_k\rangle\delta_{k,\ell}\langle\alpha_\ell| = \sum_{k=1}^n |\alpha_k\rangle\langle\alpha_k| = I \end{aligned} \quad (1.186)$$

as well as

$$U^\dagger U = \sum_{\ell=1}^n |\ell\rangle\langle\alpha_\ell| \sum_{k=1}^n |\alpha_k\rangle\langle k| = \sum_{k=1}^n |k\rangle\langle k| = I. \quad (1.187)$$

A unitary operator maps every orthonormal basis $|k\rangle$ into another orthonormal basis $|\alpha_k\rangle$. For if $|\alpha_k\rangle = U|k\rangle$, then the vectors $|\alpha_k\rangle$ are orthonormal $\langle\alpha_k|\alpha_\ell\rangle = \delta_{k,\ell}$ (exercise 1.22). They also are complete because they provide a resolution of the identity operator

$$\sum_{k=1}^n |\alpha_k\rangle\langle\alpha_k| = \sum_{k=1}^n U|k\rangle\langle k|U^\dagger = UIU^\dagger = UU^\dagger = I. \quad (1.188)$$

If we multiply the ket $|\alpha_k\rangle = U|k\rangle$ by the bra $\langle k|$ and then sum over the index k , we get

$$\sum_{k=1}^n |\alpha_k\rangle\langle k| = \sum_{k=1}^n U|k\rangle\langle k| = U \sum_{k=1}^n |k\rangle\langle k| = U. \quad (1.189)$$

An operator U is unitary if and only if it maps every orthonormal basis into an orthonormal basis.

The matrix $U_{k'k} = \langle k'|U|k\rangle$

$$\langle k'|U|k\rangle = \langle k'| \sum_{k''=1}^n |\alpha_{k''}\rangle\langle k''|k\rangle = \langle k'|\alpha_k\rangle \quad (1.190)$$

is unitary

$$\sum_{k=1}^n U_{k'k}U_{k''k}^* = \sum_{k=1}^n \langle k'|\alpha_k\rangle\langle\alpha_k|k''\rangle = \langle k'|k''\rangle = \delta_{k',k''}. \quad (1.191)$$

Inner products do not change under unitary transformations because

$\langle g|f\rangle = \langle g|U^\dagger U|f\rangle = \langle Ug|U|f\rangle = \langle Ug|Uf\rangle$ which in pre-Dirac notation is $(g, f) = (g, U^\dagger Uf) = (Ug, Uf)$.

Unitary matrices have unimodular determinants, $|\det U| = 1$, because the determinant of the product of two matrices is the product of their determinants (1.231) and because transposition doesn't change the value of a determinant (1.214) and because the inverse of a unitary matrix is its inverse $U^\dagger = U^{-1}$

$$\begin{aligned} 1 &= \det I = \det(UU^{-1}) = \det(UU^\dagger) = \det U \det U^\dagger \\ &= \det U(\det(U^\dagger))^* = \det U(\det U)^* = |\det(U)|^2. \end{aligned} \quad (1.192)$$

A unitary matrix that is real is **orthogonal** and satisfies

$$OO^\top = O^\top O = I. \quad (1.193)$$

1.18 Hilbert spaces

We have mainly been talking about linear operators that act on finite-dimensional vector spaces and that can be represented by matrices. But infinite-dimensional vector spaces and the linear operators that act on them play central roles in electrodynamics and quantum mechanics. For instance, the Hilbert space \mathcal{H} of all wave functions $\psi(\mathbf{x}, t)$ that are square integrable over three-dimensional space at all times t is of infinite dimension.

In one space dimension, the state $|x'\rangle$ represents a particle at position x' and is an eigenstate of the hermitian position operator x with eigenvalue x' , that is, $x|x'\rangle = x'|x'\rangle$. These states form a basis that is orthogonal in the sense that $\langle x|x'\rangle = 0$ for $x \neq x'$ and normalized in the sense that $\langle x|x'\rangle = \delta(x - x')$ in which $\delta(x - x')$ is Dirac's delta function. The delta function $\delta(x - x')$ actually is a **functional** $\delta_{x'}$ that maps any suitably smooth function f into its value $\delta_{x'}[f]$ at x'

$$\delta_{x'}[f] = \int \delta(x - x') f(x) dx = f(x'). \quad (1.194)$$

Another basis for the Hilbert space of one-dimensional quantum mechanics is made of the states $|p\rangle$ of well-defined momentum. The state $|p'\rangle$ represents a particle or system with momentum p' . It is an eigenstate of the hermitian momentum operator p with eigenvalue p' , that is, $p|p'\rangle = p'|p'\rangle$. The momentum states also are orthonormal in Dirac's sense, $\langle p|p'\rangle = \delta(p - p')$.

The operator that translates a system in space by a distance a is

$$U(a) = \int |x+a\rangle\langle x| dx. \quad (1.195)$$

It maps the state $|x'\rangle$ to the state $|x'+a\rangle$ and is unitary (exercise 1.23). Remarkably, this translation operator is an exponential of the momentum operator $U(a) = \exp(-ipa/\hbar)$ in which $\hbar = h/2\pi = 1.054 \times 10^{-34}$ Js is Planck's constant divided by 2π .

In two-dimensions with basis states $|x, y\rangle$ that are orthonormal in Dirac's sense $\langle x, y|x', y'\rangle = \delta(x-x')\delta(y-y')$, the unitary operator

$$U(\theta) = \int |x \cos \theta - y \sin \theta, x \sin \theta + y \cos \theta\rangle\langle x, y| dx dy \quad (1.196)$$

rotates a system in space by the angle θ . This rotation operator is the exponential $U(\theta) = \exp(-i\theta L_z/\hbar)$ in which the z component of the angular momentum is $L_z = xp_y - yp_x$.

We may carry most of our intuition about matrices over to these unitary transformations that change from one infinite basis to another. But we must keep in mind that infinite sums and integrals do not always converge.

1.19 Antiunitary, antilinear operators

Certain maps on states $|\psi\rangle \rightarrow |\psi'\rangle$, such as those involving time reversal, are implemented by operators K that are **antilinear**

$$K(z\psi + w\phi) = K(z|\psi\rangle + w|\phi\rangle) = z^*K|\psi\rangle + w^*K|\phi\rangle = z^*K\psi + w^*K\phi \quad (1.197)$$

and **antiunitary**

$$(K\phi, K\psi) = \langle K\phi|K\psi\rangle = (\phi, \psi)^* = \langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle = (\psi, \phi). \quad (1.198)$$

The adjoint K^\dagger of an antiunitary operator K is defined by $\langle K^\dagger\phi|\psi\rangle = \langle\phi|K|\psi\rangle^*$ so that $\langle K^\dagger K\phi|\psi\rangle = \langle K\phi|K\psi\rangle^* = \langle\phi|\psi\rangle^{**} = \langle\phi|\psi\rangle$, which ensures that that $K^\dagger K = KK^\dagger = 1$.

1.20 Symmetry in quantum mechanics

In quantum mechanics, a symmetry is a map of states $|\psi\rangle \rightarrow |\psi'\rangle$ and $|\phi\rangle \rightarrow |\phi'\rangle$ that preserves probabilities

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\phi|\psi\rangle|^2. \quad (1.199)$$

Eugene Wigner (1902–1995) showed that every symmetry in quantum mechanics can be represented either by an operator U that is linear and unitary or by an operator K that is antilinear and antiunitary. The antilinear, antiunitary case occurs when a symmetry involves time reversal. Most symmetries are represented by operators that are linear and unitary. Unitary operators are of great importance in quantum mechanics. They represent rotations, translations, Lorentz transformations, and internal-symmetry transformations.

1.21 Determinants

The **determinant** of a 2×2 matrix A

$$\det A = |A| = A_{11}A_{22} - A_{21}A_{12} \quad (1.200)$$

is a sum of signed products of an element of one row and column multiplied by an element of the other row and column. The sign of each product is determined by the order of the indexes, specifically by the 2×2 antisymmetric ($e_{ij} = -e_{ji}$) matrix $e_{12} = 1 = -e_{21}$ with $e_{11} = e_{22} = 0$

$$\det A = \sum_{i=1}^2 \sum_{j=1}^2 e_{ij} A_{i1} A_{j2} = \sum_{i=1}^2 \sum_{j=1}^2 e_{ij} A_{1i} A_{2j}. \quad (1.201)$$

It's also true that

$$e_{k\ell} \det A = \sum_{i=1}^2 \sum_{j=1}^2 e_{ij} A_{ik} A_{j\ell}. \quad (1.202)$$

Example 1.32 (Area of a parallelogram) Two 2-vectors $V = (V_1, V_2)$ and $W = (W_1, W_2)$ define a parallelogram whose area is the absolute value of the 2×2 determinant

$$\text{area}(V, W) = \left| \det \begin{pmatrix} V_1 & V_2 \\ W_1 & W_2 \end{pmatrix} \right| = |V_1 W_2 - V_2 W_1|. \quad (1.203)$$

To check this formula, rotate the coordinates so that the 2-vector V runs from the origin along the x -axis. Then $V_2 = 0$, and the determinant is $V_1 W_2$ which is the base V_1 of the parallelogram times its height W_2 . \square

The determinant of a 3×3 matrix A

$$\det A = \sum_{i,j,k=1}^3 e_{ijk} A_{i1} A_{j2} A_{k3} = \sum_{i,j,k=1}^3 e_{ijk} A_{1i} A_{2j} A_{3k} \quad (1.204)$$

is a sum of signed products of elements A_{ik} in which every row index i and every column index k occurs exactly once. The sign of each product is determined by the order of the indexes, specifically by the totally antisymmetric Levi-Civita symbol e_{ijk} whose nonzero values are

$$e_{123} = e_{231} = e_{312} = 1 \quad \text{and} \quad e_{213} = e_{132} = e_{321} = -1. \quad (1.205)$$

The symbol e_{ijk} vanishes whenever an index appears twice

$$e_{111} = e_{112} = e_{113} = e_{222} = e_{221} = e_{223} = e_{333} = e_{331} = e_{332} = 0. \quad (1.206)$$

Doing the first of the sums (1.204) over i explicitly, we get

$$\begin{aligned} \det A &= \sum_{i=1}^3 A_{i1} \sum_{j,k=1}^3 e_{ijk} A_{j2} A_{k3} \\ &= A_{11} \sum_{j,k=2}^3 e_{1jk} A_{j2} A_{k3} + A_{21} \sum_{j,k=1,\neq 2}^3 e_{2jk} A_{j2} A_{k3} + A_{31} \sum_{j,k=1}^2 e_{3jk} A_{j2} A_{k3} \\ &= A_{11} (A_{22}A_{33} - A_{32}A_{23}) + A_{21} (A_{32}A_{13} - A_{12}A_{33}) \\ &\quad + A_{31} (A_{12}A_{23} - A_{22}A_{13}). \end{aligned} \quad (1.207)$$

The **minor** $M_{i\ell}$ of the matrix A is the 2×2 determinant of the matrix A without row i and column ℓ , and the **cofactor** $C_{i\ell}$ is the minor $M_{i\ell}$ multiplied by $(-1)^{i+\ell}$. Thus the determinant $\det A$ is the sum over i

$$\begin{aligned} \det A &= A_{11}(-1)^2 (A_{22}A_{33} - A_{32}A_{23}) + A_{21}(-1)^3 (A_{12}A_{33} - A_{32}A_{13}) \\ &\quad + A_{31}(-1)^4 (A_{12}A_{23} - A_{22}A_{13}) \\ &= A_{11}C_{11} + A_{21}C_{21} + A_{31}C_{31} \end{aligned} \quad (1.208)$$

of A_{i1} multiplied by its cofactor C_{i1}

$$\begin{aligned} C_{11} &= (-1)^2 M_{11} = A_{22}A_{33} - A_{23}A_{32} \\ C_{21} &= (-1)^3 M_{21} = A_{32}A_{13} - A_{12}A_{33} \\ C_{31} &= (-1)^4 M_{31} = A_{12}A_{23} - A_{22}A_{13}. \end{aligned} \quad (1.209)$$

Example 1.33 (Volume of a parallelepiped) The determinant of a 3×3 matrix is the dot product of the vector of its first row with the cross-product

of the vectors of its second and third rows

$$\begin{vmatrix} U_1 & U_2 & U_3 \\ V_1 & V_2 & V_3 \\ W_1 & W_2 & W_3 \end{vmatrix} = \sum_{ijk=1}^3 e_{ijk} U_i V_j W_k = \sum_{i=1}^3 U_i (\mathbf{V} \times \mathbf{W})_i = \mathbf{U} \cdot (\mathbf{V} \times \mathbf{W}). \quad (1.210)$$

The absolute value of this **scalar triple product** is the volume of the parallelepiped defined by U , V , and W as one can see by placing the parallelepiped so the vector U runs from the origin along the x axis. The 3×3 determinant (1.210) then is $U_1(V_2W_3 - V_3W_2)$ which is the height of the parallelepiped times the area (1.203) of its base. \square

Laplace used the totally antisymmetric symbol $e_{i_1 i_2 \dots i_n}$ with n indices and with $e_{123\dots n} = 1$ to define the determinant of an $n \times n$ matrix A as

$$\det A = \sum_{i_1 i_2 \dots i_n=1}^n e_{i_1 i_2 \dots i_n} A_{i_1 1} A_{i_2 2} \dots A_{i_n n} \quad (1.211)$$

in which the sums over $i_1 \dots i_n$ run from 1 to n . In terms of cofactors, two forms of his expansion of this determinant are a sum over the row index i for an arbitrary fixed column index k and a sum over the column index k for a fixed row index i

$$\det A = \sum_{i=1}^n A_{ik} C_{ik} = \sum_{k=1}^n A_{ik} C_{ik}. \quad (1.212)$$

As for a 3×3 matrix, the cofactor C_{ik} is $(-1)^{i+k} M_{ik}$ in which the minor M_{ik} is the determinant of the $(n-1) \times (n-1)$ matrix A without its i th row and k th column. It's also true that

$$\begin{aligned} e_{k_1 k_2 \dots k_n} \det A &= \sum_{i_1 i_2 \dots i_n=1}^n e_{i_1 i_2 \dots i_n} A_{i_1 k_1} A_{i_2 k_2} \dots A_{i_n k_n} \\ &= \sum_{i_1 i_2 \dots i_n=1}^n e_{i_1 i_2 \dots i_n} A_{k_1 i_1} A_{k_2 i_2} \dots A_{k_n i_n}. \end{aligned} \quad (1.213)$$

In particular, since $e_{12\dots n} = 1$, the determinant of the transpose of a matrix is equal to the determinant (1.211) of the matrix

$$\det A^T = \sum_{i_1 i_2 \dots i_n=1}^n e_{i_1 i_2 \dots i_n} A_{1 i_1} A_{2 i_2} \dots A_{n i_n} = \det A. \quad (1.214)$$

The interchange $A \rightarrow A^T$ of the rows and columns of a matrix has no effect on its determinant.

The key feature of a determinant is that it is an *antisymmetric* combination of products of the elements A_{ik} of a matrix A . One implication of this antisymmetry is that the interchange of any two rows or any two columns changes the sign of the determinant. Another is that if one adds a multiple of one column to another column, for example a multiple xA_{i2} of column 2 to column 1, then the determinant

$$\det A' = \sum_{i_1 i_2 \dots i_n = 1}^n e_{i_1 i_2 \dots i_n} (A_{i_1 1} + xA_{i_1 2}) A_{i_2 2} \dots A_{i_n n} \quad (1.215)$$

is unchanged. The reason is that the extra term $\delta \det A$ vanishes

$$\delta \det A = \sum_{i_1 i_2 \dots i_n = 1}^n x e_{i_1 i_2 \dots i_n} A_{i_1 2} A_{i_2 2} \dots A_{i_n n} = 0 \quad (1.216)$$

because it is proportional to a sum of products of a factor $e_{i_1 i_2 \dots i_n}$ that is antisymmetric in i_1 and i_2 and a factor $A_{i_1 2} A_{i_2 2}$ that is symmetric in these indices. For instance, when i_1 and i_2 are 5 & 7 and 7 & 5, the two terms cancel

$$e_{57\dots i_n} A_{52} A_{72} \dots A_{i_n n} + e_{75\dots i_n} A_{72} A_{52} \dots A_{i_n n} = 0 \quad (1.217)$$

because $e_{57\dots i_n} = -e_{75\dots i_n}$. (Pierre-Simon Laplace, 1749–1827)

By repeated additions of $x_2 A_{i2}$, $x_3 A_{i3}$, and so forth to A_{i1} , we can change the first column of the matrix A to a linear combination of all the columns

$$A_{i1} \longrightarrow A_{i1} + \sum_{k=2}^n x_k A_{ik} \quad (1.218)$$

without changing $\det A$. In this linear combination, the coefficients x_k are arbitrary. The analogous operation with arbitrary y_k

$$A_{i\ell} \longrightarrow A_{i\ell} + \sum_{k=1, k \neq \ell}^n y_k A_{ik} \quad (1.219)$$

replaces the ℓ th column by a linear combination of all the columns without changing $\det A$.

Suppose that the columns of an $n \times n$ matrix A are linearly dependent (section 1.9), so that the linear combination of columns

$$\sum_{k=1}^n A_{ik} y_k = 0 \quad \text{for } i = 1, \dots, n \quad (1.220)$$

vanishes for some coefficients y_k not all zero. If $y_p \neq 0$, then by adding to column p the linear combinations $y'_k = (y_k/y_p)A_{ik}$ of all the other columns, we

could make the modified elements A'_{ip} of column p vanish without changing $\det A$. But then $\det A$ would vanish by definition (1.211). **Thus the determinant of any matrix whose columns are linearly dependent must vanish.**

Now suppose that the columns of an $n \times n$ matrix are linearly independent. Then the determinant of the matrix cannot vanish because any linearly independent set of n vectors in a vector space of n dimensions is complete (section 1.9). Thus if the columns of a matrix A are linearly independent and therefore complete, some linear combination of all columns 2 through n when added to column 1 will convert column 1 into a nonzero multiple of the n -dimensional column vector $(1, 0, 0, \dots, 0)$, say $(c_1, 0, 0, \dots, 0)$. Similar operations will convert column 2 into a nonzero multiple of the column vector $(0, 1, 0, \dots, 0)$, say $(0, c_2, 0, \dots, 0)$. Continuing in this way, we may convert the matrix A to a matrix with nonzero entries c_i along the main diagonal and zeros everywhere else. The determinant $\det A$ then is the product $c_1 c_2 \dots c_n$ of the nonzero diagonal entries c_i 's, and so $\det A$ cannot vanish.

We may extend these arguments to the rows of a matrix. The addition to row k of a linear combination of the other rows

$$A_{ki} \longrightarrow A_{ki} + \sum_{\ell=1, \ell \neq k}^n z_\ell A_{\ell i} \quad (1.221)$$

does not change the value of the determinant. In this way, one may show that the determinant of a matrix vanishes if and only if its rows are linearly dependent. The reason why these results apply to the rows as well as to the columns is that the determinant of a matrix A may be defined either in terms of the columns or in terms of the rows as in the definitions (1.211) and 1.213). These and other properties of determinants follow from a study of **permutations** (section 11.13). Detailed proofs are in (Aitken, 1959).

Let us return for a moment to Laplace's expansion (1.212) of the determinant $\det A$ of an $n \times n$ matrix A as a sum of $A_{ik}C_{ik}$ over the row index i with the column index k held fixed

$$\det A = \sum_{i=1}^n A_{ik}C_{ik} = \sum_{i=1}^n A_{ki}C_{ki} \quad (1.222)$$

in order to prove that

$$\delta_{k\ell} \det A = \sum_{i=1}^n A_{ik}C_{i\ell} = \sum_{i=1}^n A_{ki}C_{\ell i}. \quad (1.223)$$

For $k = \ell$, this formula just repeats Laplace's expansion (1.222). But for

$k \neq \ell$, it is Laplace's expansion for the determinant of a matrix that has two copies of its k th column. Since the determinant of a matrix with two identical columns vanishes, the rule (1.223) also is true for $k \neq \ell$.

This rule (1.223) provides a formula for the inverse of a matrix A whose determinant does not vanish. Such matrices are said to be **nonsingular**. The inverse A^{-1} of an $n \times n$ nonsingular matrix A is the transpose of the matrix of cofactors divided by the determinant of the matrix

$$(A^{-1})_{\ell i} = \frac{C_{i\ell}}{\det A} \quad \text{or} \quad A^{-1} = \frac{C^{\top}}{\det A}. \quad (1.224)$$

To verify this formula, we use it for A^{-1} in the product $A^{-1}A$ and note that by (1.223) the ℓk th entry of the product $A^{-1}A$ is just $\delta_{\ell k}$

$$(A^{-1}A)_{\ell k} = \sum_{i=1}^n (A^{-1})_{\ell i} A_{ik} = \sum_{i=1}^n \frac{C_{i\ell}}{\det A} A_{ik} = \delta_{\ell k}. \quad (1.225)$$

Example 1.34 (Inverting a 2×2 Matrix) Our formula (1.224) for the inverse of the general 2×2 matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (1.226)$$

gives

$$A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \quad (1.227)$$

which is the correct inverse as long as $ad \neq bc$. \square

The simple example of matrix multiplication

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} 1 & x & y \\ 0 & 1 & z \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a & xa + b & ya + zb + c \\ d & xd + e & yd + ze + f \\ g & xg + h & yg + zh + i \end{pmatrix} \quad (1.228)$$

shows that the operations (1.219) on columns that don't change the value of the determinant can be written as matrix multiplication from the right by a matrix that has unity on its main diagonal and zeros below. Now consider the matrix product

$$\begin{pmatrix} A & 0 \\ -I & B \end{pmatrix} \begin{pmatrix} I & B \\ 0 & I \end{pmatrix} = \begin{pmatrix} A & AB \\ -I & 0 \end{pmatrix} \quad (1.229)$$

in which A and B are $n \times n$ matrices, I is the $n \times n$ identity matrix, and 0 is the $n \times n$ matrix of all zeros. The second matrix on the left-hand side has unity on its main diagonal and zeros below, and so it does not change

the value of the determinant of the matrix to its left, which then must equal that of the matrix on the right-hand side:

$$\det \begin{pmatrix} A & 0 \\ -I & B \end{pmatrix} = \det \begin{pmatrix} A & AB \\ -I & 0 \end{pmatrix}. \quad (1.230)$$

By using Laplace's expansion (1.212) along the first column to evaluate the determinant on the left-hand side and his expansion along the last row to compute the determinant on the right-hand side, one finds that **the determinant of the product of two matrices is the product of the determinants**

$$\det A \det B = \det AB. \quad (1.231)$$

Example 1.35 (Two 2×2 Matrices) When the matrices A and B are both 2×2 , the two sides of (1.230) are

$$\begin{aligned} \det \begin{pmatrix} A & 0 \\ -I & B \end{pmatrix} &= \det \begin{pmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ -1 & 0 & b_{11} & b_{12} \\ 0 & -1 & b_{21} & b_{22} \end{pmatrix} \\ &= a_{11}a_{22} \det B - a_{21}a_{12} \det B = \det A \det B \end{aligned} \quad (1.232)$$

and

$$\begin{aligned} \det \begin{pmatrix} A & AB \\ -I & 0 \end{pmatrix} &= \det \begin{pmatrix} a_{11} & a_{12} & (ab)_{11} & (ab)_{12} \\ a_{21} & a_{22} & (ab)_{21} & (ab)_{22} \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \\ &= (-1)C_{42} = (-1)(-1) \det AB = \det AB \end{aligned} \quad (1.233)$$

and so they give the product rule $\det A \det B = \det AB$. \square

Often one uses the notation $|A| = \det A$ to denote a determinant. In this more compact notation, the obvious generalization of the product rule is

$$|ABC \dots Z| = |A||B| \dots |Z|. \quad (1.234)$$

The product rule (1.231) implies that $\det(A^{-1})$ is $1/\det A$ since

$$1 = \det I = \det(AA^{-1}) = \det A \det(A^{-1}). \quad (1.235)$$

Example 1.36 (Derivative of the logarithm of a determinant) We see from our formula (1.222) for $\det A$ that its derivative with respect to any given element A_{ik} is the corresponding cofactor C_{ik}

$$\frac{\partial \det A}{\partial A_{ik}} = C_{ik} \quad (1.236)$$

because the cofactors C_{ij} and C_{jk} for all j are independent of A_{ik} . Thus the derivative of the logarithm of this determinant with respect to any parameter β is the trace of $A^{-1}\partial A/\partial\beta$

$$\begin{aligned}\frac{\partial \ln \det A}{\partial \beta} &= \frac{1}{\det A} \sum_{ik} \frac{\partial \det A}{\partial A_{ik}} \frac{\partial A_{ik}}{\partial \beta} = \sum_{ik} \frac{C_{ik}}{\det A} \frac{\partial A_{ik}}{\partial \beta} \\ &= \sum_{ik} A_{ki}^{-1} \frac{\partial A_{ik}}{\partial \beta} = \text{Tr} \left(A^{-1} \frac{\partial A}{\partial \beta} \right).\end{aligned}\tag{1.237}$$

□

Example 1.37 (Numerical Tricks) Adding multiples of rows to other rows does not change the value of a determinant, and interchanging two rows only changes a determinant by a minus sign. So we can use these operations, which leave the absolute values of determinants invariant, to make a matrix **upper triangular**, a form in which its determinant is just the product of the factors on its diagonal. Thus to make the matrix

$$A = \begin{pmatrix} 1 & 2 & 1 \\ -2 & -6 & 3 \\ 4 & 2 & -5 \end{pmatrix}\tag{1.238}$$

upper triangular, we add twice the first row to the second row

$$\begin{pmatrix} 1 & 2 & 1 \\ 0 & -2 & 5 \\ 4 & 2 & -5 \end{pmatrix}$$

and then subtract four times the first row from the third

$$\begin{pmatrix} 1 & 2 & 1 \\ 0 & -2 & 5 \\ 0 & -6 & -9 \end{pmatrix}.\tag{1.239}$$

Next, we subtract three times the second row from the third

$$\begin{pmatrix} 1 & 2 & 1 \\ 0 & -2 & 5 \\ 0 & 0 & -24 \end{pmatrix}.$$

We now find as the determinant of A the product of its diagonal elements:

$$|A| = 1(-2)(-24) = 48.\tag{1.240}$$

□

Example 1.38 (Using Matlab) The Matlab command to make the matrix (1.238) is $A = [1 \ 2 \ 1; -2 \ -6 \ 3; 4 \ 2 \ -5]$. The command $d = \det(A)$ gives its determinant, $d = 48$, and $A_{\text{inv}} = A^{(-1)}$ gives its inverse

$$A_{\text{inv}} = \begin{array}{ccc} 0.5000 & 0.2500 & 0.2500 \\ 0.0417 & -0.1875 & -0.1042 \\ 0.4167 & 0.1250 & -0.0417 \end{array} .$$

□

The **permanent** of a square $n \times n$ matrix A_{ik} is the sum over all permutations $1, 2, \dots, n \rightarrow s_1, s_2, \dots, s_n$ of the products $A_{s_1 1} A_{s_2 2} \cdots A_{s_n n}$

$$\text{perm}(A) = \sum_s A_{s_1 1} A_{s_2 2} \cdots A_{s_n n}. \quad (1.241)$$

The permanent is the determinant without the minus signs.

Applied mathematicians have developed much faster ways of computing determinants and matrix inverses than those (1.212 & 1.224) due to Laplace. Sage, Octave, Matlab, Maple, Mathematica, and Python use these modern techniques, which are freely available as programs in C and FORTRAN from www.netlib.org/lapack. One of these techniques is the LU decomposition.

1.22 LU Decomposition

In 1938 Tadeusz Banachiewicz demonstrated the utility of factoring a square matrix A into the product $A = LU$ of a lower-triangular matrix L , with 1's on its main diagonal, and an upper-triangular matrix U

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ L_{21} & 1 & 0 & 0 & \cdots \\ L_{31} & L_{32} & 1 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & U_{13} & U_{14} & \cdots \\ 0 & U_{22} & U_{23} & U_{24} & \cdots \\ 0 & 0 & U_{33} & U_{34} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (1.242)$$

The product rule (1.231) says that $\det A = \det(LU) = \det L \det U$. But $\det L = 1$, and $\det U = U_{11}U_{22} \cdots U_{nn}$; so $\det A = U_{11}U_{22} \cdots U_{nn}$.

Example 1.39 (A 2×2 LU decomposition) The LU decomposition of a 2×2 matrix is

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ z & 1 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ 0 & \gamma \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ z\alpha & z\beta + \gamma \end{pmatrix}. \quad (1.243)$$

Comparing matrix elements, we see that $\alpha = a$, $\beta = b$, $z = c/\alpha = c/a$, and $\gamma = d - z\beta = d - c\beta/a = d - bc/a$. So the LU decomposition of A is

$$A = \begin{pmatrix} 1 & 0 \\ c/a & 1 \end{pmatrix} \begin{pmatrix} a & b \\ 0 & d - bc/a \end{pmatrix}. \quad (1.244)$$

Thus $\det A = a(d - bc/a)$. \square

1.23 Jacobians

When one changes variables in a multiple integral from coordinates x_1, x_2 and area element $dx_1 dx_2$, one must find the new element of area in terms of the new variables y_1, y_2 . If $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$ are unit vectors in the x_1 and x_2 directions, then as the new coordinates (y_1, y_2) change by dy_1 and dy_2 , the point they represent moves by

$$d\mathbf{y}^1 = \left(\frac{\partial x_1}{\partial y_1} \hat{\mathbf{x}}_1 + \frac{\partial x_2}{\partial y_1} \hat{\mathbf{x}}_2 \right) dy_1 \quad \text{and by} \quad d\mathbf{y}^2 = \left(\frac{\partial x_1}{\partial y_2} \hat{\mathbf{x}}_1 + \frac{\partial x_2}{\partial y_2} \hat{\mathbf{x}}_2 \right) dy_2. \quad (1.245)$$

These vectors, $d\mathbf{y}^1$ and $d\mathbf{y}^2$ define a parallelogram whose area (1.203) is the absolute value of a determinant

$$\text{area}(d\mathbf{y}^1, d\mathbf{y}^2) = \left| \det \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_2}{\partial y_1} \\ \frac{\partial x_1}{\partial y_2} & \frac{\partial x_2}{\partial y_2} \end{pmatrix} \right| dy_1 dy_2. \quad (1.246)$$

The determinant itself is a **jacobian**

$$J = J(x/y) = \frac{\partial(x_1, x_2)}{\partial(y_1, y_2)} = \det \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_2}{\partial y_1} \\ \frac{\partial x_1}{\partial y_2} & \frac{\partial x_2}{\partial y_2} \end{pmatrix}. \quad (1.247)$$

The two equal integrals are

$$\iint_{R_x} f(x_1, x_2) dx_1 dx_2 = \iint_{R_y} f \circ x(y_1, y_2) \left| \frac{\partial(x_1, x_2)}{\partial(y_1, y_2)} \right| dy_1 dy_2 \quad (1.248)$$

in which $f \circ x(y_1, y_2) = f(x_1(y_1, y_2), x_2(y_1, y_2))$ and R_x and R_y are the same region in the two coordinate systems.

In 3 dimensions, with $j = 1, 2$, and 3 , the 3 vectors

$$d\mathbf{y}^j = \left(\frac{\partial x_1}{\partial y_j} \hat{\mathbf{x}}_1 + \frac{\partial x_2}{\partial y_j} \hat{\mathbf{x}}_2 + \frac{\partial x_3}{\partial y_j} \hat{\mathbf{x}}_3 \right) dy_j \quad (1.249)$$

define a parallelepiped whose volume (1.210) is the absolute value of the determinant

$$\text{volume}(\mathbf{dy}^1, \mathbf{dy}^2, \mathbf{dy}^3) = \left| \det \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_2}{\partial y_1} & \frac{\partial x_3}{\partial y_1} \\ \frac{\partial x_1}{\partial y_2} & \frac{\partial x_2}{\partial y_2} & \frac{\partial x_3}{\partial y_2} \\ \frac{\partial x_1}{\partial y_3} & \frac{\partial x_2}{\partial y_3} & \frac{\partial x_3}{\partial y_3} \end{pmatrix} \right| dy_1 dy_2 dy_3. \quad (1.250)$$

The equal integrals are

$$\iiint_{R_x} f(\vec{x}) d^3x = \iiint_{R_y} f \circ x(\vec{y}) \left| \frac{\partial(x_1, x_2, x_3)}{\partial(y_1, y_2, y_3)} \right| d^3y \quad (1.251)$$

in which $d^3x = dx_1 dx_2 dx_3$, $d^3y = dy_1 dy_2 dy_3$, $f \circ x(\vec{y}) = f(x_1(\vec{y}), x_2(\vec{y}), x_3(\vec{y}))$, and R_x and R_y are the same region in the two coordinate systems.

For n -dimensional integrals over $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$, the rule is similar

$$\int_{R_x} f(x) d^n x = \int_{R_y} f \circ x(y) \left| \frac{\partial(x_1, \dots, x_n)}{\partial(y_1, \dots, y_n)} \right| d^n y \quad (1.252)$$

and uses the absolute value of the n -dimensional jacobian

$$J = J(x/y) = \frac{\partial(x_1, \dots, x_n)}{\partial(y_1, \dots, y_n)} = \det \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \cdots & \frac{\partial x_n}{\partial y_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_1}{\partial y_n} & \cdots & \frac{\partial x_n}{\partial y_n} \end{pmatrix}. \quad (1.253)$$

Since the determinant of the transpose of a matrix is the same (1.214) as the determinant of the matrix, some people write jacobians with their rows and columns interchanged.

1.24 Systems of linear equations

Suppose we wish to solve the system of n linear equations

$$\sum_{k=1}^n A_{ik} x_k = y_i \quad (1.254)$$

for n unknowns x_k . In matrix notation, with A an $n \times n$ matrix and x and y n -vectors, this system of equations is $Ax = y$. If the matrix A is **nonsingular**, that is, if $\det(A) \neq 0$, then it has an inverse A^{-1} given by

(1.224), and we may multiply both sides of $Ax = y$ by A^{-1} and so find $x = A^{-1}y$. When A is nonsingular, this is the unique solution to (1.254).

When A is singular, its determinant vanishes $\det(A) = 0$, and so its columns are linearly dependent (section 1.21). In this case, the linear dependence of the columns of A implies that $Az = 0$ for some non-zero vector z . Thus if x satisfies $Ax = y$, then so does $x + cz$ for any constant c because $A(x + cz) = Ax + cAz = y$. So if $\det(A) = 0$, then the equation $Ax = y$ may have solutions, but they will not be unique. Whether equation (1.254) has any solutions when $\det(A) = 0$ depends on whether the vector y can be expressed as a linear combination of the columns of A . Since these columns are linearly dependent, they span a subspace of fewer than n dimensions, and so (1.254) has solutions only when the n -vector y lies in that subspace.

A system of $m < n$ equations

$$\sum_{k=1}^n A_{ik}x_k = y_i \quad \text{for } i = 1, 2, \dots, m \quad (1.255)$$

in n unknowns is **under determined**. As long as at least m of the n columns A_{ik} of the matrix A are linearly independent, such a system always has solutions, but they may not be unique.

1.25 Linear least squares

Suppose we have a system of $m > n$ equations in n unknowns x_k

$$\sum_{k=1}^n A_{ik}x_k = y_i \quad \text{for } i = 1, 2, \dots, m. \quad (1.256)$$

This problem is **over determined** and, in general, has no solution, but it does have an approximate solution due to Carl Gauss (1777–1855).

If the matrix A and the vector y are real, then Gauss's solution is the n values x_k that minimize the sum E of the squares of the errors

$$E = \sum_{i=1}^m \left(y_i - \sum_{k=1}^n A_{ik}x_k \right)^2. \quad (1.257)$$

The minimizing values x_k make the n derivatives of E vanish

$$\frac{\partial E}{\partial x_\ell} = 0 = \sum_{i=1}^m 2 \left(y_i - \sum_{k=1}^n A_{ik}x_k \right) (-A_{i\ell}) \quad (1.258)$$

or in matrix notation $A^T y = A^T A x$. Since A is real, the matrix $A^T A$ is

nonnegative (1.43); if it also is positive (1.44), then it has an inverse, and our **least-squares solution** is

$$x = (A^T A)^{-1} A^T y. \quad (1.259)$$

If the matrix A and the vector y are complex, and if the matrix $A^\dagger A$ is positive, then one may derive (exercise 1.25) Gauss's solution

$$x = (A^\dagger A)^{-1} A^\dagger y. \quad (1.260)$$

The operators $(A^T A)^{-1} A^T$ and $(A^\dagger A)^{-1} A^\dagger$ are **pseudoinverses** (section ??).

1.26 Lagrange multipliers

The maxima and minima of a function $f(x)$ of $x = (x_1, x_2, \dots, x_n)$ are among the points at which its gradient vanishes $\nabla f(x) = 0$, that is,

$$\frac{\partial f(x)}{\partial x_j} = 0 \quad (1.261)$$

for $j = 1, \dots, n$. These are **stationary** points of f .

Example 1.40 (Minimum) For instance, if $f(x) = x_1^2 + 2x_2^2 + 3x_3^2$, then its minimum is at

$$\nabla f(x) = (2x_1, 4x_2, 6x_3) = 0 \quad (1.262)$$

that is, at $x_1 = x_2 = x_3 = 0$. □

How do we find the extrema of $f(x)$ if x also must satisfy a constraint? We use a Lagrange multiplier (Joseph-Louis Lagrange 1736–1813).

In the case of one constraint $c(x) = 0$, we need the gradient $\nabla f(x)$ to vanish in those directions dx that preserve the constraint. So $dx \cdot \nabla f(x) = 0$ for all dx that make the dot product $dx \cdot \nabla c(x)$ vanish. So the extrema of $f(x)$ subject to the constraint $c(x) = 0$ satisfy the equations

$$\nabla f(x) = \lambda \nabla c(x) \quad \text{and} \quad c(x) = 0. \quad (1.263)$$

These $n + 1$ equations define the extrema of the unconstrained function

$$L(x, \lambda) = f(x) - \lambda c(x) \quad (1.264)$$

of the $n + 1$ variables x_1, \dots, x_n, λ

$$\frac{\partial L(x, \lambda)}{\partial x_j} = \frac{\partial (f(x) - \lambda c(x))}{\partial x_j} = 0 \quad \text{and} \quad \frac{\partial L(x, \lambda)}{\partial \lambda} = -c(x) = 0. \quad (1.265)$$

The variable λ is a **Lagrange multiplier**.

In the case of k constraints $c_1(x) = 0, \dots, c_k(x) = 0$, the projection of ∇f must vanish in those directions dx that preserve all the constraints. So $dx \cdot \nabla f(x) = 0$ for all dx that make all $dx \cdot \nabla c_j(x) = 0$ for $j = 1, \dots, k$. The gradient ∇f will satisfy this requirement if it's a linear combination

$$\nabla f = \lambda_1 \nabla c_1 + \dots + \lambda_k \nabla c_k \quad (1.266)$$

of the k gradients because then $dx \cdot \nabla f$ will vanish if $dx \cdot \nabla c_j = 0$ for $j = 1, \dots, k$. The extrema also must satisfy the constraints

$$c_1(x) = 0, \dots, c_k(x) = 0. \quad (1.267)$$

The $n + k$ equations (1.266 & 1.267) define the extrema of the unconstrained function

$$L(x, \lambda) = f(x) - \lambda_1 c_1(x) \dots - \lambda_k c_k(x) \quad (1.268)$$

of the $n + k$ variables x and λ

$$\frac{\partial L(x, \lambda)}{\partial x_i} = \frac{\partial f(x)}{\partial x_i} - \lambda_1 \frac{\partial c_1(x)}{\partial x_i} \dots - \lambda_k \frac{\partial c_k(x)}{\partial x_i} = 0 \quad (1.269)$$

and

$$\frac{\partial L(x, \lambda)}{\partial \lambda_j} = -c_j(x) = 0 \quad \text{for } j = 1, \dots, k. \quad (1.270)$$

Example 1.41 (Constrained Extrema and Eigenvectors) Suppose we want to find the extrema of a real, symmetric quadratic form

$$f(x) = x^T A x = \sum_{i,j=1}^n x_i A_{ij} x_j \quad (1.271)$$

subject to the constraint $c(x) = x \cdot x - 1$ which says that the n -vector x is of unit length. We form the function

$$L(x, \lambda) = x^T A x - \lambda (x \cdot x - 1) \quad (1.272)$$

and since the matrix A is real and symmetric, we find its unconstrained extrema as

$$\frac{\partial L(x, \lambda)}{\partial x_i} = 2 \sum_{k=1}^n A_{ik} x_k - 2\lambda x_i = 0 \quad \text{and} \quad x \cdot x = 1. \quad (1.273)$$

The extrema of $f(x) = x^T A x$ subject to the constraint $c(x) = x \cdot x - 1$ are the **normalized eigenvectors**

$$A x = \lambda x \quad \text{and} \quad x \cdot x = 1 \quad (1.274)$$

of the real, symmetric matrix A . □

1.27 Eigenvectors and eigenvalues

If a linear operator A maps a nonzero vector $|u\rangle$ into a multiple of itself

$$A|u\rangle = \lambda|u\rangle \quad (1.275)$$

then the vector $|u\rangle$ is an **eigenvector** of A with **eigenvalue** λ . (The German adjective *eigen* means *own*, *special*, or *proper*.)

If the vectors $|k\rangle$ for $k = 1, \dots, n$ form an orthonormal basis for the vector space in which A acts, then we can write the identity operator (1.150) for the space as $I = |1\rangle\langle 1| + \dots + |n\rangle\langle n|$. By inserting this formula for I into the eigenvector equation (1.275), we get

$$\sum_{\ell=1}^n \langle k|A|\ell\rangle \langle \ell|u\rangle = \lambda \langle k|u\rangle. \quad (1.276)$$

In matrix notation, with $A_{k\ell} = \langle k|A|\ell\rangle$ and $u_\ell = \langle \ell|u\rangle$, this is $Au = \lambda u$.

A subspace $c_\ell|u_\ell\rangle + \dots + c_r|u_r\rangle$ spanned by any set of eigenvectors $|u_k\rangle$ of a matrix A is left invariant by its action, that is

$$A \left(\sum_{k \in S} c_k |u_k\rangle \right) = \sum_{k \in S} c_k A|u_k\rangle = \sum_{k \in S} c_k \lambda_k |u_k\rangle = \sum_{k \in S} c'_k |u_k\rangle \quad (1.277)$$

with $c'_k = c_k \lambda_k$. Eigenvectors span **invariant subspaces**.

Example 1.42 (Eigenvalues of an Orthogonal Matrix) The matrix equation

$$\begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} = e^{\pm i\theta} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} \quad (1.278)$$

tells us that the eigenvectors of this 2×2 orthogonal matrix are $(1, \pm i)$ with eigenvalues $e^{\pm i\theta}$. The eigenvalues λ of a unitary (and of an orthogonal) matrix are unimodular, $|\lambda| = 1$, (exercise 1.26). □

Example 1.43 (Eigenvalues of an Antisymmetric Matrix) Let us consider an eigenvector equation for a matrix A that is antisymmetric

$$\sum_{k=1}^n A_{ik} u_k = \lambda u_i. \quad (1.279)$$

The antisymmetry $A_{ik} = -A_{ki}$ of A implies that

$$\sum_{i,k=1}^n u_i A_{ik} u_k = 0. \quad (1.280)$$

Thus the last two relations imply that

$$0 = \sum_{i,k=1}^n u_i A_{ik} u_k = \lambda \sum_{i=1}^n u_i^2 = 0. \quad (1.281)$$

Thus either the eigenvalue λ or the dot product of the eigenvector with itself vanishes. \square

1.28 Eigenvectors of a square matrix

Let A be an $n \times n$ matrix with complex entries A_{ik} . A vector V with n entries V_k (not all zero) is an **eigenvector** of A with **eigenvalue** λ if

$$\sum_{k=1}^n A_{ik} V_k = \lambda V_i \quad \text{or} \quad AV = \lambda V \quad (1.282)$$

in matrix notation. Every $n \times n$ matrix A has n eigenvectors $V^{(\ell)}$ and eigenvalues λ_ℓ

$$AV^{(\ell)} = \lambda_\ell V^{(\ell)} \quad (1.283)$$

for $\ell = 1 \dots n$. To see why, we write the top equation (1.282) as

$$\sum_{k=1}^n (A_{ik} - \lambda \delta_{ik}) V_k = 0 \quad (1.284)$$

or in matrix notation as $(A - \lambda I)V = 0$ in which I is the $n \times n$ identity matrix with entries $I_{ik} = \delta_{ik}$. This equation (1.284) says that the columns of the matrix $A - \lambda I$, considered as vectors, are linearly dependent (section 1.9) because the coefficients V_k are not all zero. The columns of a matrix $A - \lambda I$ are linearly dependent if and only if the determinant $|A - \lambda I|$ vanishes (section 1.21). Thus a solution of the eigenvalue equation (1.282) exists if and only if the determinant of $A - \lambda I$ vanishes

$$\det(A - \lambda I) = |A - \lambda I| = 0. \quad (1.285)$$

This vanishing of the determinant of $A - \lambda I$ is the **characteristic equation** of the matrix A . For an $n \times n$ matrix A , it is a polynomial equation of the n th degree in the unknown eigenvalue λ

$$\begin{aligned} 0 &= |A - \lambda I| = |A| + \cdots + (-1)^{n-1} \lambda^{n-1} \text{Tr} A + (-1)^n \lambda^n \\ &= P(\lambda, A) = \sum_{k=0}^n p_k \lambda^k \end{aligned} \quad (1.286)$$

in which $p_0 = |A|$, $p_{n-1} = (-1)^{n-1} \text{Tr} A$, and $p_n = (-1)^n$.

All the p_k 's are basis independent. For if S is any nonsingular matrix, then multiplication rules (1.231 & 1.235) for determinants imply that the determinant $|A - \lambda I|$ is invariant when A undergoes a similarity transformation (1.71 & (1.290) 1.296) $A \rightarrow A' = S^{-1} A S$

$$\begin{aligned} P(\lambda, A') &= P(\lambda, S^{-1} A S) = |S^{-1} A S - \lambda I| = |S^{-1} (A - \lambda I) S| \\ &= |S^{-1}| |A - \lambda I| |S| = |A - \lambda I| = P(\lambda, A). \end{aligned} \quad (1.287)$$

By the fundamental theorem of algebra (section 6.9), the characteristic equation (1.286) always has n roots or solutions λ_ℓ lying somewhere in the complex plane. Thus the **characteristic polynomial** $P(\lambda, A)$ has the factored form

$$P(\lambda, A) = (\lambda_1 - \lambda)(\lambda_2 - \lambda) \cdots (\lambda_n - \lambda). \quad (1.288)$$

For every root λ_ℓ , there is a nonzero eigenvector $V^{(\ell)}$ whose components $V_k^{(\ell)}$ are the coefficients that make the n vectors $A_{ik} - \lambda_\ell \delta_{ik}$ that are the columns of the matrix $A - \lambda_\ell I$ sum to zero in (1.284). Thus **every $n \times n$ matrix has n eigenvalues λ_ℓ and n eigenvectors $V^{(\ell)}$** .

The $n \times n$ diagonal matrix $A_{k\ell}^{(d)} = \delta_{k\ell} \lambda_\ell$ is the **canonical form** of the matrix A . The matrix $V_{k\ell} = V_k^{(\ell)}$ whose columns are the eigenvectors $V^{(\ell)}$ of A is the **modal matrix**. The equation $A V = V A^{(d)}$

$$\sum_{k=1}^n A_{ik} V_{k\ell} = \sum_{k=1}^n A_{ik} V_k^{(\ell)} = \lambda_\ell V_i^{(\ell)} = \sum_{k=1}^n V_{ik} \delta_{k\ell} \lambda_\ell = \sum_{k=1}^n V_{ik} A_{k\ell}^{(d)} \quad (1.289)$$

presents the n solutions of the eigenvector equation (1.282).

If the eigenvectors $V_{k\ell}$ are linearly independent, then the matrix V , of which they are the columns, is nonsingular and has an inverse V^{-1} . The similarity transformation

$$V^{-1} A V = A^{(d)} \quad (1.290)$$

then diagonalizes the matrix A .

Example 1.44 (The Canonical Form of a 3×3 Matrix) If in Matlab we set $A = [0 \ 1 \ 2; 3 \ 4 \ 5; 6 \ 7 \ 8]$ and enter $[V, D] = \text{eig}(A)$, then we get

$$V = \begin{pmatrix} 0.1648 & 0.7997 & 0.4082 \\ 0.5058 & 0.1042 & -0.8165 \\ 0.8468 & -0.5913 & 0.4082 \end{pmatrix} \quad \text{and} \quad A_d = \begin{pmatrix} 13.3485 & 0 & 0 \\ 0 & -1.3485 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and one may check that $AV = VA_d$ and that $V^{-1}AV = A_d$. \square

Setting $\lambda = 0$ in the factored form (1.288) of $P(\lambda, A)$ and in the characteristic equation (1.286), we see that **the determinant of every $n \times n$ matrix is the product of its n eigenvalues**

$$P(0, A) = |A| = p_0 = \lambda_1 \lambda_2 \dots \lambda_n. \quad (1.291)$$

These n roots are usually all different, and when they are, the eigenvectors $V^{(\ell)}$ are linearly independent. The first eigenvector is trivially linearly independent. Let's assume that the first $k < n$ eigenvectors are linearly independent; we'll show that the first $k+1$ eigenvectors are linearly independent. If they were linearly dependent, then there would be $k+1$ numbers c_ℓ , not all zero, such that

$$\sum_{\ell=1}^{k+1} c_\ell V^{(\ell)} = 0. \quad (1.292)$$

First we multiply this equation from the left by the linear operator A and use the eigenvalue equation (1.283)

$$A \sum_{\ell=1}^{k+1} c_\ell V^{(\ell)} = \sum_{\ell=1}^{k+1} c_\ell AV^{(\ell)} = \sum_{\ell=1}^{k+1} c_\ell \lambda_\ell V^{(\ell)} = 0. \quad (1.293)$$

Now we multiply the same equation (1.292) by λ_{k+1}

$$\sum_{\ell=1}^{k+1} c_\ell \lambda_{k+1} V^{(\ell)} = 0 \quad (1.294)$$

and subtract the product (1.294) from (1.293). The terms with $\ell = k+1$ cancel leaving

$$\sum_{\ell=1}^k c_\ell (\lambda_\ell - \lambda_{k+1}) V^{(\ell)} = 0 \quad (1.295)$$

in which all the factors $(\lambda_\ell - \lambda_{k+1})$ are different from zero since by assumption all the eigenvalues are different. But this last equation says that the

first k eigenvectors are linearly dependent, which contradicts our assumption that they were linearly independent. This contradiction tells us that **if all n eigenvectors of an $n \times n$ square matrix have different eigenvalues, then they are linearly independent**. Similarly, if any $k < n$ eigenvectors of an $n \times n$ square matrix have different eigenvalues, then they are linearly independent.

An eigenvalue λ that is a single root of the characteristic equation (1.286), i.e., that occurs only once in its factored form (1.288), is associated with a single eigenvector and is called a **simple eigenvalue**. An eigenvalue λ that is a root of multiplicity n of the characteristic equation is associated with n eigenvectors; it is said to be an **n -fold degenerate eigenvalue** or to have **algebraic multiplicity n** . Its **geometric multiplicity** is the number $n' \leq n$ of linearly independent eigenvectors with eigenvalue λ . A matrix with $n' < n$ for any eigenvalue λ is **defective**. Thus an $n \times n$ matrix with fewer than n linearly independent eigenvectors is defective. **So every nondefective square matrix A can be diagonalized by a similarity transformation** (1.290)

$$V^{-1}AV = A^{(d)}. \quad (1.296)$$

The elements of the main diagonal of the matrix $A^{(d)}$ are the eigenvalues of the matrix A . Thus the trace of every nondefective matrix A is the sum of its eigenvalues, $\text{Tr}A = \text{Tr}A^{(d)} = \lambda_1 + \cdots + \lambda_n$. The columns of the matrix V are the eigenvectors of the matrix A .

Since the determinant of every matrix A is the product (1.291) of its eigenvalues, $\det A = |A| = \lambda_1 \lambda_2 \cdots \lambda_n$, the determinant of every nondefective matrix is the exponential of the trace of its logarithm

$$\det A = \exp[\text{Tr}(\log A)]. \quad (1.297)$$

Example 1.45 (A Defective 2×2 Matrix) Each of the 2×2 matrices

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (1.298)$$

has only one linearly independent eigenvector and so is defective. \square

1.29 A matrix obeys its characteristic equation

Every square matrix obeys its characteristic equation (1.286). That is, the characteristic equation

$$P(\lambda, A) = |A - \lambda I| = \sum_{k=0}^n p_k \lambda^k = 0 \quad (1.299)$$

remains true when the matrix A replaces the variable λ

$$P(A, A) = \sum_{k=0}^n p_k A^k = 0. \quad (1.300)$$

To see why, we use the formula (1.224) for the inverse of the matrix $A - \lambda I$

$$(A - \lambda I)^{-1} = \frac{C(\lambda, A)^{\top}}{|A - \lambda I|} \quad (1.301)$$

in which $C(\lambda, A)^{\top}$ is the transpose of the matrix of cofactors of the matrix $A - \lambda I$. Since $|A - \lambda I| = P(\lambda, A)$, we have, rearranging,

$$(A - \lambda I) C(\lambda, A)^{\top} = |A - \lambda I| I = P(\lambda, A) I. \quad (1.302)$$

The transpose of the matrix of cofactors of the matrix $A - \lambda I$ is a polynomial in λ with coefficients C_0, \dots, C_{n-1} that are matrices

$$C(\lambda, A)^{\top} = C_0 + C_1 \lambda + \dots + C_{n-1} \lambda^{n-1}. \quad (1.303)$$

Combining these last two equations (1.302 & 1.303) with the characteristic equation (1.299), we have

$$\begin{aligned} (A - \lambda I) C(\lambda, A)^{\top} &= AC_0 + (AC_1 - C_0)\lambda + (AC_2 - C_1)\lambda^2 + \dots \\ &\quad + (AC_{n-1} - C_{n-2})\lambda^{n-1} - C_{n-1}\lambda^n \quad (1.304) \\ &= \sum_{k=0}^n p_k \lambda^k I. \end{aligned}$$

Equating equal powers of λ on both sides of this equation, we find

$$\begin{aligned} AC_0 &= p_0 I \\ AC_1 - C_0 &= p_1 I \\ AC_2 - C_1 &= p_2 I \\ &\dots = \dots \\ AC_{n-1} - C_{n-2} &= p_{n-1} I \\ -C_{n-1} &= p_n I. \end{aligned} \quad (1.305)$$

We now multiply from the left the first of these equations by I , the second by A , the third by A^2 , \dots , and the last by A^n and then add the resulting equations. All the terms on the left-hand sides cancel, while the sum of those on the right gives $p_0I + p_1A + \dots + p_nA^n = P(A, A)$. Thus a square matrix A obeys its characteristic equation

$$0 = \sum_{k=0}^n p_k A^k = |A|I + p_1A + \dots + (-1)^{n-1}(\text{Tr}A)A^{n-1} + (-1)^n A^n \quad (1.306)$$

a result known as the **Cayley-Hamilton theorem** (Arthur Cayley, 1821–1895, and William Hamilton, 1805–1865). This derivation is due to Israel Gelfand (1913–2009) (Gelfand, 1961, pp. 89–90).

Because every $n \times n$ matrix A obeys its characteristic equation, its n th power A^n can be expressed as a linear combination of its lesser powers

$$A^n = (-1)^{n-1}(|A|I + p_1A + p_2A^2 + \dots + (-1)^{n-1}(\text{Tr}A)A^{n-1}). \quad (1.307)$$

For instance, the square A^2 of every 2×2 matrix is given by

$$A^2 = -|A|I + (\text{Tr}A)A. \quad (1.308)$$

Example 1.46 (Spin-one-half rotation matrix) If $\boldsymbol{\theta}$ is a real 3-vector and $\boldsymbol{\sigma}$ is the 3-vector of Pauli matrices (1.36), then the square of the traceless 2×2 matrix $A = \boldsymbol{\theta} \cdot \boldsymbol{\sigma}$ is

$$(\boldsymbol{\theta} \cdot \boldsymbol{\sigma})^2 = -|\boldsymbol{\theta} \cdot \boldsymbol{\sigma}|I = - \begin{vmatrix} \theta_3 & \theta_1 - i\theta_2 \\ \theta_1 + i\theta_2 & -\theta_3 \end{vmatrix} I = \theta^2 I \quad (1.309)$$

in which $\theta^2 = \boldsymbol{\theta} \cdot \boldsymbol{\theta}$. One may use this identity to show (exercise 1.28) that

$$\exp(-i\boldsymbol{\theta} \cdot \boldsymbol{\sigma}/2) = \cos(\theta/2)I - i\hat{\boldsymbol{\theta}} \cdot \boldsymbol{\sigma} \sin(\theta/2) \quad (1.310)$$

in which $\hat{\boldsymbol{\theta}}$ is a unit 3-vector. For a spin-one-half object, this matrix represents an active right-handed rotation of θ radians about the axis $\hat{\boldsymbol{\theta}}$. \square

1.30 Functions of matrices

What sense can we make of a function f of an $n \times n$ matrix A ? and how would we compute it? One way is to use the characteristic equation (1.307) to express every power of A in terms of I, A, \dots, A^{n-1} and the coefficients $p_0 = |A|, p_1, p_2, \dots, p_{n-2}$, and $p_{n-1} = (-1)^{n-1}\text{Tr}A$. Then if $f(x)$ is a polynomial or a function with a convergent power series

$$f(x) = \sum_{k=0}^{\infty} c_k x^k \quad (1.311)$$

in principle we may express $f(A)$ in terms of n functions $f_k(\mathbf{p})$ of the coefficients $\mathbf{p} \equiv (p_0, \dots, p_{n-1})$ as

$$f(A) = \sum_{k=0}^{n-1} f_k(\mathbf{p}) A^k. \quad (1.312)$$

The identity (1.310) for $\exp(-i\boldsymbol{\theta} \cdot \boldsymbol{\sigma}/2)$ is an $n = 2$ example of this technique which can become challenging when $n > 3$.

Example 1.47 (The 3×3 Rotation Matrix) In exercise (1.29), one finds the characteristic equation (1.306) for the 3×3 matrix $-i\boldsymbol{\theta} \cdot \mathbf{J}$ in which $(J_k)_{ij} = i\epsilon_{ikj}$, and ϵ_{ijk} is totally antisymmetric with $\epsilon_{123} = 1$. The generators J_k satisfy the commutation relations $[J_i, J_j] = i\epsilon_{ijk}J_k$ in which sums over repeated indices from 1 to 3 are understood. In exercise (1.30), one uses the characteristic equation for $-i\boldsymbol{\theta} \cdot \mathbf{J}$ to show that the 3×3 real orthogonal matrix $\exp(-i\boldsymbol{\theta} \cdot \mathbf{J})$, which represents a right-handed rotation by θ radians about the axis $\hat{\boldsymbol{\theta}}$, is

$$\exp(-i\boldsymbol{\theta} \cdot \mathbf{J}) = \cos \theta I - i\hat{\boldsymbol{\theta}} \cdot \mathbf{J} \sin \theta + (1 - \cos \theta) \hat{\boldsymbol{\theta}}(\hat{\boldsymbol{\theta}})^\top \quad (1.313)$$

or

$$\exp(-i\boldsymbol{\theta} \cdot \mathbf{J})_{ij} = \delta_{ij} \cos \theta - \sin \theta \epsilon_{ijk} \hat{\theta}_k + (1 - \cos \theta) \hat{\theta}_i \hat{\theta}_j \quad (1.314)$$

in terms of indices. □

Direct use of the characteristic equation can become unwieldy for larger values of n . Fortunately, another trick is available if A is a nondefective square matrix, and if the power series (1.311) for $f(x)$ converges. For then A is related to its diagonal form $A^{(d)}$ by the similarity transformation (1.290) of its model matrix V , and we may define $f(A)$ as

$$f(A) = V f(A^{(d)}) V^{-1}. \quad (1.315)$$

in which $f(A^{(d)})$ is the diagonal matrix with entries $f(a_\ell)$

$$f(A^{(d)}) = \begin{pmatrix} f(a_1) & 0 & 0 & \dots \\ 0 & f(a_2) & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & f(a_n) \end{pmatrix} \quad (1.316)$$

and a_1, a_2, \dots, a_n are the eigenvalues of the matrix A . This definition makes sense if $f(A)$ is a series in powers of A because then

$$f(A) = \sum_{k=0}^{\infty} c_k A^k = \sum_{k=0}^{\infty} c_k \left(V A^{(d)} V^{-1} \right)^k. \quad (1.317)$$

So since $V^{-1}V = I$, we have $(VA^{(d)}V^{-1})^k = V(A^{(d)})^k V^{-1}$ and thus

$$f(A) = V \left[\sum_{k=0}^{\infty} c_k (A^{(d)})^k \right] V^{-1} = Vf(A^{(d)})V^{-1} \quad (1.318)$$

which is (1.315).

Example 1.48 (Momentum operators generate spatial translations) The position operator x and the momentum operator p obey the commutation relation $[x, p] = xp - px = i\hbar$. Thus the a -derivative $\dot{x}(a)$ of the operator $x(a) = e^{iap/\hbar} x e^{-iap/\hbar}$ is unity

$$\dot{x}(a) = e^{iap/\hbar} (i/\hbar)[p, x] e^{-iap/\hbar} = e^{iap/\hbar} e^{-iap/\hbar} = 1. \quad (1.319)$$

Since $x(0) = x$, we see that the unitary transformation $U(a) = e^{iap/\hbar}$ moves x to $x + a$

$$e^{iap/\hbar} x e^{-iap/\hbar} = x(a) = x(0) + \int_0^a \dot{x}(a') da' = x + a. \quad (1.320)$$

□

Example 1.49 (Glauber's identity) The commutator of the annihilation operator a and the creation operator a^\dagger for a given mode is the number 1

$$[a, a^\dagger] = a a^\dagger - a^\dagger a = 1. \quad (1.321)$$

Thus a and a^\dagger commute with their commutator $[a, a^\dagger] = 1$ just as x and p commute with their commutator $[x, p] = i\hbar$.

Suppose that A and B are any two operators that commute with their commutator $[A, B] = AB - BA$

$$[A, [A, B]] = [B, [A, B]] = 0. \quad (1.322)$$

As in the $[x, p]$ example (1.48), we define $A_B(t) = e^{-tB} A e^{tB}$ and note that because $[B, [A, B]] = 0$, its t -derivative is simply

$$\dot{A}_B(t) = e^{-tB} [A, B] e^{tB} = [A, B]. \quad (1.323)$$

Since $A_B(0) = A$, an integration gives

$$A_B(t) = A + \int_0^t \dot{A}_B(t) dt = A + \int_0^t [A, B] dt = A + t[A, B]. \quad (1.324)$$

Multiplication from the left by e^{tB} now gives $e^{tB} A_B(t)$ as

$$e^{tB} A_B(t) = A e^{tB} = e^{tB} (A + t[A, B]). \quad (1.325)$$

Now we define

$$G(t) = e^{tA} e^{tB} e^{-t(A+B)} \quad (1.326)$$

and use our formula (1.325) to compute its t -derivative as

$$\begin{aligned} \dot{G}(t) &= e^{tA} (A e^{tB} + e^{tB} B - e^{tB}(A+B)) e^{-t(A+B)} \\ &= e^{tA} (e^{tB} (A + t[A, B]) + e^{tB} B - e^{tB}(A+B)) e^{-t(A+B)} \\ &= e^{tA} e^{tB} t[A, B] e^{t(A+B)} = t[A, B] G(t) = t G(t) [A, B]. \end{aligned} \quad (1.327)$$

Since $\dot{G}(t)$, $G(t)$, and $[A, B]$ all commute with each other, we can integrate this operator equation

$$\frac{d}{dt} \log G(t) = \frac{\dot{G}(t)}{G(t)} = t[A, B] \quad (1.328)$$

from 0 to 1 and get since $G(0) = 1$

$$\log G(1) - \log G(0) = \log G(1) = \frac{1}{2} [A, B]. \quad (1.329)$$

Thus $G(1) = e^{[A, B]/2}$ and so

$$e^A e^B e^{-(A+B)} = e^{\frac{1}{2}[A, B]} \quad \text{or} \quad e^A e^B = e^{A+B+\frac{1}{2}[A, B]} \quad (1.330)$$

which is Glauber's identity. \square

Example 1.50 (Chemical reactions) The chemical reactions $[A] \xrightarrow{a} [B]$, $[B] \xrightarrow{b} [A]$, and $[B] \xrightarrow{c} [C]$ make the concentrations $[A] \equiv A$, $[B] \equiv B$, and $[C] \equiv C$ of three kinds of molecules vary with time as

$$\dot{A} = -aA + bB, \quad \dot{B} = aA - (b+c)B \quad \text{and} \quad \dot{C} = cB. \quad (1.331)$$

We can group these concentrations into a 3-vector $V = (A, B, C)$ and write the three equations (1.331) as $\dot{V} = K V$ in which K is the matrix

$$K = \begin{pmatrix} -a & b & 0 \\ a & -b-c & 0 \\ 0 & c & 0 \end{pmatrix}. \quad (1.332)$$

The solution to the differential equation $\dot{V} = K V$ is $V(t) = e^{Kt} V(0)$.

The eigenvalues of the matrix K are the roots of the cubic equation $\det(K - \lambda I) = 0$. One root vanishes, and the other two are the roots of the quadratic equation $\lambda^2 + (a+b+c)\lambda + ac = 0$. Their sum is the trace $\text{Tr}K = -(a+b+c)$. They are real when a, b , and c are positive but are complex when $4ac > (a+b+c)^2$. The eigenvectors are complete unless $4ac = (a+b+c)^2$, but are not orthogonal unless $c = 0$.

The time evolution of the concentrations $[A]$ (dashdot), $[B]$ (solid), and $[C]$ (dashes) are plotted in Fig. 1.1 for the initial conditions $[A] = 1$ and $[B] = [C] = 0$ and rates $a = 0.15$, $b = 0.1$, and $c = 0.1$. The Matlab code is in the repository `Linear_algebra` at github.com/kevinecahill.

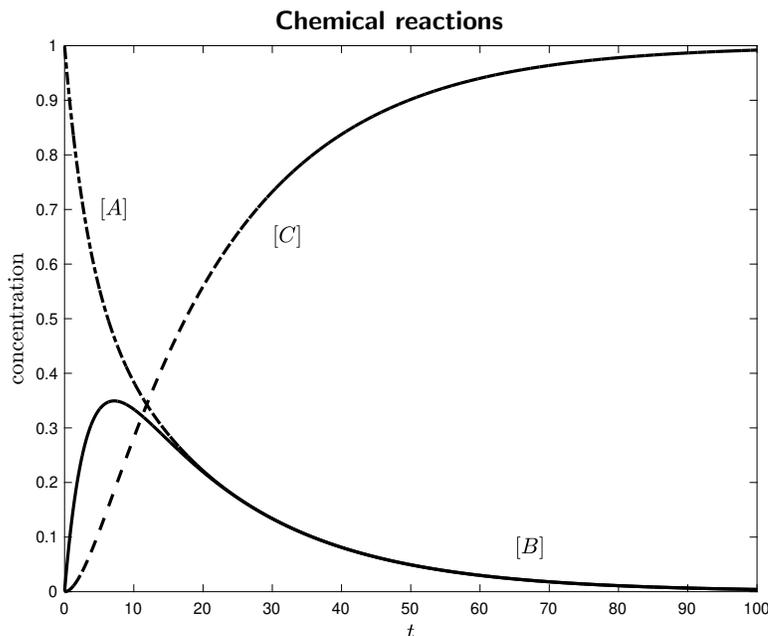


Figure 1.1 The concentrations $[A]$ (dashdot), $[B]$ (solid), and $[C]$ (dashes) as given by the matrix equation $\dot{V}(t) = e^{Kt} V(0)$ for the initial conditions $[A] = 1$ and $[B] = [C] = 0$ and rates $a = 0.15$, $b = 0.1$, and $c = 0.1$.

□

Example 1.51 (Time-evolution operator) In quantum mechanics, the time-evolution operator is the exponential $\exp(-iHt/\hbar)$ where $H = H^\dagger$ is a hermitian linear operator, the hamiltonian (William Rowan Hamilton 1805–1865), and $\hbar = h/(2\pi) = 1.054 \times 10^{-34}$ Js where h is Planck’s constant (Max Planck 1858–1947). As we’ll see in the next section, hermitian operators are never defective, so H can be diagonalized by a similarity transformation

$$H = SH^{(d)}S^{-1}. \quad (1.333)$$

The diagonal elements of the diagonal matrix $H^{(d)}$ are the **energies** E_ℓ of the states of the system described by the hamiltonian H . The time-evolution operator $U(t)$ then is

$$U(t) = S \exp(-iH^{(d)}t/\hbar) S^{-1}. \quad (1.334)$$

For a three-state system with angular frequencies $\omega_i = E_i/\hbar$, it is

$$U(t) = S \begin{pmatrix} e^{-i\omega_1 t} & 0 & 0 \\ 0 & e^{-i\omega_2 t} & 0 \\ 0 & 0 & e^{-i\omega_3 t} \end{pmatrix} S^{-1}. \quad (1.335)$$

□

Example 1.52 (Entropy) The **entropy** S of a system described by a density operator ρ is the trace $S = -k \operatorname{Tr}(\rho \ln \rho)$ in which $k = 1.38 \times 10^{-23}$ J/K is the constant named after Ludwig Boltzmann (1844–1906). The density operator ρ is hermitian, nonnegative, and of unit trace. Since ρ is hermitian, the matrix that represents it is never defective (section 1.31), and so it can be diagonalized by a similarity transformation $\rho = S \rho^{(d)} S^{-1}$. By (1.27), $\operatorname{Tr} ABC = \operatorname{Tr} BCA$, so we can write S as

$$S = -k \operatorname{Tr} \left(S \rho^{(d)} S^{-1} S \ln(\rho^{(d)}) S^{-1} \right) = -k \operatorname{Tr} \left(\rho^{(d)} \ln(\rho^{(d)}) \right). \quad (1.336)$$

A vanishing eigenvalue $\rho_k^{(d)} = 0$ contributes nothing to this trace since $\lim_{x \rightarrow 0} x \ln x = 0$. If the system has three states, populated with probabilities ρ_i , the elements of $\rho^{(d)}$, then the sum

$$\begin{aligned} S &= -k (\rho_1 \ln \rho_1 + \rho_2 \ln \rho_2 + \rho_3 \ln \rho_3) \\ &= k [\rho_1 \ln(1/\rho_1) + \rho_2 \ln(1/\rho_2) + \rho_3 \ln(1/\rho_3)] \end{aligned} \quad (1.337)$$

is its entropy. □

Example 1.53 (Logarithm of a determinant) Since every nondefective $n \times n$ matrix A may be diagonalized by a similarity transformation, its determinant is the product of its eigenvalues and its trace is the sum of them, and so the logarithm of its determinant is the trace of its logarithm

$$\ln \det A = \ln(\lambda_1 \dots \lambda_n) = \ln(\lambda_1) + \dots + \ln(\lambda_n) = \operatorname{Tr}(\ln A). \quad (1.338)$$

When none of A 's eigenvalues vanishes, this relation implies the earlier result (1.237) that the variation of A 's determinant is

$$\delta \det A = \det A \operatorname{Tr}(A^{-1} \delta A). \quad (1.339)$$

□

1.31 Hermitian matrices

Hermitian matrices have very nice properties. By definition (1.34), a hermitian matrix A is square and unchanged by hermitian conjugation $A^\dagger = A$.

Since it is square, the results of section 1.28 ensure that an $n \times n$ hermitian matrix A has n eigenvectors $|k\rangle$ with eigenvalues a_k

$$A|k\rangle = a_k|k\rangle. \quad (1.340)$$

In fact, all its eigenvalues are real. To see why, we take the adjoint

$$\langle k|A^\dagger = a_k^*\langle k| \quad (1.341)$$

and use the property $A^\dagger = A$ to find

$$\langle k|A^\dagger = \langle k|A = a_k^*\langle k|. \quad (1.342)$$

We now form the inner product of both sides of this equation with the ket $|k\rangle$ and use the eigenvalue equation (1.340) to get

$$\langle k|A|k\rangle = a_k\langle k|k\rangle = a_k^*\langle k|k\rangle \quad (1.343)$$

which (since $\langle k|k\rangle > 0$) tells us that the eigenvalues are real

$$a_k^* = a_k. \quad (1.344)$$

Since $A^\dagger = A$, the matrix elements of A between two of its eigenvectors satisfy

$$a_m^*\langle m|k\rangle = (a_m\langle k|m\rangle)^* = \langle k|A|m\rangle^* = \langle m|A^\dagger|k\rangle = \langle m|A|k\rangle = a_k\langle m|k\rangle \quad (1.345)$$

which implies that

$$(a_m^* - a_k)\langle m|k\rangle = 0. \quad (1.346)$$

But by (1.344), the eigenvalues a_m are real, and so we have

$$(a_m - a_k)\langle m|k\rangle = 0 \quad (1.347)$$

which tells us that when the eigenvalues are different, the eigenvectors are orthogonal. In the absence of a symmetry, the eigenvalues are usually different and the eigenvectors mutually orthogonal.

When two or more eigenvectors $|k_\alpha\rangle$ of a hermitian matrix have the same eigenvalue a_k , their eigenvalues are said to be **degenerate**. In this case, any linear combination of the degenerate eigenvectors also will be an eigenvector with the same eigenvalue a_k

$$A \left(\sum_{\alpha \in D} c_\alpha |k_\alpha\rangle \right) = a_k \left(\sum_{\alpha \in D} c_\alpha |k_\alpha\rangle \right) \quad (1.348)$$

where D is the set of labels α of the eigenvectors with the same eigenvalue. If the degenerate eigenvectors $|k_\alpha\rangle$ are linearly independent, then we may

use the Gram-Schmidt procedure (1.120–1.130) to choose the coefficients c_α so as to construct degenerate eigenvectors that are orthogonal to each other and to the nondegenerate eigenvectors. We then may normalize these mutually orthogonal eigenvectors.

But two related questions arise: Are the degenerate eigenvectors $|k_\alpha\rangle$ linearly independent? And if so, what orthonormal linear combinations of them should we choose for a given physical problem? Let's consider the second question first.

We know that unitary transformations preserve the orthonormality of a basis (section 1.17). Any unitary transformation that commutes with a matrix A

$$[A, U] = 0 \quad (1.349)$$

represents a symmetry of A and maps each set of orthonormal degenerate eigenvectors of A into another set of orthonormal degenerate eigenvectors of A with the same eigenvalue because

$$AU|k_\alpha\rangle = UA|k_\alpha\rangle = a_k U|k_\alpha\rangle. \quad (1.350)$$

So there's a huge spectrum of choices for the orthonormal degenerate eigenvectors of A with the same eigenvalue. What is the right set for a given physical problem?

A sensible way to proceed is to add to the matrix A a second hermitian matrix B multiplied by a tiny, real scale factor ϵ

$$A(\epsilon) = A + \epsilon B. \quad (1.351)$$

The matrix B must completely break whatever symmetry led to the degeneracy in the eigenvalues of A . Ideally, the matrix B should be one that represents a modification of A that is physically plausible and relevant to the problem at hand. The hermitian matrix $A(\epsilon)$ then will have n different eigenvalues $a_k(\epsilon)$ and n orthonormal nondegenerate eigenvectors

$$A(\epsilon)|k_\beta, \epsilon\rangle = a_{k_\beta}(\epsilon)|k_\beta, \epsilon\rangle. \quad (1.352)$$

These eigenvectors $|k_\beta, \epsilon\rangle$ of $A(\epsilon)$ are orthogonal to each other

$$\langle k_\beta, \epsilon | k_{\beta'}, \epsilon \rangle = \delta_{\beta, \beta'} \quad (1.353)$$

and to the eigenvectors of $A(\epsilon)$ with other eigenvalues, and they remain so as we take the limit

$$|k_\beta\rangle = \lim_{\epsilon \rightarrow 0} |k_\beta, \epsilon\rangle. \quad (1.354)$$

We may choose them as the orthogonal degenerate eigenvectors of A . Since

one can always find a crooked hermitian matrix B that breaks any particular symmetry, it follows that every $n \times n$ hermitian matrix A has n orthonormal eigenvectors that are complete in the vector space in which A acts. (Any n linearly independent vectors span their n -dimensional vector space, as explained in section 1.10.)

Now let's return to the first question and show by a different argument that an $n \times n$ hermitian matrix has n orthogonal eigenvectors. To do this, we first note that the space $S_{\perp,k}$ of vectors $|y\rangle$ orthogonal to an eigenvector $|k\rangle$ of a hermitian operator A

$$A|k\rangle = a_k|k\rangle \quad (1.355)$$

is **invariant** under the action of A , that is, $\langle k|y\rangle = 0$ implies

$$\langle k|A|y\rangle = a_k\langle k|y\rangle = 0. \quad (1.356)$$

Thus if the vector $|y\rangle$ is in the space $S_{\perp,k}$ of vectors orthogonal to an eigenvector $|k\rangle$ of a hermitian operator A , then the vector $A|y\rangle$ also is in the space $S_{\perp,k}$. This space is invariant under the action of A .

Now a hermitian operator A acting on an n -dimensional vector space S is represented by an $n \times n$ hermitian matrix, and so it has at least one eigenvector $|1\rangle$. The subspace $S_{\perp,1}$ of S consisting of all vectors orthogonal to $|1\rangle$ is an $(n-1)$ -dimensional vector space S_{n-1} that is invariant under the action of A . On this space S_{n-1} , the operator A is represented by an $(n-1) \times (n-1)$ hermitian matrix A_{n-1} . This matrix has at least one eigenvector $|2\rangle$. The subspace $S_{\perp,2}$ of S_{n-1} consisting of all vectors orthogonal to $|2\rangle$ is an $(n-2)$ -dimensional vector space S_{n-2} that is invariant under the action of A . On S_{n-2} , the operator A is represented by an $(n-2) \times (n-2)$ hermitian matrix A_{n-2} which has at least one eigenvector $|3\rangle$. By construction, the vectors $|1\rangle$, $|2\rangle$, and $|3\rangle$ are mutually orthogonal. Continuing in this way, we see that A has n orthogonal eigenvectors $|k\rangle$ for $k = 1, 2, \dots, n$. Thus **hermitian matrices are nondefective**.

The n orthogonal eigenvectors $|k\rangle$ of an $n \times n$ matrix A can be normalized and used to write the $n \times n$ identity operator I as

$$I = \sum_{k=1}^n |k\rangle\langle k|. \quad (1.357)$$

On multiplying from the left by the matrix A , we find

$$A = AI = A \sum_{k=1}^n |k\rangle\langle k| = \sum_{k=1}^n a_k |k\rangle\langle k| \quad (1.358)$$

which is the diagonal form of the hermitian matrix A . This expansion of A as a sum over outer products of its eigenstates multiplied by their eigenvalues exhibits the possible values a_k of the physical quantity represented by the matrix A when selective, nondestructive measurements $|k\rangle\langle k|$ of the quantity A are made.

The hermitian matrix A is diagonal in the basis of its eigenstates $|k\rangle$

$$A_{kj} = \langle k|A|j\rangle = a_k\delta_{kj}. \quad (1.359)$$

But in any other basis $|\alpha_k\rangle$, the matrix A appears as

$$A_{k\ell} = \langle \alpha_k|A|\alpha_\ell\rangle = \sum_{n=1}^n \langle \alpha_k|n\rangle a_n \langle n|\alpha_\ell\rangle. \quad (1.360)$$

The unitary matrix $U_{kn} = \langle \alpha_k|n\rangle$ relates the matrix $A_{k\ell}$ in an arbitrary basis to its diagonal form $A^{(d)} = U^\dagger A U$ which is the diagonal matrix $A_{nm}^{(d)} = \langle n|A|m\rangle = a_n \delta_{nm}$. An arbitrary $n \times n$ hermitian matrix A can be diagonalized by a unitary transformation.

A matrix H that is **real and symmetric** is hermitian; so is one H' that is **imaginary and antisymmetric**; and so is their sum $H + H'$ which is neither real nor imaginary nor symmetric nor antisymmetric. A real, symmetric matrix R can be diagonalized by an **orthogonal transformation**

$$R = O R^{(d)} O^\top \quad (1.361)$$

in which the matrix O is a real unitary matrix, i.e., an orthogonal matrix (1.193).

Example 1.54 (The Seesaw Mechanism) Suppose we wish to find the eigenvalues of the real, symmetric mass matrix

$$\mathcal{M} = \begin{pmatrix} 0 & m \\ m & M \end{pmatrix} \quad (1.362)$$

in which m is an ordinary mass and M is a huge mass. The eigenvalues μ of this hermitian mass matrix satisfy $\det(\mathcal{M} - \mu I) = \mu(\mu - M) - m^2 = 0$ with solutions $\mu_\pm = \left(M \pm \sqrt{M^2 + 4m^2}\right)/2$. The larger mass $\mu_+ \approx M + m^2/M$ is approximately the huge mass M and the smaller mass $\mu_- \approx -m^2/M$ is tiny. The physical mass of a fermion is the absolute value of its mass parameter, here m^2/M .

The product of the two eigenvalues is the constant $\mu_+\mu_- = \det \mathcal{M} = -m^2$ so as μ_- goes down, μ_+ must go up. Minkowski, Yanagida, and Gell-Mann, Ramond, and Slansky invented this “**seesaw**” mechanism as an explanation

of why neutrinos have such small masses, less than 1 eV/ c^2 . If $mc^2 = 10$ MeV, and $\mu_-c^2 \approx 0.01$ eV, which is a plausible light-neutrino mass, then the rest energy of the huge mass would be $Mc^2 = 10^7$ GeV suggesting new physics at that scale. But if we set $mc^2 = 0.28$ MeV and use $m_\nu = 0.45$ eV as an average neutrino mass, then the big mass is only $Mc^2 = 173$ GeV, the mass of the top. Also, the small masses of the neutrinos may be related to the weakness of their interactions. \square

If we return to the orthogonal transformation (1.361) and multiply column ℓ of the matrix O and row ℓ of the matrix O^\top by $\sqrt{|R_\ell^{(d)}|}$, then we arrive at the **congruency transformation** of Sylvester's theorem

$$R = C \hat{R}^{(d)} C^\top \quad (1.363)$$

in which the diagonal entries $\hat{R}_\ell^{(d)}$ are either ± 1 or 0 because the matrices $C_{k\ell} = \sqrt{|R_\ell^{(d)}|} O_{k\ell}$ and C^\top have absorbed the factors $|R_\ell^{(d)}|$.

Example 1.55 (Principle of equivalence) If G is a real, symmetric 4×4 matrix then there's a real 4×4 matrix $D = C^{\top-1}$ such that

$$G_d = D^\top G D = \begin{pmatrix} g_1 & 0 & 0 & 0 \\ 0 & g_2 & 0 & 0 \\ 0 & 0 & g_3 & 0 \\ 0 & 0 & 0 & g_4 \end{pmatrix} \quad (1.364)$$

in which the diagonal entries g_i are ± 1 or 0. Thus there's a real 4×4 matrix D that casts any real symmetric metric g_{ik} of spacetime with three positive and one negative eigenvalues into the diagonal metric $\eta_{j\ell}$ of flat spacetime by the congruence

$$g_d = D^\top g D = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \eta \quad (1.365)$$

at any given point x of spacetime. Usually one needs different D 's at different points of spacetime. The principle of equivalence (section 13.25) says that in the new free-fall coordinates, all physical laws take the same form as in special relativity without acceleration or gravitation in a suitably small region of spacetime about the point x . \square

1.32 Normal matrices

The largest set of matrices that can be diagonalized by a unitary transformation is the set of **normal** matrices. These are square matrices that commute with their adjoints

$$[V, V^\dagger] = VV^\dagger - V^\dagger V = 0. \quad (1.366)$$

This broad class of matrices includes not only hermitian matrices but also unitary matrices since

$$[U, U^\dagger] = UU^\dagger - U^\dagger U = I - I = 0. \quad (1.367)$$

A matrix $V = U^\dagger V^{(d)} U$ that can be diagonalized by a unitary transformation U commutes with its adjoint $V^\dagger = U^\dagger V^{(d)*} U$ and so is normal because the commutator of any two diagonal matrices vanishes

$$[V, V^\dagger] = [U^\dagger V^{(d)} U, U^\dagger V^{(d)*} U] = U^\dagger [V^{(d)}, V^{(d)*}] U = 0. \quad (1.368)$$

To see why a normal matrix can be diagonalized by a unitary transformation, we consider an $n \times n$ normal matrix V which since it is square has n eigenvectors $|k\rangle$ with eigenvalues v_k

$$(V - v_k I) |k\rangle = 0 \quad (1.369)$$

(section 1.28). The square of the norm (1.89) of this vector must vanish

$$\| (V - v_k I) |k\rangle \|^2 = \langle k | (V - v_k I)^\dagger (V - v_k I) |k\rangle = 0. \quad (1.370)$$

But since V is normal, we also have

$$\langle k | (V - v_k I) (V - v_k I)^\dagger |k\rangle = 0. \quad (1.371)$$

So the square of the norm of the vector $(V^\dagger - v_k^* I) |k\rangle = (V - v_k I)^\dagger |k\rangle$ also vanishes $\| (V^\dagger - v_k^* I) |k\rangle \|^2 = 0$ which tells us that $|k\rangle$ also is an eigenvector of V^\dagger with eigenvalue v_k^*

$$V^\dagger |k\rangle = v_k^* |k\rangle \quad \text{and so} \quad \langle k | V = v_k \langle k|. \quad (1.372)$$

If now $|m\rangle$ is an eigenvector of V with eigenvalue v_m

$$V |m\rangle = v_m |m\rangle \quad (1.373)$$

then

$$\langle k | V |m\rangle = v_m \langle k | m\rangle \quad (1.374)$$

and also by (1.372)

$$\langle k | V |m\rangle = v_k \langle k | m\rangle. \quad (1.375)$$

Subtracting (1.374) from (1.375), we get

$$(v_k - v_m) \langle k|m \rangle = 0 \quad (1.376)$$

which shows that **any two eigenvectors of a normal matrix V with different eigenvalues are orthogonal.**

To see that a normal $n \times n$ matrix V has n orthogonal eigenvectors, we first note that if $|y\rangle$ is any vector that is orthogonal to any eigenvector $|k\rangle$ of the matrix V , that is both $\langle k|y\rangle = 0$ and $V|k\rangle = v_k|k\rangle$, then the property (1.372) implies that

$$\langle k|V|y\rangle = v_k \langle k|y\rangle = 0. \quad (1.377)$$

Thus the space of vectors orthogonal to an eigenvector of a normal matrix V is invariant under the action of V . The argument following the analogous equation (1.356) applies also to normal matrices and shows that **every $n \times n$ normal matrix has n orthonormal eigenvectors.** It follows then from the argument of equations (1.357–1.360) that every $n \times n$ normal matrix V can be diagonalized by an $n \times n$ unitary matrix U

$$V = UV^{(d)}U^\dagger \quad (1.378)$$

whose k th column $U_{\ell k} = \langle \alpha_\ell | k \rangle$ is the eigenvector $|k\rangle$ in the arbitrary basis $|\alpha_\ell\rangle$ of the matrix $V_{m\ell} = \langle \alpha_m | V | \alpha_\ell \rangle$ as in (1.360).

Since the eigenstates $|k\rangle$ of a normal matrix V

$$V|k\rangle = v_k|k\rangle \quad (1.379)$$

are complete and orthonormal, we can write the identity operator I as

$$I = \sum_{k=1}^n |k\rangle \langle k|. \quad (1.380)$$

The product VI is V itself, so

$$V = VI = V \sum_{k=1}^n |k\rangle \langle k| = \sum_{k=1}^n v_k |k\rangle \langle k|. \quad (1.381)$$

It follows therefore that if f is a function, then $f(V)$ is

$$f(V) = \sum_{k=1}^n f(v_k) |k\rangle \langle k| \quad (1.382)$$

which is simpler than the corresponding formula (1.315) for an arbitrary nondefective matrix. This is a good way to think about functions of normal matrices.

Example 1.56 (Time-evolution operator) How do we handle the operator $\exp(-iHt/\hbar)$ that translates states in time by t ? The hamiltonian H is hermitian and so is normal. Its orthonormal eigenstates $|k\rangle$ have energy E_k

$$H|k\rangle = E_k|k\rangle. \quad (1.383)$$

So we apply (1.382) with $V \rightarrow H$ and get

$$e^{-iHt/\hbar} = \sum_{k=1}^n e^{-iE_k t/\hbar} |k\rangle\langle k| \quad (1.384)$$

which lets us compute the time evolution of any state $|\psi\rangle$ as

$$e^{-iHt/\hbar}|\psi\rangle = \sum_{k=1}^n e^{-iE_k t/\hbar} |k\rangle\langle k|\psi\rangle \quad (1.385)$$

if we know the eigenstates $|k\rangle$ and eigenvalues E_k of the hamiltonian H . \square

The determinant $|V|$ of a normal matrix V satisfies the identities

$$|V| = \exp[\text{Tr}(\ln V)], \quad \ln |V| = \text{Tr}(\ln V), \quad \text{and} \quad \delta \ln |V| = \text{Tr}(V^{-1}\delta V). \quad (1.386)$$

1.33 Compatible normal matrices

Two normal matrices A and B that **commute**

$$[A, B] \equiv AB - BA = 0 \quad (1.387)$$

are said to be **compatible**. Since these operators are normal, they have complete sets of orthonormal eigenvectors. If $|u\rangle$ is an eigenvector of A with eigenvalue z , then so is $B|u\rangle$ since

$$AB|u\rangle = BA|u\rangle = Bz|u\rangle = zB|u\rangle. \quad (1.388)$$

We have seen that any normal matrix A can be written as a sum (1.34) of outer products

$$A = \sum_{k=1}^n |a_k\rangle a_k \langle a_k| \quad (1.389)$$

of its orthonormal eigenvectors $|a_k\rangle$ which are complete in the n -dimensional vector space \mathcal{S} on which A acts. Suppose now that the eigenvalues a_k of A are nondegenerate, and that B is another normal matrix acting on \mathcal{S} and that the matrices A and B are compatible. Then in the basis provided by

the eigenvectors $|a_k\rangle$ of the matrix A , the the normal matrix A obeys the relation (1.372) $\langle a_\ell|A = a_\ell\langle a_\ell|$, and so the matrix B must satisfy

$$0 = \langle a_\ell|AB - BA|a_k\rangle = (a_\ell - a_k) \langle a_\ell|B|a_k\rangle \quad (1.390)$$

which says that $\langle a_\ell|B|a_k\rangle$ is zero unless $a_\ell = a_k$. Thus if the eigenvalues a_ℓ of the operator A are nondegenerate, then the operator B is diagonal

$$B = IBI = \sum_{\ell=1}^n |a_\ell\rangle\langle a_\ell|B \sum_{k=1}^n |a_k\rangle\langle a_k| = \sum_{\ell=1}^n |a_\ell\rangle\langle a_\ell|B|a_\ell\rangle\langle a_\ell| \quad (1.391)$$

in the $|a_\ell\rangle$ basis. Moreover B maps each eigenket $|a_k\rangle$ of A into a multiple of itself

$$B|a_k\rangle = \sum_{\ell=1}^n |a_\ell\rangle\langle a_\ell|B|a_\ell\rangle\langle a_\ell|a_k\rangle = \sum_{\ell=1}^n |a_\ell\rangle\langle a_\ell|B|a_\ell\rangle\delta_{\ell k} = \langle a_k|B|a_k\rangle|a_k\rangle \quad (1.392)$$

which shows that each eigenvector $|a_k\rangle$ of the matrix A also is an eigenvector of the matrix B with eigenvalue $\langle a_k|B|a_k\rangle$. Thus **two compatible normal matrices can be simultaneously diagonalized** if one of them has nondegenerate eigenvalues.

If A 's eigenvalues a_ℓ are degenerate, each eigenvalue a_ℓ may have d_ℓ orthonormal eigenvectors $|a_\ell, k\rangle$ for $k = 1, \dots, d_\ell$. In this case, the matrix elements $\langle a_\ell, k|B|a_m, k'\rangle$ of B are zero unless the eigenvalues are the same, $a_\ell = a_m$. The matrix representing the operator B in this basis consists of square, $d_\ell \times d_\ell$, normal submatrices $\langle a_\ell, k|B|a_\ell, k'\rangle$ arranged along its main diagonal; it is said to be in **block-diagonal form**. Since each submatrix is a $d_\ell \times d_\ell$, normal matrix, we may find linear combinations $|a_\ell, b_k\rangle$ of the degenerate eigenvectors $|a_\ell, k\rangle$ that are orthonormal eigenvectors of both compatible operators

$$A|a_\ell, b_k\rangle = a_\ell|a_\ell, b_k\rangle \quad \text{and} \quad B|a_\ell, b_k\rangle = b_k|a_\ell, b_k\rangle. \quad (1.393)$$

Thus one can simultaneously diagonalize any two compatible operators.

The converse also is true: If the operators A and B can be simultaneously diagonalized as in (1.393), then they commute

$$AB|a_\ell, b_k\rangle = Ab_k|a_\ell, b_k\rangle = a_\ell b_k|a_\ell, b_k\rangle = a_\ell B|a_\ell, b_k\rangle = BA|a_\ell, b_k\rangle \quad (1.394)$$

and so are compatible. Normal matrices can be simultaneously diagonalized if and only if they are compatible, i.e., if and only if they commute.

In quantum mechanics, compatible hermitian operators represent physical observables that can be measured simultaneously to arbitrary precision (in principle). A set of compatible hermitian operators A, B, C, \dots is said to be

complete if to every set of eigenvalues a_j, b_k, c_ℓ, \dots there is only a single eigenvector $|a_j, b_k, c_\ell, \dots\rangle$.

Example 1.57 (Compatible Photon Observables) For example, the state of a photon is completely characterized by its momentum and its angular momentum about its direction of motion. For a photon, the momentum operator \mathbf{P} and the dot product $\mathbf{J} \cdot \mathbf{P}$ of the angular momentum \mathbf{J} with the momentum form a complete set of compatible hermitian observables. Incidentally, because its mass is zero, the angular momentum \mathbf{J} of a photon about its direction of motion can have only two values $\pm\hbar$, which correspond to its two possible states of circular polarization. \square

Example 1.58 (Thermal density operator) A **density operator** ρ is the most general description of a quantum-mechanical system. It is hermitian, positive definite, and of unit trace. Since it is hermitian, it can be diagonalized (section 1.31)

$$\rho = \sum_n |n\rangle \langle n| \rho_n \langle n| \tag{1.395}$$

and its eigenvalues $\rho_n = \langle n| \rho |n\rangle$ are real. Each ρ_n is the probability that the system is in the state $|n\rangle$ and so is nonnegative. The unit-trace rule

$$\sum_n \rho_n = 1. \tag{1.396}$$

ensures that these probabilities add up to one—the system is in some state.

The mean value of an operator F is the trace, $\langle F \rangle = \text{Tr}(\rho F)$. So the average energy E is the trace, $E = \langle H \rangle = \text{Tr}(\rho H)$. The **entropy operator** S is the negative logarithm of the density operator multiplied by Boltzmann's constant, $S = -k \ln \rho$, and the mean entropy S is $S = \langle S \rangle = -k \text{Tr}(\rho \ln \rho)$.

A density operator that describes a system in thermal equilibrium at a constant temperature T is time independent and so commutes with the hamiltonian, $[\rho, H] = 0$. Since ρ and H commute, they are compatible operators (1.387), and so they can be simultaneously diagonalized. Each eigenstate $|n\rangle$ of ρ is an eigenstate of H ; its energy E_n is its eigenvalue, $H|n\rangle = E_n|n\rangle$.

If we have no information about the state of the system other than its mean energy E , then we take ρ to be the density operator that maximizes the mean entropy S while respecting the constraints $c_1 = \sum_n \rho_n - 1 = 0$ and $c_2 = \text{Tr}(\rho H) - E = 0$. We introduce two Lagrange multipliers (section 1.26)

and maximize the unconstrained function

$$\begin{aligned} L(\rho, \lambda_1, \lambda_2) &= S - \lambda_1 c_1 - \lambda_2 c_2 & (1.397) \\ &= -k \sum_n \rho_n \ln \rho_n - \lambda_1 \left(\sum_n \rho_n - 1 \right) - \lambda_2 \left(\sum_n \rho_n E_n - E \right) \end{aligned}$$

by setting its derivatives with respect to ρ_n , λ_1 , and λ_2 equal to zero

$$\frac{\partial L}{\partial \rho_n} = -k (\ln \rho_n + 1) - \lambda_1 - \lambda_2 E_n = 0 \quad (1.398)$$

$$\frac{\partial L}{\partial \lambda_1} = \sum_n \rho_n - 1 = 0 \quad (1.399)$$

$$\frac{\partial L}{\partial \lambda_2} = \sum_n \rho_n E_n - E = 0. \quad (1.400)$$

The first (1.398) of these conditions implies that

$$\rho_n = \exp[-(\lambda_1 + \lambda_2 E_n + k)/k]. \quad (1.401)$$

We satisfy the second condition (1.399) by choosing λ_1 so that

$$\rho_n = \frac{\exp(-\lambda_2 E_n/k)}{\sum_n \exp(-\lambda_2 E_n/k)}. \quad (1.402)$$

Setting $\lambda_2 = 1/T$, we define the temperature T so that ρ satisfies the third condition (1.400). Its eigenvalue ρ_n then is

$$\rho_n = \frac{\exp(-E_n/kT)}{\sum_n \exp(-E_n/kT)}. \quad (1.403)$$

In terms of the inverse temperature $\beta \equiv 1/(kT)$, the density operator is

$$\rho = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})} \quad (1.404)$$

which is the **Boltzmann distribution**, also called the **canonical ensemble**. \square

Example 1.59 (Grand canonical ensemble) Lagrange's function for the density operator of a system of maximum entropy $S = -k\text{Tr}(\rho \ln \rho)$ given a fixed mean energy $E = \text{Tr}(\rho H)$ and a fixed mean number of particles

$\langle N \rangle = \text{Tr}(\rho N)$, in which N is the number operator $N|n\rangle = N_n|n\rangle$, is

$$\begin{aligned} L(\rho, \lambda_1, \lambda_2, \lambda_3) = & -k \sum_n \rho_n \ln \rho_n - \lambda_1 \left(\sum_n \rho_n - 1 \right) \\ & - \lambda_2 \left(\sum_n \rho_n E_n - E \right) - \lambda_3 \left(\sum_n \rho_n N_n - \langle N \rangle \right). \end{aligned} \quad (1.405)$$

Setting the partial derivative of L with respect to ρ_n

$$\frac{\partial L}{\partial \rho_n} = -k (\ln \rho_n + 1) - \lambda_1 - \lambda_2 E_n - \lambda_3 N_n = 0 \quad (1.406)$$

as well as the partial derivatives of L with respect to the three Lagrange multipliers λ_i equal to zero, we get

$$\rho = \frac{e^{-\beta(H-\mu N)}}{\text{Tr}(e^{-\beta(H-\mu N)})} \quad (1.407)$$

in which μ is the **chemical potential**. □

Example 1.60 (Anticommuting operators) Fermion operators like $\alpha a + \beta a^\dagger$ and $\gamma b + \delta b^\dagger$ that anticommute, $\{\alpha a + \beta a^\dagger, \gamma b + \delta b^\dagger\} = 0$, are not compatible. Each has complex eigenvalues and eigenvectors, but no complex vector is an eigenvector of both $\alpha a + \beta a^\dagger$ and $\gamma b + \delta b^\dagger$. For that one needs Grassmann eigenvalues and eigenvectors Section 20.12. □

1.34 Singular-value decompositions

Every complex $m \times n$ rectangular matrix A is the product of an $m \times m$ unitary matrix U , an $m \times n$ rectangular matrix Σ that is zero except on its main diagonal on which A 's nonnegative singular values S_k are arranged, and an $n \times n$ unitary matrix V^\dagger

$$A = U \Sigma V^\dagger \quad \text{or} \quad A_{ik} = \sum_{\ell=1}^{\min(m,n)} U_{i\ell} S_\ell V_{\ell k}^\dagger. \quad (1.408)$$

This singular-value decomposition is a key theorem of matrix algebra.

Suppose A is a linear operator that maps vectors in an n -dimensional vector space V_n into vectors in an m -dimensional vector space V_m . Each of the spaces V_n and V_m has infinitely many orthonormal bases $\{|a_j\rangle \in V_n\}$

and $\{|b_k\rangle \in V_m\}$ labeled by parameters a and b . Each pair of bases provides a resolution of the identity operator I_n for V_n and I_m for V_m

$$I_n = \sum_{j=1}^n |a_j\rangle\langle a_j| \quad \text{and} \quad I_m = \sum_{k=1}^m |b_k\rangle\langle b_k| \quad (1.409)$$

and lets us write linear operator A as

$$A = I_m A I_n = \sum_{k=1}^m \sum_{j=1}^n |b_k\rangle\langle b_k| A |a_j\rangle\langle a_j| \quad (1.410)$$

in which the $\langle b_k|A|a_j\rangle$ are the elements of a complex $m \times n$ matrix.

The singular-value decomposition of the linear operator A is a choice of two special bases $|a_j\rangle$ and $|b_j\rangle$ that make $\langle b_k|A|a_j\rangle = S_j \delta_{kj}$ and so express A as

$$A = \sum_j |b_j\rangle S_j \langle a_j| \quad (1.411)$$

in which the sum is over the singular values S_j , which are positive.

The kets $|a_j\rangle$ of the special basis of the domain space V_n are the normalized eigenstates of the hermitian operator $A^\dagger A$

$$A^\dagger A |a_j\rangle = e_j |a_j\rangle. \quad (1.412)$$

These states $|a_j\rangle$ are orthogonal because $A^\dagger A$ is hermitian. The eigenvalue e_j is the squared length of the ket $A|a_j\rangle$ and so is positive or zero

$$\langle a_j|A^\dagger A|a_j\rangle = e_j \langle a_j|a_j\rangle = e_j \geq 0. \quad (1.413)$$

The singular values are the square roots of these eigenvalues

$$S_j = \sqrt{e_j} = \sqrt{\langle a_j|A^\dagger A|a_j\rangle}. \quad (1.414)$$

The kets $|b_j\rangle$ of the special basis of the image space V_m are the suitably normalized images of the eigenstates $|a_j\rangle$ that have positive singular values $S_j > 0$

$$|b_j\rangle = \frac{A|a_j\rangle}{S_j}. \quad (1.415)$$

If $S_j = 0$, then there is no ket $|b_j\rangle$. The special kets $|b_j\rangle$ are orthonormal

$$\langle b_k|b_j\rangle = \frac{1}{S_k S_j} \langle a_k|A^\dagger A|a_j\rangle = \frac{e_j}{S_k S_j} \langle a_k|a_j\rangle = \frac{e_j}{S_k S_j} \delta_{kj} = \delta_{kj}. \quad (1.416)$$

The number of positive singular values, $S_j > 0$, is at most n . It also is at most m because each nonzero ket $|b_j\rangle$ is an orthonormal vector in the space

V_m which has only m dimensions. So the number of positive singular values, $S_j > 0$, is at most $\min(m, n)$, the smaller of m and n .

The singular-value decomposition of the linear operator A then is the sum

$$A = AI_n = A \sum_{j=1}^n |a_j\rangle\langle a_j| = \sum_{j=1}^n A |a_j\rangle\langle a_j| = \sum_{j, S_j > 0} |b_j\rangle S_j \langle a_j| \quad (1.417)$$

in which at most $\min(m, n)$ of the singular values are positive.

Example 1.61 (Making the matrix from its singular values and eigenstates) Suppose the special bras $|a_j\rangle$ are

$$\langle a_1| = \frac{1}{\sqrt{2}} (1 \ 0 \ 0 \ 1) \quad \text{and} \quad \langle a_2| = \frac{1}{\sqrt{2}} (0 \ 1 \ 1 \ 0) \quad (1.418)$$

and the kets $|b_j\rangle$ are

$$|b_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad \text{and} \quad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \quad (1.419)$$

If the singular values are $S_1 = 3$, $S_2 = 2$, and $S_3 = 0$, then the matrix A is

$$\begin{aligned} A &= \frac{3}{2} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} (1 \ 0 \ 0 \ 1) + \sqrt{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0 \ 1 \ 1 \ 0) \\ &= \begin{pmatrix} \frac{3}{2} & 0 & 0 & \frac{3}{2} \\ 0 & \sqrt{2} & \sqrt{2} & 0 \\ \frac{3}{2} & 0 & 0 & \frac{3}{2} \end{pmatrix}. \end{aligned} \quad (1.420)$$

□

In terms of any two bases, $|k\rangle$ for $k = 1, \dots, m$ for the space V_m and $|\ell\rangle$ for $\ell = 1, \dots, n$ for the space V_n , and their identity operators

$$I_m = \sum_{k=1}^m |k\rangle\langle k| \quad \text{and} \quad I_n = \sum_{\ell=1}^n |\ell\rangle\langle \ell| \quad (1.421)$$

the singular-value decomposition of the linear operator A is

$$\begin{aligned} A &= \sum_{k=1}^m |k\rangle\langle k| A \sum_{\ell=1}^n |\ell\rangle\langle \ell| = \sum_{k=1}^m \sum_{j=1}^n \sum_{\ell=1}^n |k\rangle\langle k| b_j \rangle S_j \langle a_j| \ell \rangle \langle \ell| \\ &= \sum_{k=1}^m \sum_{i=1}^m \sum_{j=1}^n \sum_{\ell=1}^n |k\rangle\langle k| b_i \rangle S_i \delta_{ij} \langle a_j| \ell \rangle \langle \ell| = U \Sigma V^\dagger. \end{aligned} \quad (1.422)$$

In this expansion, the k, i matrix element of the $m \times m$ unitary matrix U is $U_{ki} = \langle k|b_i\rangle$, the i, j element of the $m \times n$ matrix Σ is $\Sigma_{ij} = S_j \delta_{ij}$, and the j, ℓ matrix element of the $n \times n$ unitary matrix V^\dagger is $V_{j\ell}^\dagger = \langle a_j|\ell\rangle$. Thus $V_{\ell j}^* = \langle a_j|\ell\rangle$, and so $V_{\ell j} = \langle a_j|\ell\rangle^* = \langle \ell|a_j\rangle$.

The vectors $|b_j\rangle$ and $|a_j\rangle$ respectively are the left and right singular vectors. Incidentally, the singular-value decomposition (1.417) shows that the left singular vectors $|b_j\rangle$ are the eigenvectors of AA^\dagger

$$\begin{aligned} AA^\dagger &= \sum_{j=1}^n |b_j\rangle S_j \langle a_j| \sum_{k=1}^n |a_k\rangle S_k \langle b_k| = \sum_{j,k=1}^n |b_j\rangle S_j \langle a_j|a_k\rangle S_k \langle b_k| \\ &= \sum_{j,k=1}^n |b_j\rangle S_j \delta_{jk} S_k \langle b_k| = \sum_{j=1}^n |b_j\rangle S_j^2 \langle b_j| \end{aligned} \quad (1.423)$$

just as (1.412) the right singular vectors $|a_j\rangle$ are the eigenvectors of $A^\dagger A$.

The kets $|a_j\rangle$ whose singular values vanish, $S_j = 0$, are annihilated by A , $A|a_j\rangle = 0$, and so span the **null space** or **kernel** of the linear operator A .

Example 1.62 (Singular-Value Decomposition of a 2×1 Matrix) If G is the 2×1 matrix

$$G = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (1.424)$$

then its singular value decomposition as given by the Matlab command `[U,S,V] = svd(G)` is

$$G = USV^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{pmatrix} (1). \quad (1.425)$$

□

Example 1.63 (Singular-Value Decomposition of a 2×3 Matrix) If A is

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (1.426)$$

then the positive hermitian matrix $A^\dagger A$ is

$$A^\dagger A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad (1.427)$$

The normalized eigenvectors and eigenvalues of $A^\dagger A$ are

$$|a_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad |a_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |a_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \quad (1.428)$$

and their eigenvalues are $e_1 = 2$, $e_2 = 1$, and $e_3 = 0$. The third eigenvalue e_3 had to vanish because A is a 3×2 matrix.

The vector $A|a_1\rangle$ (as a row vector) is $(0, \sqrt{2})$, and its norm is $\sqrt{2}$, so the normalized vector is $|b_1\rangle = (0, 1)$. Similarly, the vector $|b_2\rangle$ is $A|a_2\rangle = (1, 0)$. The SVD of A then is

$$A = \sum_{n=1}^2 |b_j\rangle S_j \langle a_j| = U \Sigma V^\dagger \quad (1.429)$$

where $S_n = \sqrt{e_n}$. The unitary matrices are $U_{k,n} = \langle k|b_n\rangle$ and $V_{\ell,j} = \langle \ell|a_j\rangle$ are

$$U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (1.430)$$

and the diagonal matrix Σ is

$$\Sigma = \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \quad (1.431)$$

So finally the SVD of $A = U \Sigma V^\dagger$ is

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ -1 & 0 & 1 \end{pmatrix}. \quad (1.432)$$

The null space or kernel of A is the set of vectors that are real multiples $c|a_3\rangle$ of the eigenvector $|a_3\rangle$ which has a zero eigenvalue, $e_3 = 0$. It is the third column of the matrix V displayed in (1.430). \square

Example 1.64 (Matlab's singular-value decomposition) Matlab's command `[U,S,V] = svd(X)` performs the singular-value decomposition (SVD) of the matrix X . For instance

```
>> X = rand(3,3) + i*rand(3,3)
```

```

      0.6551 + 0.2551i    0.4984 + 0.8909i    0.5853 + 0.1386i
X = 0.1626 + 0.5060i    0.9597 + 0.9593i    0.2238 + 0.1493i
      0.1190 + 0.6991i    0.3404 + 0.5472i    0.7513 + 0.2575i
>> [U,S,V] = svd(X)
```

$$\begin{aligned}
 & \begin{array}{ccc}
 -0.3689 - 0.4587i & 0.4056 - 0.2075i & 0.4362 - 0.5055i \\
 -0.3766 - 0.5002i & -0.5792 - 0.2810i & 0.0646 + 0.4351i \\
 -0.2178 - 0.4626i & 0.1142 + 0.6041i & -0.5938 - 0.0901i
 \end{array} \\
 \\
 \mathbf{S} = & \begin{array}{ccc}
 2.2335 & 0 & 0 \\
 0 & 0.7172 & 0 \\
 0 & 0 & 0.3742
 \end{array} \\
 \\
 \mathbf{V} = & \begin{array}{ccc}
 -0.4577 & 0.5749 & 0.6783 \\
 -0.7885 - 0.0255i & -0.6118 - 0.0497i & -0.0135 + 0.0249i \\
 -0.3229 - 0.2527i & 0.3881 + 0.3769i & -0.5469 - 0.4900i .
 \end{array}
 \end{aligned}$$

The singular values are 2.2335, 0.7172, and 0.3742. \square

We may use the SVD to solve, when possible, the matrix equation

$$A|x\rangle = |y\rangle \quad (1.433)$$

for the n -dimensional vector $|x\rangle$ in terms of the m -dimensional vector $|y\rangle$ and the $m \times n$ matrix A . Using the SVD expansion (1.417), we have

$$\sum_{j=1}^{\min(m,n)} |b_j\rangle S_j \langle a_j|x\rangle = |y\rangle. \quad (1.434)$$

The orthonormality (1.416) of the vectors $|b_j\rangle$ then tells us that

$$S_j \langle a_j|x\rangle = \langle b_j|y\rangle. \quad (1.435)$$

If the singular value is positive, $S_j > 0$, then we may divide by it to get $\langle a_j|x\rangle = \langle b_j|y\rangle/S_j$ and so find the solution

$$|x\rangle = \sum_{j=1}^{\min(m,n)} \frac{\langle b_j|y\rangle}{S_j} |a_j\rangle. \quad (1.436)$$

But this solution is not always available or unique.

For instance, if for some ℓ the inner product $\langle b_\ell|y\rangle \neq 0$ while the singular value $S_\ell = 0$, then there is no solution to equation (1.433). This problem occurs when $m > n$ because there are at most $n < m$ nonzero singular values.

Example 1.65 Suppose A is the 3×2 matrix

$$A = \begin{pmatrix} r_1 & p_1 \\ r_2 & p_2 \\ r_3 & p_3 \end{pmatrix} \quad (1.437)$$

and the vector $|y\rangle$ is the cross-product $|y\rangle = \mathbf{L} = \mathbf{r} \times \mathbf{p}$. Then no solution $|x\rangle$ exists to the equation $A|x\rangle = |y\rangle$ (unless \mathbf{r} and \mathbf{p} are parallel) because $A|x\rangle$ is a linear combination of the vectors \mathbf{r} and \mathbf{p} while $|y\rangle = \mathbf{L}$ is perpendicular to both \mathbf{r} and \mathbf{p} . \square

Even when the matrix A is square, the equation (1.433) sometimes has no solutions. For instance, if A is a square defective matrix (section 1.28), then $A|x\rangle = |y\rangle$ will fail to have a solution when the vector $|y\rangle$ lies outside the space spanned by the linearly dependent eigenvectors of the matrix A .

And when $n > m$, as in for instance

$$\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \quad (1.438)$$

the solution (1.436) is never unique, for we may add to it any linear combination of the vectors $|a_j\rangle$ that have zero as their singular values

$$|x\rangle = \sum_{j=1}^{\min(m,n)} \frac{\langle b_j|y\rangle}{S_n} |a_j\rangle + \sum_{j,S_j=0} x_j |a_j\rangle \quad (1.439)$$

of which there are at least $n - m$.

Example 1.66 (CKM matrix) In the standard model, the mass matrices of the u, c, t and d, s, b quarks are 3×3 complex matrices M_u and M_d with singular-value decompositions $M_u = U_u \Sigma_u V_u^\dagger$ and $M_d = U_d \Sigma_d V_d^\dagger$ whose singular-values are the quark masses. The unitary CKM matrix $U_u^\dagger U_d$ (Cabibbo, Kobayashi, Maskawa) describes transitions among the quarks mediated by the W^\pm gauge bosons. By redefining the quark fields, one may make the CKM matrix real, apart from a phase that violates charge-conjugation-parity (CP) symmetry. \square

The adjoint of a complex symmetric matrix M is its complex conjugate, $M^\dagger = M^*$. So by (1.412), its right singular vectors $|n\rangle$ are the eigenstates of M^*M

$$M^*M|n\rangle = S_n^2|n\rangle \quad (1.440)$$

and by (1.423) its left singular vectors $|m_n\rangle$ are the eigenstates of MM^*

$$MM^*|m_n\rangle = (M^*M)^*|m_n\rangle = S_n^2|m_n\rangle. \quad (1.441)$$

Thus its left singular vectors are the complex conjugates of its right singular vectors, $|m_n\rangle = |n\rangle^*$. So in its SVD $M = U\Sigma V^\dagger$, the unitary matrix V is the complex conjugate of the unitary matrix U , and the SVD of M is (Autonne, 1915)

$$M = U\Sigma U^\dagger. \quad (1.442)$$

1.35 Moore-Penrose pseudoinverse

Although a matrix A has an inverse A^{-1} if and only if it is square and has a nonzero determinant, one may use the singular-value decomposition to make a pseudoinverse A^+ for an arbitrary $m \times n$ matrix A . If the singular-value decomposition of the matrix A is

$$A = U\Sigma V^\dagger \quad (1.443)$$

then the Moore-Penrose pseudoinverse is.

$$A^+ = V\Sigma^+ U^\dagger \quad (1.444)$$

in which Σ^+ is the transpose of the matrix Σ with every nonzero entry replaced by its (multiplicative) inverse (and the zeros left as they are). One may show that the pseudoinverse ($A^+ = \text{pinv}(A)$ in Matlab) satisfies the four relations

$$\begin{aligned} AA^+A &= A, & A^+AA^+ &= A^+, \\ (AA^+)^\dagger &= AA^+, & (A^+A)^\dagger &= A^+A \end{aligned} \quad (1.445)$$

and that it is the only matrix that does so. (Eliakim H. Moore 1862–1932, Roger Penrose 1931–)

Suppose that all the singular values of the $m \times n$ matrix A are positive. In this case, if A has more rows than columns, so that $m > n$, then the product A^+A is the $n \times n$ identity matrix I_n

$$A^+A = V^\dagger\Sigma^+\Sigma V = V^\dagger I_n V = I_n \quad (1.446)$$

and AA^+ is an $m \times m$ matrix that is not the identity matrix I_m . If instead A has more columns than rows, so that $n > m$, then AA^+ is the $m \times m$ identity matrix I_m

$$AA^+ = U\Sigma\Sigma^+U^\dagger = UI_mU^\dagger = I_m \quad (1.447)$$

and A^+A is an $n \times n$ matrix that is not the identity matrix I_n . If the matrix A is square with positive singular values, then it has a true inverse A^{-1} which is equal to its pseudoinverse

$$A^{-1} = A^+. \quad (1.448)$$

If the columns of A are linearly independent, then the matrix $A^\dagger A$ has an inverse, and the pseudoinverse is

$$A^+ = (A^\dagger A)^{-1} A^\dagger. \quad (1.449)$$

The solution (1.260) to the complex least-squares method used this pseudoinverse.

If the rows of A are linearly independent, then the matrix AA^\dagger has an inverse, and the pseudoinverse is

$$A^+ = A^\dagger (AA^\dagger)^{-1}. \quad (1.450)$$

If both the rows and the columns of A are linearly independent, then the matrix A has an inverse A^{-1} which is its pseudoinverse

$$A^{-1} = A^+. \quad (1.451)$$

Example 1.67 (The pseudoinverse of a 2×1 matrix) The Matlab command `pinv(G)` gives the pseudoinverse G^+ of the matrix

$$G = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (1.452)$$

with singular-value decomposition (1.425) as

$$G^+ = V\Sigma^+U^\dagger = (1) \begin{pmatrix} 1/\sqrt{2} & 0 \\ 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}. \quad (1.453)$$

□

Example 1.68 (The pseudoinverse of a 2×3 matrix) The pseudoinverse A^+ of the matrix

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (1.454)$$

with singular-value decomposition (1.432) is

$$\begin{aligned} A^+ &= V\Sigma^+U^\dagger \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \\ 0 & 1/2 \end{pmatrix} \end{aligned} \quad (1.455)$$

which satisfies the four conditions (1.445). The product AA^+ gives the 2×2 identity matrix

$$AA^+ = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \\ 0 & 1/2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.456)$$

which is an instance of (1.447). Moreover, the rows of A are linearly independent, and so the simple rule (1.450) works:

$$\begin{aligned} A^+ &= A^\dagger (AA^\dagger)^{-1} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 2 & 0 \end{pmatrix}^{-1} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \\ 0 & 1/2 \end{pmatrix} \end{aligned} \quad (1.457)$$

which is (1.455).

The columns of the matrix A are not linearly independent, however, and so the simple rule (1.449) fails. Thus the product A^+A

$$A^+A = \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (1.458)$$

is not the 3×3 identity matrix which it would be if (1.449) held. \square

1.36 Tensor products and entanglement

Tensor products are used to describe composite systems. The tensor product of a vector space S spanned by n orthonormal kets $|i\rangle$ and a vector space T spanned by m orthonormal kets $|k\rangle$ is a vector space $S \otimes T$ spanned by nm orthonormal kets $|i\rangle \otimes |k\rangle$. The inner product of two such kets $|i\rangle \otimes |k\rangle$ and $|i'\rangle \otimes |k'\rangle$ is

$$\langle i' | \otimes \langle k' | \rangle |i\rangle \otimes |k\rangle = \langle i' | i \rangle \langle k' | k \rangle = \delta_{i',i} \delta_{k',k}. \quad (1.459)$$

Tensor product states are often written without \otimes as $|i\rangle \otimes |k\rangle = |i\rangle |k\rangle = |i, k\rangle$.

An arbitrary vector in the space $S \otimes T$ is of the form

$$|\psi\rangle = \sum_{i=1}^n \sum_{k=1}^m \psi_{i,k} |i\rangle \otimes |k\rangle = \sum_{i=1}^n \sum_{k=1}^m |i, k\rangle \langle i, k|\psi\rangle. \quad (1.460)$$

The inner product of this vector with another vector in the tensor-product space $S \otimes T$

$$|\phi\rangle = \sum_{i=1}^n \sum_{k=1}^m \phi_{i,k} |i\rangle \otimes |k\rangle = \sum_{i=1}^n \sum_{k=1}^m |i, k\rangle \langle i, k|\phi\rangle \quad (1.461)$$

is

$$\langle\phi|\psi\rangle = \sum_{i',i=1}^n \sum_{k',k=1}^m \langle i', k'|i, k\rangle \phi_{i',k'}^* \psi_{i,k} = \sum_{i=1}^n \sum_{k=1}^m \phi_{i,k}^* \psi_{i,k}. \quad (1.462)$$

Vectors $|\phi_S, \chi_T\rangle$ that are tensor products $|\phi_S\rangle \otimes |\chi_T\rangle$ of a vector $|\phi_S\rangle \in S$ and a vector $|\chi_T\rangle \in T$

$$|\phi_S\rangle \otimes |\chi_T\rangle = \left(\sum_{i=1}^n \phi_i |i\rangle \right) \otimes \left(\sum_{k=1}^m \chi_k |k\rangle \right) = \sum_{i=1}^n \sum_{k=1}^m \phi_i \chi_k |i, k\rangle \quad (1.463)$$

are **separable**. States represented by vectors that are not separable are said to be **entangled**. Most states in a tensor-product space $S \otimes T$ are entangled.

If A is an $n \times n$ matrix with elements A_{ij} and B is an $m \times m$ matrix with elements $B_{k\ell}$, then their **tensor product** $C = A \otimes B$ is an $nm \times nm$ matrix with elements $C_{ik,j\ell} = A_{ij} B_{k\ell}$. This tensor-product matrix $A \otimes B$ maps a vector $V_{j\ell}$ into the vector

$$W_{ik} = \sum_{j=1}^n \sum_{\ell=1}^m C_{ik,j\ell} V_{j\ell} = \sum_{j=1}^n \sum_{\ell=1}^m A_{ij} B_{k\ell} V_{j\ell} \quad (1.464)$$

in which the second double index $j\ell$ of C and the second indices of A and B match the double index $j\ell$ of the vector V .

A tensor-product operator is a product of operators that act on different vector spaces. Suppose that an operator A acts on a space S spanned by n kets $|i\rangle$, and that an operator B acts on a space T spanned by m kets $|k\rangle$, and that both operators map vectors into their spaces S and T . Then we may write A as

$$A = I_S A I_S = \sum_{i,j=1}^n |i\rangle \langle i| A |j\rangle \langle j| \quad (1.465)$$

and B as

$$B = I_T B I_T = \sum_{k,s=1}^m |k\rangle \langle k| B |\ell\rangle \langle \ell|. \quad (1.466)$$

Their tensor product $A \otimes B$ is

$$\begin{aligned} A \otimes B &= \sum_{i,j=1}^n \sum_{k,\ell=1}^m |i\rangle \otimes |k\rangle \langle i| A |j\rangle \langle k| B |\ell\rangle \langle j| \otimes \langle \ell| \\ &= \sum_{i,j=1}^n \sum_{k,\ell=1}^m |i,k\rangle \langle i| A |j\rangle \langle k| B |\ell\rangle \langle j,\ell| \psi\rangle. \end{aligned} \quad (1.467)$$

and it acts on the tensor-product vector space $S \otimes T$ which is spanned by the tensor-product kets $|i,k\rangle = |i\rangle |k\rangle = |i\rangle \otimes |k\rangle$ and has dimension nm .

Just as separable states are special, so too tensor-product operators are special cases of the more general linear operator on the space $S \otimes T$

$$D = \sum_{i,j=1}^n \sum_{k,\ell=1}^m |i,k\rangle \langle i,k| D |j,\ell\rangle \langle j,\ell| \quad (1.468)$$

which maps an arbitrary vector (1.460) into the vector

$$D |\psi\rangle = \sum_{i,j=1}^n \sum_{k,\ell=1}^m |i,k\rangle \langle i,k| D |j,\ell\rangle \langle j,\ell| \psi\rangle. \quad (1.469)$$

Example 1.69 (States of the hydrogen atom) Suppose the state $|n,\ell,m\rangle$ is an eigenvector of the hamiltonian H , the square \mathbf{L}^2 of the orbital angular momentum \mathbf{L} , and the third component of the orbital angular momentum L_3 of a hydrogen atom without spin:

$$\begin{aligned} H |n,\ell,m\rangle &= E_n |n,\ell,m\rangle \\ \mathbf{L}^2 |n,\ell,m\rangle &= \hbar^2 \ell(\ell+1) |n,\ell,m\rangle \\ L_3 |n,\ell,m\rangle &= \hbar m |n,\ell,m\rangle. \end{aligned} \quad (1.470)$$

The state $|n,\ell,m\rangle = |n\rangle \otimes |\ell,m\rangle$ is separable. Suppose the states $|\sigma\rangle$ for $\sigma = \pm$ are eigenstates of the third component S_3 of the operator \mathbf{S} that represents the spin of the electron

$$S_3 |\sigma\rangle = \sigma \frac{\hbar}{2} |\sigma\rangle. \quad (1.471)$$

The separable, tensor-product states

$$|n,\ell,m,\sigma\rangle \equiv |n,\ell,m\rangle \otimes |\sigma\rangle \equiv |n,\ell,m\rangle |\sigma\rangle \quad (1.472)$$

represent a hydrogen atom including the spin of its electron. These separable states are eigenvectors of all four operators H , \mathbf{L}^2 , L_3 , and S_3 :

$$\begin{aligned} H|n, \ell, m, \sigma\rangle &= E_n|n, \ell, m, \sigma\rangle & \mathbf{L}^2|n, \ell, m, \sigma\rangle &= \hbar^2\ell(\ell+1)|n, \ell, m, \sigma\rangle \\ L_3|n, \ell, m, \sigma\rangle &= \hbar m|n, \ell, m, \sigma\rangle & S_3|n, \ell, m, \sigma\rangle &= \sigma\frac{1}{2}\hbar|n, \ell, m, \sigma\rangle. \end{aligned} \quad (1.473)$$

Suitable linear combinations of these states are eigenstates of the square \mathbf{J}^2 of the composite angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ as well as of J_3 , L_3 , and S_3 . Many of these states are entangled. \square

Example 1.70 (Adding two spins) The smallest positive value of angular momentum is $\hbar/2$. The spin-one-half angular momentum operators \mathbf{S} are represented by three 2×2 matrices, $S_a = \frac{1}{2}\hbar\sigma_a$, the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.474)$$

which are both hermitian and unitary. They map the basis vectors

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (1.475)$$

to $\sigma_1|\pm\rangle = |\mp\rangle$, $\sigma_2|\pm\rangle = \pm i|\mp\rangle$, and $\sigma_3|\pm\rangle = \pm|\pm\rangle$.

Suppose two spin operators $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$ act on two spin-one-half systems with states $|\pm\rangle_1$ that are eigenstates of $S_3^{(1)}$ and states $|\pm\rangle_2$ that are eigenstates of $S_3^{(2)}$

$$S_3^{(1)}|\pm\rangle_1 = \pm\frac{1}{2}\hbar|\pm\rangle_1 \quad \text{and} \quad S_3^{(2)}|\pm\rangle_2 = \pm\frac{1}{2}\hbar|\pm\rangle_2. \quad (1.476)$$

Then the tensor-product states $|\pm, \pm\rangle = |\pm\rangle_1|\pm\rangle_2 = |\pm\rangle_1 \otimes |\pm\rangle_2$ are eigenstates of both $S_3^{(1)}$ and $S_3^{(2)}$

$$S_3^{(1)}|\pm, s_2\rangle = \pm\frac{1}{2}\hbar|\pm, s_2\rangle \quad \text{and} \quad S_3^{(2)}|s_1, \pm\rangle = \pm\frac{1}{2}\hbar|s_1, \pm\rangle. \quad (1.477)$$

These states also are eigenstates of the third component of the spin operator of the combined system

$$S_3 = S_3^{(1)} + S_3^{(2)} \quad \text{that is} \quad S_3|s_1, s_2\rangle = \frac{1}{2}\hbar(s_1 + s_2)|s_1, s_2\rangle. \quad (1.478)$$

Thus $S_3|+, +\rangle = \hbar|+, +\rangle$, and $S_3|-, -\rangle = -\hbar|-, -\rangle$, while $S_3|+, -\rangle = 0$ and $S_3|-, +\rangle = 0$.

Using the notation (1.475), we can compute the effect of the operator \mathbf{S}^2 on the state $|++\rangle$. We find for S_1^2

$$\begin{aligned} S_1^2|++\rangle &= \left(S_1^{(1)} + S_1^{(2)}\right)^2|++\rangle = \frac{\hbar^2}{4} \left(\sigma_1^{(1)} + \sigma_1^{(2)}\right)^2|++\rangle \\ &= \frac{1}{2}\hbar^2 \left(1 + \sigma_1^{(1)}\sigma_1^{(2)}\right)|++\rangle = \frac{1}{2}\hbar^2 \left(|++\rangle + \sigma_1^{(1)}|+\rangle\sigma_1^{(2)}|+\rangle\right) \\ &= \frac{1}{2}\hbar^2 (|++\rangle + |--\rangle) \end{aligned} \quad (1.479)$$

and leave S_2^2 and S_3^2 to exercise 1.36. \square

Example 1.71 (Entangled states) A neutral pion π^0 has zero angular momentum and negative parity. Its mass is $135 \text{ MeV}/c^2$ and 99% of them decay into two photons with a mean lifetime of $8.5 \times 10^{-17} \text{ s}$. A π^0 at rest decays into two photons moving in opposite directions along the same axis, and the spins of the photons must be either parallel to their momenta $|+, +\rangle$, positive helicity, or antiparallel to their momenta $|-, -\rangle$, negative helicity. Parity reverses helicity, and so the state of negative parity and zero angular momentum is

$$|\gamma, \gamma\rangle = \frac{1}{\sqrt{2}} \left(|+, +\rangle - |-, -\rangle \right). \quad (1.480)$$

The two photons have the same helicity. If the helicity of one photon is measured to be positive, then a measurement of the other photon will show it to have positive helicity. The state is entangled.

One π^0 in 17 million will decay into a positron and an electron in a state of zero angular momentum. The spin part of the final state is

$$|e^+, e^-\rangle = \frac{1}{\sqrt{2}} \left(|+, -\rangle - |-, +\rangle \right). \quad (1.481)$$

If the spin along any axis of one of the electrons is measured to be positive, then a measurement of the spin of the other electron along the same axis will be negative. The state is entangled. \square

1.37 Density operators

A general quantum-mechanical system is represented by a **density operator** ρ that is hermitian $\rho^\dagger = \rho$, of unit trace $\text{Tr}\rho = 1$, and positive $\langle\psi|\rho|\psi\rangle \geq 0$ for all kets $|\psi\rangle$.

If the state $|\psi\rangle$ is normalized, then $\langle\psi|\rho|\psi\rangle$ is the nonnegative probability

that the system is in that state. This probability is real because the density matrix is hermitian. If $\{|k\rangle\}$ is any complete set of orthonormal states

$$I = \sum_k |k\rangle\langle k| \quad (1.482)$$

then the probability that the system is in the state $|k\rangle$ is

$$p_k = \langle k|\rho|k\rangle = \text{Tr}(\rho|k\rangle\langle k|). \quad (1.483)$$

Since $\text{Tr}\rho = 1$, the sum of these probabilities is unity

$$\sum_k p_k = \sum_k \langle k|\rho|k\rangle = \text{Tr}\left(\rho \sum_k |k\rangle\langle k|\right) = \text{Tr}(\rho I) = \text{Tr}\rho = 1. \quad (1.484)$$

A system that is measured to be in a state $|k\rangle$ cannot simultaneously be measured to be in an orthogonal state $|\ell\rangle$. The probabilities sum to unity because the system must be in some state.

Since the density operator ρ is hermitian and positive, it has a complete, orthonormal set of eigenvectors $|k\rangle$ all of which have nonnegative eigenvalues, $\rho|k\rangle = \rho_k|k\rangle$ with $\rho_k \geq 0$. They afford for it an expansion in their outer products

$$\rho = \sum_k \rho_k |k\rangle\langle k| \quad (1.485)$$

each weighted by the probability ρ_k that the system is in the state $|k\rangle$.

A system composed of two systems, one with basis kets $|i\rangle$ and the other with basis kets $|k\rangle$, has basis states $|i, k\rangle = |i\rangle|k\rangle$ and can be described by the density operator

$$\rho = \sum_{ijkl} |i, k\rangle\langle i, k|\rho|j, \ell\rangle\langle j, \ell|. \quad (1.486)$$

The density operator for the first system is the trace of ρ over the states $|k\rangle$ of the second system

$$\rho_1 = \sum_k \langle k|\rho|k\rangle = \sum_{ijk} |i\rangle\langle i, k|\rho|j, k\rangle\langle j| \quad (1.487)$$

and similarly the density operator for the second system is the trace of ρ over the states $|i\rangle$ of the first system

$$\rho_2 = \sum_i \langle i|\rho|i\rangle = \sum_{jkl} |k\rangle\langle i, k|\rho|i, \ell\rangle\langle \ell|. \quad (1.488)$$

For $n = 1$ and 2 , the **entanglement entropy** of system n , is the entropy $S_n = -k\text{Tr}(\rho_n \log \rho_n)$ of the reduced density matrix ρ_n .

Classical entropy is an **extensive** quantity like volume, mass, and energy. The classical entropy of a composite system is the sum of the classical entropies of its parts. But quantum entropy $S = -k\text{Tr}(\rho \log \rho)$ is not necessarily extensive. The quantum entropy of an entangled system can be less than the sum of the entanglement entropies of its parts. The quantum entropy of each of the eigenstates $|\gamma, \gamma\rangle$ and $|e^+, e^-\rangle$ of example 1.71 is zero, but the sum of the entanglement entropies of their parts is $2k \log 2$ in both cases.

1.38 Schmidt decomposition

Suppose $|\psi\rangle$ is an arbitrary vector in the tensor product of the vector spaces B and C

$$|\psi\rangle = \sum_{i=1}^n \sum_{k=1}^m A_{ik} |i\rangle \otimes |k\rangle. \quad (1.489)$$

The arbitrary matrix A has a singular-value decomposition (1.408)

$$A_{ik} = \sum_{\ell=1}^{\min(n,m)} U_{i\ell} S_{\ell} V_{\ell k}^{\dagger}. \quad (1.490)$$

In terms of this SVD, the vector $|\psi\rangle$ is

$$\begin{aligned} |\psi\rangle &= \sum_{i=1}^n \sum_{k=1}^m \sum_{\ell=1}^{\min(n,m)} U_{i\ell} S_{\ell} V_{\ell k}^{\dagger} |i\rangle \otimes |k\rangle \\ &= \sum_{\ell=1}^{\min(n,m)} S_{\ell} |U, \ell\rangle \otimes |V^{\dagger}, \ell\rangle \end{aligned} \quad (1.491)$$

where the state $|U, \ell\rangle$ is

$$|U, \ell\rangle = \sum_{i=1}^n U_{i\ell} |i\rangle \quad (1.492)$$

and is in the vector space B , and the state $|V^{\dagger}, \ell\rangle$ is

$$|V^{\dagger}, \ell\rangle = \sum_{k=1}^m V_{\ell k}^{\dagger} |k\rangle \quad (1.493)$$

and is in the vector space C . The states $|U, \ell\rangle$ and $|V^{\dagger}, \ell\rangle$ are orthonormal

$$\langle U, \ell | U, \ell' \rangle = \delta_{\ell\ell'} \quad \text{and} \quad \langle V^{\dagger}, \ell | V^{\dagger}, \ell' \rangle = \delta_{\ell\ell'} \quad (1.494)$$

because the matrices U and V are unitary.

The outer product of a tensor-product state (1.489) is a pure-state density operator

$$\rho = |\psi\rangle\langle\psi| = \sum_{\ell\ell'} S_\ell S_{\ell'} (|U, \ell\rangle \otimes |V^\dagger, \ell\rangle) (\langle U, \ell' | \otimes \langle V^\dagger, \ell' |). \quad (1.495)$$

Taking the trace over a complete set of orthonormal states in B or C , we get the density operator ρ in the spaces B or C

$$\begin{aligned} \rho_B = \text{Tr}_C(\rho) &= \sum_{\ell''} \langle V^\dagger, \ell'' | \rho | V^\dagger, \ell'' \rangle = \sum_{\ell} S_\ell^2 |U, \ell\rangle \langle U, \ell| \\ \rho_C = \text{Tr}_B(\rho) &= \sum_{\ell''} \langle U, \ell'' | \rho | U, \ell'' \rangle = \sum_{\ell} S_\ell^2 |V^\dagger, \ell\rangle \langle V^\dagger, \ell|. \end{aligned} \quad (1.496)$$

The density operators ρ_B and ρ_C have the same eigenvalues and therefore the same von Neumann entropy

$$\begin{aligned} s(\rho_B) &= -k \text{Tr}_B(\rho_B \log \rho_B) = -k \sum_{\ell} S_\ell^2 \log(S_\ell^2) \\ s(\rho_C) &= -k \text{Tr}_C(\rho_C \log \rho_C) = -k \sum_{\ell} S_\ell^2 \log(S_\ell^2). \end{aligned} \quad (1.497)$$

The nonzero, positive singular values S_ℓ are called Schmidt coefficients. The number of them is the Schmidt rank or Schmidt number of the state $|\psi\rangle$. The state $|\psi\rangle$ is entangled if and only if its Schmidt rank is greater than unity. For instance, the density operators $|\gamma, \gamma\rangle\langle\gamma, \gamma|$ and $|e^+, e^-\rangle\langle e^+, e^-|$ of example 1.71 have Schmidt rank 2.

1.39 Correlation functions

We can define two Schwarz inner products for a density matrix ρ . If $|f\rangle$ and $|g\rangle$ are two states, then the inner product

$$(f, g) \equiv \langle f | \rho | g \rangle \quad (1.498)$$

for $g = f$ is nonnegative, $(f, f) = \langle f | \rho | f \rangle \geq 0$, and satisfies the other conditions (1.82, 1.83, & 1.85) for a Schwarz inner product.

The second Schwarz inner product applies to operators A and B and is defined (Titulaer and Glauber, 1965) as

$$(A, B) = \text{Tr}(\rho A^\dagger B) = \text{Tr}(B \rho A^\dagger) = \text{Tr}(A^\dagger B \rho). \quad (1.499)$$

This inner product is nonnegative when $A = B$ and obeys the other rules (1.82, 1.83, & 1.85) for a Schwarz inner product.

These two degenerate inner products are not inner products in the strict sense of (1.82–1.88), but they are Schwarz inner products, and so (1.102–1.103) they satisfy the Schwarz inequality (1.103)

$$(f, f)(g, g) \geq |(f, g)|^2. \quad (1.500)$$

Applied to the first, vector, inner product (1.498), the Schwarz inequality gives

$$\langle f|\rho|f\rangle\langle g|\rho|g\rangle \geq |\langle f|\rho|g\rangle|^2 \quad (1.501)$$

which is a useful property of density matrices. Application of the Schwarz inequality to the second inner product (1.499) gives (Titulaer and Glauber, 1965)

$$\text{Tr}(\rho A^\dagger A) \text{Tr}(\rho B^\dagger B) \geq \left| \text{Tr}(\rho A^\dagger B) \right|^2. \quad (1.502)$$

The operator $E_i(x)$ that represents the i th component of the electric field at the point x is the hermitian sum of the positive-frequency part $E_i^{(+)}(x)$ and its adjoint $E_i^{(-)}(x) = (E_i^{(+)}(x))^\dagger$

$$E_i(x) = E_i^{(+)}(x) + E_i^{(-)}(x). \quad (1.503)$$

Glauber has defined the first-order correlation function $G_{ij}^{(1)}(x, y)$ as (Glauber, 1963b)

$$G_{ij}^{(1)}(x, y) = \text{Tr}(\rho E_i^{(-)}(x) E_j^{(+)}(y)) \quad (1.504)$$

or in terms of the operator inner product (1.499) as

$$G_{ij}^{(1)}(x, y) = \left(E_i^{(+)}(x), E_j^{(+)}(y) \right). \quad (1.505)$$

By setting $A = E_i^{(+)}(x)$ and $B = E_j^{(+)}(y)$ in the Schwarz inequality (1.502), we find that the correlation function $G_{ij}^{(1)}(x, y)$ is bounded by

$$\left| G_{ij}^{(1)}(x, y) \right|^2 \leq G_{ii}^{(1)}(x, x) G_{jj}^{(1)}(y, y). \quad (1.506)$$

Interference fringes are sharpest when this inequality is saturated

$$\left| G_{ij}^{(1)}(x, y) \right|^2 = G_{ii}^{(1)}(x, x) G_{jj}^{(1)}(y, y) \quad (1.507)$$

which can occur only if the correlation function $G_{ij}^{(1)}(x, y)$ factorizes (Titulaer and Glauber, 1965)

$$G_{ij}^{(1)}(x, y) = \mathcal{E}_i^*(x) \mathcal{E}_j(y) \quad (1.508)$$

as it does when the density operator is an outer product of coherent states

$$\rho = |\{\alpha_k\}\rangle\langle\{\alpha_k\}| \quad (1.509)$$

which are eigenstates of $E_i^{(+)}(x)$ with eigenvalue $\mathcal{E}_i(x)$ (Glauber, 1963b,a)

$$E_i^{(+)}(x)|\{\alpha_k\}\rangle = \mathcal{E}_i(x)|\{\alpha_k\}\rangle. \quad (1.510)$$

The higher-order correlation functions

$$G_{i_1 \dots i_{2n}}^{(n)}(x_1 \dots x_{2n}) = \text{Tr} \left(\rho E_{i_1}^{(-)}(x_1) \dots E_{i_n}^{(-)}(x_n) E_{i_{n+1}}^{(+)}(x_{n+1}) \dots E_{i_{2n}}^{(+)}(x_{2n}) \right) \quad (1.511)$$

satisfy similar inequalities (Glauber, 1963b) which also follow from the Schwarz inequality (1.502). (Roy Jay Glauber, 1925–2019)

1.40 Rank of a matrix

Four equivalent definitions of the **rank** $R(A)$ of an $m \times n$ matrix A are:

1. the number of its linearly independent rows,
2. the number of its linearly independent columns,
3. the number of its nonzero singular values, and
4. the number of rows in its biggest square nonsingular submatrix.

A matrix of rank zero has no nonzero singular values and so is zero.

Example 1.72 (Rank) The 3×4 matrix

$$A = \begin{pmatrix} 1 & 0 & 1 & -2 \\ 2 & 2 & 0 & 2 \\ 4 & 3 & 1 & 1 \end{pmatrix} \quad (1.512)$$

has three rows, so its rank can be at most 3. But twice the first row added to thrice the second row equals twice the third row, $2r_1 + 3r_2 - 2r_3 = 0$, so $R(A) \leq 2$. The first two rows obviously are not parallel, so they are linearly independent. Thus the number of linearly independent rows of A is 2, and so A has rank 2. \square

1.41 Software

High-quality software for virtually all numerical problems in linear algebra are available in the linear-algebra package Lapack. Lapack codes in Fortran and C++ are available at netlib.org/lapack/ and at math.nist.gov/tnt/. Apple's Xcode command `-framework accelerate` links this software into `gnu`

executables. The Basic Linear Algebra Subprograms (BLAS) on which Lapack is based are also available in Java at icl.cs.utk.edu/f2j/ and at math.nist.gov/javanumerics/.

Matlab solves a wide variety of numerical problems. A free GNU version is available at gnu.org/software/octave/. Maple and Mathematica are good commercial programs for numerical and symbolic problems. Python (python.org), Scientific Python (scipy.org), Sage (sagemath.org), and Cadabra (cadabra.science) are websites of free software of broad (and universal, Python) applicability. Maxima, xMaxima, and wxMaxima (maxima.sourceforge.net) are free Lisp programs that excel at computer algebra. Intel gives software to students and teachers (software.intel.com).

Exercises

- 1.1 What is the most general function of three Grassmann numbers $\theta_1, \theta_2, \theta_3$?
- 1.2 Derive the cyclicity (1.27) of the trace from Eq. (1.26).
- 1.3 Show that $(AB)^T = B^T A^T$, which is Eq.(1.30).
- 1.4 Show that a real hermitian matrix is symmetric.
- 1.5 Show that $(AB)^\dagger = B^\dagger A^\dagger$, which is Eq.(1.33).
- 1.6 Show that the matrix (1.45) is positive on the space of all real 2-vectors but not on the space of all complex 2-vectors.
- 1.7 Show that the two 4×4 matrices (1.50) satisfy Grassmann's algebra (1.11) for $n = 2$.
- 1.8 Show that the operators $a_i = \theta_i$ defined in terms of the Grassmann matrices (1.50) and their adjoints $a_i^\dagger = \theta_i^\dagger$ satisfy the anticommutation relations (1.51) of the creation and annihilation operators for a system with two fermionic states.
- 1.9 Derive (1.70) from (1.67–1.69).
- 1.10 Fill in the steps leading to the formulas (1.78) for the vectors b'_1 and b'_2 and the formula (1.79) for the matrix a' .
- 1.11 Show that the antilinearity (1.85) of the inner product follows from its first two properties (1.82 & 1.83).
- 1.12 Show that the Minkowski product $(x, y) = \mathbf{x} \cdot \mathbf{y} - x^0 y^0$ of two 4-vectors x and y is an inner product obeying the rules (1.82, 1.83, and 1.88).
- 1.13 Show that if $f = 0$, then the linearity (1.83) of the inner product implies that (f, f) and (g, f) vanish.
- 1.14 Show that the condition (1.84) of being positive definite implies non-degeneracy (1.88).

- 1.15 Show that the nonnegativity (1.86) of the Schwarz inner product implies the condition (1.87). Hint: the inequality $(f - \lambda g, f - \lambda g) \geq 0$ must hold for every complex λ and for all vectors f and g .
- 1.16 Show that the inequality (1.110) follows from the Schwarz inequality (1.109).
- 1.17 Show that the inequality (1.112) follows from the Schwarz inequality (1.111).
- 1.18 Use the Gram-Schmidt method to find orthonormal linear combinations of the three vectors

$$\mathbf{s}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{s}_2 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{s}_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \quad (1.513)$$

- 1.19 Now use the Gram-Schmidt method to find orthonormal linear combinations of the same three vectors but in a different order

$$\mathbf{s}'_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{s}'_2 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{s}'_3 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \quad (1.514)$$

Did you get the same orthonormal vectors as in the previous exercise?

- 1.20 Derive the linearity (1.132) of the outer product from its definition (1.131).
- 1.21 Show that a linear operator A that is represented by a hermitian matrix (1.174) in an orthonormal basis satisfies $(g, Af) = (Ag, f)$.
- 1.22 Show that a unitary operator maps one orthonormal basis into another.
- 1.23 Show that the integral (1.195) defines a unitary operator that maps the state $|x'\rangle$ to the state $|x' + a\rangle$.
- 1.24 For the 2×2 matrices

$$A = \begin{pmatrix} 1 & 2 \\ 3 & -4 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix} \quad (1.515)$$

verify equations (1.229–1.231).

- 1.25 Derive the least-squares solution (1.260) for complex A , x , and y when the matrix $A^\dagger A$ is positive.
- 1.26 Show that the eigenvalues λ of a unitary matrix are unimodular, that is, $|\lambda| = 1$.
- 1.27 What are the eigenvalues and eigenvectors of the two defective matrices (1.298)?
- 1.28 Use (1.309) to derive expression (1.310) for the 2×2 rotation matrix $\exp(-i\boldsymbol{\theta} \cdot \boldsymbol{\sigma}/2)$.

- 1.29 Compute the characteristic equation for the matrix $-i\boldsymbol{\theta} \cdot \mathbf{J}$ in which the generators are $(J_k)_{ij} = i\epsilon_{ikj}$ and ϵ_{ijk} is totally antisymmetric with $\epsilon_{123} = 1$.
- 1.30 Use the characteristic equation of exercise 1.29 to derive identities (1.313) and (1.314) for the 3×3 real orthogonal matrix $\exp(-i\boldsymbol{\theta} \cdot \mathbf{J})$.
- 1.31 Show that the sum of the eigenvalues of a normal antisymmetric matrix vanishes.
- 1.32 Consider the 2×3 matrix A

$$A = \begin{pmatrix} 1 & 2 & 3 \\ -3 & 0 & 1 \end{pmatrix}. \quad (1.516)$$

Perform the singular value decomposition $A = USV^T$, where V^T the transpose of V . Use Matlab or another program to find the singular values and the real orthogonal matrices U and V .

- 1.33 Consider the 6×9 matrix A with elements $A_{j,k} = x + x^j + i(y - y^k)$ in which $x = 1.1$ and $y = 1.02$. Use Matlab or another program to find the singular values, and the first left and right singular vectors.
- 1.34 Show that the totally antisymmetric Levi-Civita symbol ϵ_{ijk} where $\epsilon_{123} = 1$ satisfies the useful relation

$$\sum_{i=1}^3 \epsilon_{ijk} \epsilon_{inm} = \delta_{jn} \delta_{km} - \delta_{jm} \delta_{kn}. \quad (1.517)$$

- 1.35 Consider the hamiltonian $H = \frac{1}{2}\hbar\omega\sigma_3$ where σ_3 is defined in (1.474). The entropy S of this system at temperature T is $S = -k\text{Tr}[\rho \ln(\rho)]$ in which the density operator ρ is

$$\rho = \frac{e^{-H/(kT)}}{\text{Tr}[e^{-H/(kT)}]}. \quad (1.518)$$

Find expressions for the density operator ρ and its entropy S .

- 1.36 Use example 1.70 to find the action of the operator $\mathbf{S}^2 = (\mathbf{S}^{(1)} + \mathbf{S}^{(2)})^2$ on the four states $|\pm\pm\rangle$ and then find the eigenstates and eigenvalues of \mathbf{S}^2 in the space spanned by these four states.
- 1.37 A system that has three fermionic states has three creation operators a_i^\dagger and three annihilation operators a_k which satisfy the anticommutation relations $\{a_i, a_k^\dagger\} = \delta_{ik}$ and $\{a_i, a_k\} = \{a_i^\dagger, a_k^\dagger\} = 0$ for $i, k = 1, 2, 3$. The eight states of the system are $|t, u, v\rangle \equiv (a_1^\dagger)^t (a_2^\dagger)^u (a_3^\dagger)^v |0, 0, 0\rangle$. We can represent them by eight 8-vectors each of which has seven 0's with a 1 in position $4t + 2u + v + 1$. How big should the matrices that

represent the creation and annihilation operators be? Write down the three matrices that represent the three creation operators.

- 1.38 Show that the Schwarz inner product (1.498) is degenerate because it can violate (1.88) for certain density operators and certain pairs of states.
- 1.39 Show that the Schwarz inner product (1.499) is degenerate because it can violate (1.88) for certain density operators and certain pairs of operators.
- 1.40 The coherent state $|\{\alpha(\mathbf{k}, \ell)\}\rangle$ is an eigenstate of the annihilation operator $a(\mathbf{k}, \ell)$ with eigenvalue $\alpha(\mathbf{k}, \ell)$ for each wavenumber \mathbf{k} and polarization ℓ , i.e., $a(\mathbf{k}, \ell)|\{\alpha(\mathbf{k}, \ell)\}\rangle = \alpha(\mathbf{k}, \ell)|\{\alpha(\mathbf{k}, \ell)\}\rangle$. The positive-frequency part $E_i^{(+)}(t, \mathbf{x})$ of the electric field is a sum over \mathbf{k} and ℓ

$$E_i^{(+)}(t, \mathbf{x}) = \sum_{\mathbf{k}} \sum_{\ell=1}^2 a(\mathbf{k}, \ell) e_i(\mathbf{k}, \ell) e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)} \quad (1.519)$$

in which $\mathbf{e}(\mathbf{k}, \ell) = \mathbf{k} \times \boldsymbol{\epsilon}(\mathbf{k}, \ell)$ and $\boldsymbol{\epsilon}(\mathbf{k}, \ell)$ is proportional to a polarization vector. Show that $|\{\alpha(\mathbf{k}, \ell)\}\rangle$ is an eigenstate of $E_i^{(+)}(t, \mathbf{x})$ as in (1.510) and find its eigenvalue $\mathcal{E}_i^{(+)}(t, \mathbf{x})$.

- 1.41 Show that if X is a nondefective, nonsingular square matrix, then the variation of the logarithm of its determinant is $\delta \ln(\det X) = \text{Tr}(X^{-1} \delta X)$.

2

Vector Calculus

2.1 Derivatives and partial derivatives

The **derivative** of a function $f(x)$ at a point x is the limit of the ratio

$$\frac{df(x)}{dx} = \lim_{x' \rightarrow x} \frac{f(x') - f(x)}{x' - x}. \quad (2.1)$$

Example 2.1 (Derivative of a monomial) Setting $x' = x + \epsilon$ and letting $\epsilon \rightarrow 0$, we compute the derivative of x^n as

$$\frac{dx^n}{dx} = \lim_{\epsilon \rightarrow 0} \frac{(x + \epsilon)^n - x^n}{\epsilon} \approx \frac{x^n + \epsilon n x^{n-1} - x^n}{\epsilon} = n x^{n-1}. \quad (2.2)$$

Similarly, adding fractions, we find

$$\frac{dx^{-n}}{dx} = \lim_{\epsilon \rightarrow 0} \frac{(x + \epsilon)^{-n} - x^{-n}}{\epsilon} \approx \frac{x^{-n} - (x^n + \epsilon n x^{n-1})}{\epsilon x^{2n}} = -n x^{-n-1}. \quad (2.3)$$

□

The **partial derivative** of a function with respect to a given variable is the whole derivative of the function with its other variables held constant. For instance, the partial derivatives of the function $f(x, y, z) = x^\ell y^n / z^m$ with respect to x and z are

$$\frac{\partial f(x, y, z)}{\partial x} = \ell \frac{x^{\ell-1} y^n}{z^m} \quad \text{and} \quad \frac{\partial f(x, y, z)}{\partial z} = -m \frac{x^\ell y^n}{z^{m+1}}. \quad (2.4)$$

One often uses primes or dots to denote derivatives as in

$$f' = \frac{df}{dx}, \quad f'' = \frac{d^2 f}{dx^2} \equiv \frac{d}{dx} \left(\frac{df}{dx} \right), \quad \dot{f} = \frac{df}{dt}, \quad \text{and} \quad \ddot{f} = \frac{d^2 f}{dt^2}. \quad (2.5)$$

For higher or partial derivatives, one sometimes uses superscripts

$$f^{(k)} = \frac{d^k f}{dx^k} \quad \text{and} \quad f^{(k, \ell)} = \frac{\partial^{k+\ell} f}{\partial x^k \partial y^\ell} \quad (2.6)$$

or subscripts, sometimes preceded by commas

$$f_x = f_{,x} = \frac{\partial f}{\partial x} \quad \text{and} \quad f_{xyy} = f_{,xyy} = \frac{\partial^3 f}{\partial x \partial y^2}. \quad (2.7)$$

If variables $x = x_1, \dots, x_n$ are labeled by indexes, derivatives can be labeled by subscripted indexes, sometimes preceded by commas

$$f_{,k} = \partial_k f = \frac{\partial f}{\partial x_k} \quad \text{and} \quad f_{,k\ell} = \partial_k \partial_\ell f = \frac{\partial^2 f}{\partial x_k \partial x_\ell}. \quad (2.8)$$

2.2 Gradient

The change $d\mathbf{p}$ in a point \mathbf{p} due to changes du_1, du_2, du_3 in its **orthogonal** coordinates u_1, u_2, u_3 is a linear combination

$$\begin{aligned} d\mathbf{p} &= \frac{\partial \mathbf{p}}{\partial u_1} du_1 + \frac{\partial \mathbf{p}}{\partial u_2} du_2 + \frac{\partial \mathbf{p}}{\partial u_3} du_3 \\ &= \mathbf{e}_1 du_1 + \mathbf{e}_2 du_2 + \mathbf{e}_3 du_3 \end{aligned} \quad (2.9)$$

of vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ that are orthogonal

$$\mathbf{e}_i \cdot \mathbf{e}_k = h_i h_k \delta_{ik}. \quad (2.10)$$

In terms of the orthonormal vectors $\hat{\mathbf{e}}_j = \mathbf{e}_j/h_j$, the change $d\mathbf{p}$ is

$$d\mathbf{p} = h_1 \hat{\mathbf{e}}_1 du_1 + h_2 \hat{\mathbf{e}}_2 du_2 + h_3 \hat{\mathbf{e}}_3 du_3. \quad (2.11)$$

The orthonormal vectors $\hat{\mathbf{e}}_j$ have cyclic cross products

$$\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_j = \sum_{k=1}^3 \epsilon_{ijk} \hat{\mathbf{e}}_k \quad (2.12)$$

in which ϵ_{ijk} is the antisymmetric Levi-Civita symbol (1.205) with $\epsilon_{123} = 1$.

In rectangular coordinates, the change $d\mathbf{p}$ in a physical point \mathbf{p} due to changes $dx, dy,$ and dz in its coordinates is $d\mathbf{p} = \hat{\mathbf{x}} dx + \hat{\mathbf{y}} dy + \hat{\mathbf{z}} dz$, and the scale factors are all unity $h_x = h_y = h_z = 1$. In cylindrical coordinates, the change $d\mathbf{p}$ in a point \mathbf{p} due to changes $d\rho, d\phi,$ and dz in its coordinates is $d\mathbf{p} = \hat{\boldsymbol{\rho}} d\rho + \rho \hat{\boldsymbol{\phi}} d\phi + \hat{\mathbf{z}} dz$, and the scale factors are $h_\rho = 1, h_\phi = \rho,$ and $h_z = 1$. In spherical coordinates, the change is $d\mathbf{p} = \hat{\mathbf{r}} dr + r \hat{\boldsymbol{\theta}} d\theta + r \sin \theta \hat{\boldsymbol{\phi}} d\phi$, and the scale factors are $h_r = 1, h_\theta = r,$ and $h_\phi = r \sin \theta$. In these orthogonal coordinates, the change in a point is

$$d\mathbf{p} = \begin{cases} \hat{\mathbf{x}} dx + \hat{\mathbf{y}} dy + \hat{\mathbf{z}} dz \\ \hat{\boldsymbol{\rho}} d\rho + \rho \hat{\boldsymbol{\phi}} d\phi + \hat{\mathbf{z}} dz \\ \hat{\mathbf{r}} dr + r \hat{\boldsymbol{\theta}} d\theta + r \sin \theta \hat{\boldsymbol{\phi}} d\phi \end{cases}. \quad (2.13)$$

Since in cylindrical and spherical coordinates a point \mathbf{p} is

$$\mathbf{p} = \rho \cos \phi \hat{\mathbf{x}} + \rho \sin \phi \hat{\mathbf{y}} + z \hat{\mathbf{z}} = r \sin \theta \cos \phi \hat{\mathbf{x}} + r \sin \theta \sin \phi \hat{\mathbf{y}} + r \cos \theta \hat{\mathbf{z}}, \quad (2.14)$$

the cylindrical and spherical basis vectors are (exercise 2.1)

$$\begin{aligned} \hat{\boldsymbol{\rho}} &= \cos \phi \hat{\mathbf{x}} + \sin \phi \hat{\mathbf{y}} & \hat{\mathbf{r}} &= \sin \theta \cos \phi \hat{\mathbf{x}} + \sin \theta \sin \phi \hat{\mathbf{y}} + \cos \theta \hat{\mathbf{z}} \\ \hat{\boldsymbol{\phi}} &= -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}} & \hat{\boldsymbol{\theta}} &= \cos \theta \cos \phi \hat{\mathbf{x}} + \cos \theta \sin \phi \hat{\mathbf{y}} - \sin \theta \hat{\mathbf{z}} \\ \hat{\mathbf{z}} &= \hat{\mathbf{z}} & \hat{\boldsymbol{\phi}} &= -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}}. \end{aligned} \quad (2.15)$$

The **gradient** ∇f of a scalar function f is defined so that its dot product $\nabla f \cdot d\mathbf{p}$ with the change $d\mathbf{p}$ in the point \mathbf{p} is the change df in f

$$\begin{aligned} \nabla f \cdot d\mathbf{p} &= (\nabla f_1 \hat{\mathbf{e}}_1 + \nabla f_2 \hat{\mathbf{e}}_2 + \nabla f_3 \hat{\mathbf{e}}_3) \cdot (\hat{\mathbf{e}}_1 h_1 du_1 + \hat{\mathbf{e}}_2 h_2 du_2 + \hat{\mathbf{e}}_3 h_3 du_3) \\ &= \nabla f_1 h_1 du_1 + \nabla f_2 h_2 du_2 + \nabla f_3 h_3 du_3 \\ &= df = \frac{\partial f}{\partial u_1} du_1 + \frac{\partial f}{\partial u_2} du_2 + \frac{\partial f}{\partial u_3} du_3. \end{aligned} \quad (2.16)$$

Thus the gradient in orthogonal coordinates is

$$\nabla f = \frac{\hat{\mathbf{e}}_1}{h_1} \frac{\partial f}{\partial u_1} + \frac{\hat{\mathbf{e}}_2}{h_2} \frac{\partial f}{\partial u_2} + \frac{\hat{\mathbf{e}}_3}{h_3} \frac{\partial f}{\partial u_3}, \quad (2.17)$$

and in rectangular, cylindrical, and spherical coordinates it is

$$\nabla f = \begin{cases} \hat{\mathbf{x}} \frac{\partial f}{\partial x} + \hat{\mathbf{y}} \frac{\partial f}{\partial y} + \hat{\mathbf{z}} \frac{\partial f}{\partial z} \\ \hat{\boldsymbol{\rho}} \frac{\partial f}{\partial \rho} + \frac{\hat{\boldsymbol{\phi}}}{\rho} \frac{\partial f}{\partial \phi} + \hat{\mathbf{z}} \frac{\partial f}{\partial z} \\ \hat{\mathbf{r}} \frac{\partial f}{\partial r} + \frac{\hat{\boldsymbol{\theta}}}{r} \frac{\partial f}{\partial \theta} + \frac{\hat{\boldsymbol{\phi}}}{r \sin \theta} \frac{\partial f}{\partial \phi} \end{cases}. \quad (2.18)$$

In particular the gradient of $1/r$ is

$$\nabla \left(\frac{1}{r} \right) = -\frac{\hat{\mathbf{r}}}{r^2} \quad \text{and} \quad \nabla \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) = -\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3}. \quad (2.19)$$

In the last two formulas, the differentiation is with respect to \mathbf{r} , not \mathbf{r}' .

2.3 Divergence

The **divergence** of a vector \mathbf{v} in an infinitesimal cube C is defined as the integral S of \mathbf{v} over the surface of the cube divided by its volume $V = h_1 h_2 h_3 du_1 du_2 du_3$. The surface integral S is the sum of the integrals of v_1 , v_2 , and v_3 over the cube's three forward faces $v_1 h_2 du_2 h_3 du_3 + v_2 h_1 du_1 h_3 du_3 +$

$v_3 h_1 du_1 h_2 du_2$ minus the sum of the integrals of v_1 , v_2 , and v_3 over the cube's three opposite faces. The surface integral is then

$$S = \left[\frac{\partial(v_1 h_2 h_3)}{\partial u_1} + \frac{\partial(v_2 h_1 h_3)}{\partial u_2} + \frac{\partial(v_3 h_1 h_2)}{\partial u_3} \right] du_1 du_2 du_3. \quad (2.20)$$

So the divergence $\nabla \cdot \mathbf{v}$ is the ratio S/V

$$\nabla \cdot \mathbf{v} = \frac{S}{V} = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial(v_1 h_2 h_3)}{\partial u_1} + \frac{\partial(v_2 h_1 h_3)}{\partial u_2} + \frac{\partial(v_3 h_1 h_2)}{\partial u_3} \right]. \quad (2.21)$$

In rectangular coordinates, the divergence of a vector $\mathbf{v} = (v_x, v_y, v_z)$ is

$$\nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}. \quad (2.22)$$

In cylindrical coordinates, it is

$$\nabla \cdot \mathbf{v} = \frac{1}{\rho} \left[\frac{\partial(v_\rho \rho)}{\partial \rho} + \frac{\partial v_\phi}{\partial \phi} + \frac{\partial(v_z \rho)}{\partial z} \right] = \frac{1}{\rho} \frac{\partial(\rho v_\rho)}{\partial \rho} + \frac{1}{\rho} \frac{\partial v_\phi}{\partial \phi} + \frac{\partial v_z}{\partial z}, \quad (2.23)$$

and in spherical coordinates it is

$$\nabla \cdot \mathbf{v} = \frac{1}{r^2} \frac{\partial(v_r r^2)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(v_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi}. \quad (2.24)$$

By assembling a suitable number of infinitesimal cubes, one may create a three-dimensional region of arbitrary shape and volume. The sum of the products of the divergence $\nabla \cdot \mathbf{v}$ in each cube times its volume dV is the sum of the surface integrals dS over the faces of these tiny cubes. The integrals over the interior faces cancel leaving just the integral over the surface ∂V of the whole volume V . Thus we arrive at Stokes's theorem

$$\int_V \nabla \cdot \mathbf{v} dV = \int_{\partial V} \mathbf{v} \cdot d\mathbf{a} \quad (2.25)$$

in which $d\mathbf{a}$ is an infinitesimal, outward, area element of the surface that is the boundary ∂V of the volume V .

Example 2.2 (Delta function) The integral of the divergence of the negative gradient $\hat{\mathbf{r}}/r^2$ (2.19) of $1/r$ over any sphere, however small, centered at the origin is 4π

$$\int \nabla \cdot \left(\frac{\hat{\mathbf{r}}}{r^2} \right) dV = \int \frac{\hat{\mathbf{r}}}{r^2} \cdot d\mathbf{a} = \int \frac{\hat{\mathbf{r}}}{r^2} \cdot r^2 \hat{\mathbf{r}} d\Omega = \int d\Omega = 4\pi. \quad (2.26)$$

Similarly, the integral of the divergence of $(\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|^3$ over any sphere,

however small, centered at \mathbf{r}' is 4π

$$\begin{aligned} \int \nabla \cdot \left(\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right) dV &= \int \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \cdot d\mathbf{a} \\ &= \int \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \cdot |\mathbf{r} - \mathbf{r}'|^2 \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} d\Omega = \int d\Omega = 4\pi. \end{aligned} \quad (2.27)$$

These divergences, vanishing for $\mathbf{r} \neq 0$ and for $\mathbf{r} - \mathbf{r}' \neq 0$, are examples of **delta functions** (sections 2.6 and 3.11)

$$\nabla \cdot \left(\frac{\hat{\mathbf{r}}}{r^2} \right) = 4\pi\delta^3(\mathbf{r}) \quad \text{and} \quad \nabla \cdot \left(\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right) = 4\pi\delta^3(\mathbf{r} - \mathbf{r}') \quad (2.28)$$

because if $f(\mathbf{r})$ is any suitably smooth function, then the integral over any volume that includes the point \mathbf{r}' is

$$\int f(\mathbf{r}) \nabla \cdot \left(\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \right) d^3r = 4\pi f(\mathbf{r}'). \quad (2.29)$$

□

Example 2.3 (Gauss's laws) Gauss's laws are that the divergence of the magnetic induction vanishes and that the divergence $\nabla \cdot \mathbf{E}$ of the electric field is the charge density ρ divided by the electric constant $\epsilon_0 = 8.854 \times 10^{-12}$ F/m

$$\nabla \cdot \mathbf{B} = 0 \quad \text{and} \quad \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}. \quad (2.30)$$

So by Stokes's theorem, the integral of the electric field over a surface ∂V that bounds a volume V is the charge inside divided by ϵ_0

$$\int_{\partial V} \mathbf{E} \cdot d\mathbf{a} = \int_V \nabla \cdot \mathbf{E} dV = \int_V \frac{\rho}{\epsilon_0} dV = \frac{Q_V}{\epsilon_0}. \quad (2.31)$$

□

2.4 Laplacian

The laplacian is the divergence (2.21) of the gradient (2.17). So in orthogonal coordinates it is

$$\Delta f \equiv \nabla^2 f \equiv \nabla \cdot \nabla f = \frac{1}{h_1 h_2 h_3} \left[\sum_{k=1}^3 \frac{\partial}{\partial u_k} \left(\frac{h_1 h_2 h_3}{h_k^2} \frac{\partial f}{\partial u_k} \right) \right]. \quad (2.32)$$

In rectangular coordinates, the laplacian is

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}. \quad (2.33)$$

In cylindrical coordinates, it is

$$\Delta f = \frac{1}{\rho} \left[\frac{\partial}{\partial \rho} \left(\rho \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho} \frac{\partial^2 f}{\partial \phi^2} + \rho \frac{\partial^2 f}{\partial z^2} \right] = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2}, \quad (2.34)$$

and in spherical coordinates it is

$$\begin{aligned} \Delta f &= \frac{1}{r^2 \sin \theta} \left[\frac{\partial}{\partial r} \left(r^2 \sin \theta \frac{\partial f}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{\partial}{\partial \phi} \left(\frac{1}{\sin \theta} \frac{\partial f}{\partial \phi} \right) \right] \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \quad (2.35) \\ &= \frac{1}{r} \frac{\partial^2}{\partial r^2} (rf) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}. \end{aligned}$$

Example 2.4 (Delta function as laplacian of $1/r$) By combining the gradient (2.19) of $1/r$ with the representation (2.28) of the delta function as a divergence, we can write delta functions as laplacians (with respect to \mathbf{r})

$$-\Delta \left(\frac{1}{r} \right) = 4\pi \delta^3(\mathbf{r}) \quad \text{and} \quad -\Delta \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) = 4\pi \delta^3(\mathbf{r} - \mathbf{r}'). \quad (2.36)$$

□

Example 2.5 (Electric field of a uniformly charged sphere) The electric field $\mathbf{E} = -\nabla\phi - \dot{\mathbf{A}}$ in static problems is just the gradient $\mathbf{E} = -\nabla\phi$ of the scalar potential ϕ . Gauss's law (2.30) then gives us Poisson's equation $\nabla \cdot \mathbf{E} = -\Delta\phi = \rho/\epsilon_0$. Writing the laplacian in spherical coordinates (2.35) and using spherical symmetry, we find

$$-\frac{1}{r} \frac{d^2}{dr^2} (r\phi) = \frac{\rho}{\epsilon_0} \quad (2.37)$$

in which ρ is the uniform charge density of the sphere. Integrating twice and letting the constant a be $\phi(r)$ at $r = 0$, we find the potential inside the sphere to be $\phi(r) = a - \rho r^2/(6\epsilon_0)$. Outside the sphere, the charge density vanishes, and so the second r -derivative of $r\phi$ vanishes, $(r\phi)'' = 0$. Integrating twice, we get for the potential outside the sphere $\phi(r) = b/r$ after dropping a constant term because $\phi(r) \rightarrow 0$ as $r \rightarrow \infty$. The interior and exterior solutions for the electric field $\mathbf{E} = -\nabla\phi$ agree where they meet on the surface of the sphere at $r = R$

$$\mathbf{E} = \hat{\mathbf{r}} \frac{\rho R}{3\epsilon_0} = \hat{\mathbf{r}} \frac{b}{R^2}. \quad (2.38)$$

Thus $b = \rho R^3/(3\epsilon_0)$. Matching the interior potential to the exterior potential

on the surface of the sphere gives $a = \rho R^2/(2\epsilon_0)$. So the potential of a uniformly charged sphere of radius R is

$$\phi(r) = \begin{cases} \rho(R^2 - r^2/3)/(2\epsilon_0) & r \leq R \\ \rho R^3/(3\epsilon_0 r) & r \geq R \end{cases}. \quad (2.39)$$

□

2.5 Curl

The directed area $d\mathbf{S}$ of an infinitesimal rectangle whose sides are the tiny perpendicular vectors $h_i \hat{\mathbf{e}}_i du_i$ and $h_j \hat{\mathbf{e}}_j du_j$ (fixed i and j) is their cross-product (2.12)

$$d\mathbf{S} = h_i \hat{\mathbf{e}}_i du_i \times h_j \hat{\mathbf{e}}_j du_j = \sum_{k=1}^3 \epsilon_{ijk} \hat{\mathbf{e}}_k h_i h_j du_i du_j. \quad (2.40)$$

The line integral of the vector \mathbf{f} along the perimeter of this infinitesimal rectangle is

$$\oint \mathbf{f} \cdot d\mathbf{l} = \left(\frac{\partial(h_j f_j)}{\partial u_i} - \frac{\partial(h_i f_i)}{\partial u_j} \right) du_i du_j. \quad (2.41)$$

The **curl** $\nabla \times \mathbf{f}$ of a vector \mathbf{f} is defined to be the vector whose dot product with the area (2.40) is the line integral (2.41)

$$(\nabla \times \mathbf{f}) \cdot d\mathbf{S} = (\nabla \times \mathbf{f})_k h_i h_j du_i du_j = \left(\frac{\partial(h_j f_j)}{\partial u_i} - \frac{\partial(h_i f_i)}{\partial u_j} \right) du_i du_j \quad (2.42)$$

in which i, j, k are 1, 2, 3 or a cyclic permutation of 1, 2, 3. Thus the k th component of the curl is

$$(\nabla \times \mathbf{f})_k = \sum_{i,j=1}^3 \frac{\epsilon_{ijk}}{h_i h_j} \frac{\partial(h_j f_j)}{\partial u_i}, \quad (2.43)$$

and the curl is the vector field

$$\nabla \times \mathbf{f} = \sum_{i,j,k=1}^3 \epsilon_{ijk} \frac{\hat{\mathbf{e}}_k}{h_i h_j} \frac{\partial(h_j f_j)}{\partial u_i}. \quad (2.44)$$

In rectangular coordinates, the scale factors are all unity, and the i th component of the curl $\nabla \times \mathbf{f}$ is

$$(\nabla \times \mathbf{f})_i = \sum_{j,k=1}^3 \epsilon_{ijk} \frac{\partial f_k}{\partial x_j} = \sum_{j,k=1}^3 \epsilon_{ijk} \partial_j f_k. \quad (2.45)$$

We can write the curl as a determinant

$$\nabla \times \mathbf{f} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \hat{\mathbf{e}}_1 & h_2 \hat{\mathbf{e}}_2 & h_3 \hat{\mathbf{e}}_3 \\ \partial_1 & \partial_2 & \partial_3 \\ h_1 f_1 & h_2 f_2 & h_3 f_3 \end{vmatrix}. \quad (2.46)$$

In rectangular coordinates, the curl is

$$\nabla \times \mathbf{f} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \partial_x & \partial_y & \partial_z \\ f_x & f_y & f_z \end{vmatrix}. \quad (2.47)$$

In cylindrical coordinates, it is

$$\nabla \times \mathbf{f} = \frac{1}{\rho} \begin{vmatrix} \hat{\boldsymbol{\rho}} & \rho \hat{\boldsymbol{\phi}} & \hat{\mathbf{z}} \\ \partial_\rho & \partial_\phi & \partial_z \\ f_\rho & \rho f_\phi & f_z \end{vmatrix} \quad (2.48)$$

and in spherical coordinates, it is

$$\nabla \times \mathbf{f} = \frac{1}{r^2 \sin \theta} \begin{vmatrix} \hat{\mathbf{r}} & r \hat{\boldsymbol{\theta}} & r \sin \theta \hat{\boldsymbol{\phi}} \\ \partial_r & \partial_\theta & \partial_\phi \\ f_r & r f_\theta & r \sin \theta f_\phi \end{vmatrix}. \quad (2.49)$$

Example 2.6 (Magnetic field in the z direction) The curl (2.48) of the vector potential $\mathbf{A} = \frac{1}{2} B_0 \rho \hat{\boldsymbol{\phi}}$ is $\mathbf{B} = \nabla \times \mathbf{A} = B_0 \hat{\mathbf{z}}$. \square

Sums of products of two Levi-Civita symbols (1.205) yield useful identities

$$\sum_{i=1}^3 \epsilon_{ijk} \epsilon_{imn} = \delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km} \quad \text{and} \quad \sum_{i,j=1}^3 \epsilon_{ijk} \epsilon_{ijn} = 2\delta_{kn} \quad (2.50)$$

in which δ_{jm} is Kronecker's delta (1.38). Thus the curl of a curl is

$$\begin{aligned} [\nabla \times (\nabla \times \mathbf{A})]_i &= \sum_{j,k,m,n=1}^3 \epsilon_{ijk} \partial_j \epsilon_{kmn} \partial_m A_n = \sum_{j,m,n=1}^3 (\delta_{im} \delta_{jn} - \delta_{in} \delta_{jm}) \partial_j \partial_m A_n \\ &= \partial_i \nabla \cdot \mathbf{A} - \Delta A_i \quad \text{or} \quad \nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \Delta \mathbf{A}. \end{aligned} \quad (2.51)$$

By assembling a suitable set of infinitesimal rectangles $d\mathbf{S}$, we may create an arbitrary surface S . The surface integral of the dot product $\nabla \times \mathbf{f} \cdot d\mathbf{S}$ over the tiny rectangles $d\mathbf{S}$ that make up the surface S is the sum of the line integrals along the sides of these tiny rectangles. The line integrals over the interior sides cancel leaving just the line integral along the boundary ∂S

of the finite surface S . Thus the integral of the curl $\nabla \times \mathbf{f}$ of a vector \mathbf{f} over a surface is the line integral of the vector \mathbf{f} along the boundary of the surface

$$\int_S (\nabla \times \mathbf{f}) \cdot d\mathbf{S} = \int_{\partial S} \mathbf{f} \cdot d\boldsymbol{\ell} \quad (2.52)$$

which is one of Stokes's theorems.

Example 2.7 (Maxwell's equations) In empty space, Maxwell's equations in SI units are $\nabla \cdot \mathbf{E} = 0$, $\nabla \cdot \mathbf{B} = 0$, $\nabla \times \mathbf{E} = -\dot{\mathbf{B}}$, and $c^2 \nabla \times \mathbf{B} = \dot{\mathbf{E}}$. They imply that the voltage induced in a loop is the negative of the rate of change of the magnetic induction through the loop

$$V = \oint_{\partial S} \mathbf{E} \cdot d\mathbf{x} = -\dot{\Phi}_B = -\int_S \dot{\mathbf{B}} \cdot d\mathbf{a} \quad (2.53)$$

and that the magnetic induction induced in a loop is the rate of change of the electric flux through the loop divided by c^2

$$B = \int_{\partial S} \mathbf{B} \cdot d\mathbf{x} = \frac{1}{c^2} \dot{\Phi}_E = \frac{1}{c^2} \int_S \dot{\mathbf{E}} \cdot d\mathbf{a}. \quad (2.54)$$

Maxwell's equations in empty space and the curl identity (2.51) imply that

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \Delta \mathbf{E} = -\Delta \mathbf{E} = -\nabla \times \dot{\mathbf{B}} = -\ddot{\mathbf{E}}/c^2 \quad (2.55)$$

$$\nabla \times (\nabla \times \mathbf{B}) = \nabla(\nabla \cdot \mathbf{B}) - \Delta \mathbf{B} = -\Delta \mathbf{B} = \nabla \times \dot{\mathbf{E}}/c^2 = -\ddot{\mathbf{B}}/c^2 \quad (2.56)$$

or

$$\Delta \mathbf{E} = \ddot{\mathbf{E}}/c^2 \quad \text{and} \quad \Delta \mathbf{B} = \ddot{\mathbf{B}}/c^2. \quad (2.57)$$

The exponentials $\mathbf{E}(\mathbf{k}, \omega) = \boldsymbol{\epsilon} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$ and $\mathbf{B}(\mathbf{k}, \omega) = (\hat{\mathbf{k}} \times \boldsymbol{\epsilon}/c) e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$ with $\omega = |\mathbf{k}|c$ and $\hat{\mathbf{k}} \cdot \boldsymbol{\epsilon} = 0$ obey these wave equations. \square

Example 2.8 (Helmholtz decomposition) We can use the delta-function formula (2.36) to write any suitably smooth 3-dimensional vector field $\mathbf{V}(\mathbf{x})$ as

$$\mathbf{V}(\mathbf{x}) = -\int \mathbf{V}(\mathbf{r}) \Delta \left(\frac{1}{|\mathbf{r} - \mathbf{x}|} \right) d^3r \quad (2.58)$$

in which the derivatives $\nabla \cdot \nabla = \nabla^2 = \Delta$ can be both with respect to \mathbf{x} or both with respect to \mathbf{r} . Taking them to be with respect to \mathbf{x} , we have

$$\mathbf{V}(\mathbf{x}) = -\nabla^2 \int \frac{\mathbf{V}(\mathbf{r})}{|\mathbf{r} - \mathbf{x}|} d^3r. \quad (2.59)$$

We now use our formula (2.51) for the curl of a curl

$$\nabla^2 \mathbf{V} = \nabla(\nabla \cdot \mathbf{V}) - \nabla \times (\nabla \times \mathbf{V}) \quad (2.60)$$

to write $\mathbf{V}(\mathbf{x})$ as

$$\mathbf{V}(\mathbf{x}) = -\nabla \left(\nabla \cdot \int \frac{\mathbf{V}(\mathbf{r})}{|\mathbf{r} - \mathbf{x}|} d^3r \right) + \nabla \times \left(\nabla \times \int \frac{\mathbf{V}(\mathbf{r})}{|\mathbf{r} - \mathbf{x}|} d^3r \right). \quad (2.61)$$

Thus any suitably smooth 3-dimensional vector field $\mathbf{V}(\mathbf{x})$ can be written as the sum

$$\mathbf{V}(\mathbf{x}) = \nabla\phi(\mathbf{x}) + \nabla \times \mathbf{A}(\mathbf{x}) \quad (2.62)$$

of the gradient of a scalar field

$$\phi(\mathbf{x}) = -\nabla \cdot \int \frac{\mathbf{V}(\mathbf{r})}{|\mathbf{r} - \mathbf{x}|} d^3r \quad (2.63)$$

and the curl of a vector field

$$\mathbf{A}(\mathbf{x}) = \nabla \times \int \frac{\mathbf{V}(\mathbf{r})}{|\mathbf{r} - \mathbf{x}|} d^3r \quad (2.64)$$

(Hermann von Helmholtz, 1821–1894). □

2.6 Dirac's delta function

A function f is a map from numbers x to numbers $f(x)$. A **functional** F is a map from functions f to numbers $F[f]$. Dirac's delta function $\delta(x - a)$ is a functional $\delta[f, a]$ that maps a function f to its value $f(a)$ at a particular point $x = a$. We may write this suggestively as

$$\delta[f, a] = f(a) = \int f(x) \delta(x - a) dx. \quad (2.65)$$

The delta functional let's one integrate by parts

$$-f'(b) = \int f(x) \delta'(x - b) dx \quad \text{and} \quad f''(c) = \int f(x) \delta''(x - c) dx. \quad (2.66)$$

Delta functions of several variables obey the same rules. For instance, in three dimensions

$$\delta[f, \mathbf{a}] = f(\mathbf{a}) = \int f(\mathbf{x}) \delta^{(3)}(\mathbf{x} - \mathbf{a}) d^3x. \quad (2.67)$$

One may imagine $\delta(x - a)$ to be a smooth function normalized to unity and very sharply peaked at $x = a$ like the $\epsilon \rightarrow 0$ limit of the gaussians

$$\frac{1}{(\pi\epsilon^2)^{1/2}} \exp\left(-\frac{(x-b)^2}{\epsilon^2}\right) \quad \text{or} \quad \frac{1}{(\pi\epsilon^2)^{3/2}} \exp\left(-\frac{\mathbf{x}-\mathbf{c}}{\epsilon^2}\right). \quad (2.68)$$

Delta functions often are written as Fourier transforms (section 3.11).

2.7 Covariant and Contravariant Vectors

The coordinates of time and space are often variously labelled as $x^0 = t$, $x^1 = x$, $x^2 = y$, and $x^3 = z$ or as x^i for $i = 0, 1, 2, 3$ or as x . Any one-to-one, smooth change of variables from x to $x'(x)$, is a **general coordinate transformation**.

Under a general coordinate transformation $x \rightarrow x'$ derivatives transform by the chain rule as

$$\frac{\partial}{\partial x'^i} = \sum_{k=0}^3 \frac{\partial x^k}{\partial x'^i} \frac{\partial}{\partial x^k} \quad \text{for } i = 0, 1, 2, 3. \quad (2.69)$$

Any vector V_i that transforms this way

$$V'_i = \sum_{k=0}^3 \frac{\partial x^k}{\partial x'^i} V_k \quad \text{for } i = 0, 1, 2, 3. \quad (2.70)$$

under general coordinate transformations $x \rightarrow x'$ is a **covariant vector**.

The coordinate differentials dx'^i of the primed coordinates are related to those of the unprimed coordinates dx^k by the chain rule as

$$dx'^i = \sum_{k=0}^3 \frac{\partial x'^i}{\partial x^k} dx^k \quad \text{for } i = 0, 1, 2, 3. \quad (2.71)$$

Any vector V^i that transforms this way

$$V'^i = \sum_{k=0}^3 \frac{\partial x'^i}{\partial x^k} V^k \quad \text{for } i = 0, 1, 2, 3 \quad (2.72)$$

is a **contravariant vector**.

Covariant vectors ∂_i and V_i have lowered indexes. Contravariant vectors dx^i and V^i have raised indexes.

Exercises

- 2.1 Use formulas (2.13 and 2.14) to derive (2.15).
 2.2 Derive the first of the Levi-Civita identities (2.50).
 2.3 Derive the second of the Levi-Civita identities (2.50).
 2.4 Use the first of the Levi-Civita identities (2.50) to show that every 3-vector \mathbf{V} can be expressed in terms of any nonzero 3-vector \mathbf{k} as

$$\mathbf{V} = \frac{1}{\mathbf{k} \cdot \mathbf{k}} \left((\mathbf{k} \cdot \mathbf{V}) \mathbf{k} - \mathbf{k} \times (\mathbf{k} \times \mathbf{V}) \right). \quad (2.73)$$

- 2.5 Show that

$$\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{a} \nabla \cdot \mathbf{b} - \mathbf{b} \nabla \cdot \mathbf{a} + (\mathbf{b} \cdot \nabla) \mathbf{a} - (\mathbf{a} \cdot \nabla) \mathbf{b}. \quad (2.74)$$

- 2.6 Simplify $\nabla \times \nabla \phi$ and $\nabla \cdot (\nabla \times \mathbf{a})$ in which ϕ is a scalar field and \mathbf{a} is a vector field.
 2.7 Simplify $\nabla \cdot (\nabla \phi \times \nabla \psi)$ in which ϕ and ψ are scalar fields.
 2.8 Let $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla \phi - \dot{\mathbf{A}}$ and show that Maxwell's equations in vacuum (example 2.7) and the Lorentz gauge condition

$$\nabla \cdot \mathbf{A} + \dot{\phi}/c^2 = 0 \quad (2.75)$$

imply that \mathbf{A} and ϕ obey the wave equations

$$\Delta \phi - \ddot{\phi}/c^2 = 0 \quad \text{and} \quad \Delta \mathbf{A} - \ddot{\mathbf{A}}/c^2 = 0. \quad (2.76)$$

3

Fourier Series

3.1 Fourier series

The phases $\exp(inx)/\sqrt{2\pi}$ for integer n are orthonormal on an interval of length 2π

$$\int_0^{2\pi} \frac{e^{-imx}}{\sqrt{2\pi}} \frac{e^{inx}}{\sqrt{2\pi}} dx = \int_0^{2\pi} \frac{e^{i(n-m)x}}{2\pi} dx = \delta_{m,n} = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases} \quad (3.1)$$

in which $\delta_{n,m}$ is Kronecker's delta (1.38). So if a function $f(x)$ is a sum of these phases, called a **Fourier Series**,

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{inx}}{\sqrt{2\pi}}, \quad (3.2)$$

then the orthonormality (3.1) of these phases $\exp(inx)/\sqrt{2\pi}$ gives the n th coefficient f_n as the integral

$$\int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} f(x) dx = \int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} f_m \frac{e^{imx}}{\sqrt{2\pi}} dx = \sum_{m=-\infty}^{\infty} \delta_{n,m} f_m = f_n. \quad (3.3)$$

Fourier series can represent functions $f(x)$ that are square integrable on the interval $0 < x < 2\pi$ (Joseph Fourier 1768–1830).

In Dirac's notation, we interpret the phase

$$\langle x|n\rangle = \frac{e^{inx}}{\sqrt{2\pi}} \quad (3.4)$$

as the inner product of the ket $|n\rangle$ with the bra $\langle x|$, and we assume that the kets $|x\rangle$ and $|n\rangle$ form a complete sets of states that represent the identity

operator as

$$I = \int_0^{2\pi} |x\rangle\langle x| dx = \sum_{n=-\infty}^{\infty} |n\rangle\langle n|. \quad (3.5)$$

In these terms, the orthonormality integral (3.1) says that the inner product of $|n\rangle$ and $|m\rangle$ is unity when $n = m$ and zero when $n \neq m$

$$\langle m|n\rangle = \langle m|I|n\rangle = \int_0^{2\pi} \langle m|x\rangle\langle x|n\rangle dx = \int_0^{2\pi} \frac{e^{i(n-m)x}}{2\pi} dx = \delta_{m,n}. \quad (3.6)$$

Thus the kets $|n\rangle$ are orthonormal.

The representation (3.5) of the identity operator, together with the formula (3.4) for $\langle x|n\rangle$, shows that the inner product $f(x) = \langle x|f\rangle$, which is the component of the vector $|f\rangle$ in the $|x\rangle$ basis, is given by the Fourier series (3.2)

$$\begin{aligned} f(x) &= \langle x|f\rangle = \langle x|I|f\rangle = \sum_{n=-\infty}^{\infty} \langle x|n\rangle\langle n|f\rangle \\ &= \sum_{n=-\infty}^{\infty} \frac{e^{inx}}{\sqrt{2\pi}} \langle n|f\rangle = \sum_{n=-\infty}^{\infty} \frac{e^{inx}}{\sqrt{2\pi}} f_n. \end{aligned} \quad (3.7)$$

Similarly, the representation (3.5) of the identity operator shows that the inner products $f_n = \langle n|f\rangle$, which are the components of the vector $|f\rangle$ in the $|n\rangle$ basis, are the Fourier integrals (3.3)

$$f_n = \langle n|f\rangle = \langle n|I|f\rangle = \int_0^{2\pi} \langle n|x\rangle\langle x|f\rangle dx = \int_0^{2\pi} \frac{e^{-inx}}{\sqrt{2\pi}} f(x) dx. \quad (3.8)$$

The two representations (3.5) of the identity operator also give two ways of writing the inner product $\langle g|f\rangle$ of two vectors $|f\rangle$ and $|g\rangle$

$$\begin{aligned} \langle g|f\rangle &= \sum_{n=-\infty}^{\infty} \langle g|n\rangle\langle n|f\rangle = \sum_{n=-\infty}^{\infty} g_n^* f_n \\ &= \int_0^{2\pi} \langle g|x\rangle\langle x|f\rangle dx = \int_0^{2\pi} g^*(x) f(x) dx. \end{aligned} \quad (3.9)$$

When the vectors are the same, this identity shows that the sum of the squared absolute values of the Fourier coefficients f_n is equal to the integral of the squared absolute value $|f(x)|^2$

$$\langle f|f\rangle = \sum_{n=-\infty}^{\infty} |\langle n|f\rangle|^2 = \sum_{n=-\infty}^{\infty} |f_n|^2 = \int_0^{2\pi} |\langle x|f\rangle|^2 dx = \int_0^{2\pi} |f(x)|^2 dx. \quad (3.10)$$

The Fourier series (3.2 & 3.7) are **periodic** with period 2π because the phases $\langle x|n\rangle$ are periodic with period 2π , $\exp(in(x+2\pi)) = \exp(inx)$. Thus even if the function $f(x)$ which we use in (3.3 and 3.8) to make the Fourier coefficients $f_n = \langle n|f\rangle$ is not periodic, its Fourier series (3.2 and 3.7) will nevertheless be strictly periodic, as illustrated by Figs. 3.2 and 3.4.

The complex conjugate of the Fourier series (3.2 and 3.7) is

$$f^*(x) = \sum_{n=-\infty}^{\infty} f_n^* \frac{e^{-inx}}{\sqrt{2\pi}} = \sum_{n=-\infty}^{\infty} f_{-n}^* \frac{e^{inx}}{\sqrt{2\pi}} \quad (3.11)$$

so the n th Fourier coefficient $f_n(f^*)$ for $f^*(x)$ is the complex conjugate of the $-n$ th Fourier coefficient for $f(x)$

$$f_n(f^*) = f_{-n}^*(f). \quad (3.12)$$

Thus if the function $f(x)$ is real, then

$$f_n(f) = f_n(f^*) = f_{-n}^*(f) \quad \text{or} \quad f_n = f_{-n}^*. \quad (3.13)$$

Example 3.1 (Fourier Series by Inspection) The doubly exponential function $\exp(\exp(ix))$ has the Fourier series

$$\exp(e^{ix}) = \sum_{n=0}^{\infty} \frac{1}{n!} e^{inx} \quad (3.14)$$

in which $n! = n(n-1)\dots 1$ is n -factorial with $0! \equiv 1$. □

Example 3.2 (Beats) The sum of two sines $f(x) = \sin \omega_1 x + \sin \omega_2 x$ of similar frequencies $\omega_1 \approx \omega_2$ is the product (exercise 3.1)

$$f(x) = 2 \cos \frac{1}{2}(\omega_1 - \omega_2)x \sin \frac{1}{2}(\omega_1 + \omega_2)x. \quad (3.15)$$

The first factor $\cos \frac{1}{2}(\omega_1 - \omega_2)x$ is the **beat**; it modulates the second factor $\sin \frac{1}{2}(\omega_1 + \omega_2)x$ as illustrated by Fig. 3.1. □

Example 3.3 (Laplace's equation) The Fourier series (exercise 3.2)

$$f(\rho, \theta) = \sum_{n=-\infty}^{\infty} \left(\frac{\rho}{a}\right)^{|n|} \left[\int_0^{2\pi} h(\theta') \frac{e^{-in\theta'}}{\sqrt{2\pi}} d\theta' \right] \frac{e^{in\theta}}{\sqrt{2\pi}} \quad (3.16)$$

(Ritt, 1970, p. 3) obeys Laplace's equation (7.23)

$$\frac{1}{\rho} \frac{d}{d\rho} \left(\rho \frac{df}{d\rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 f}{\partial \theta^2} = 0 \quad (3.17)$$

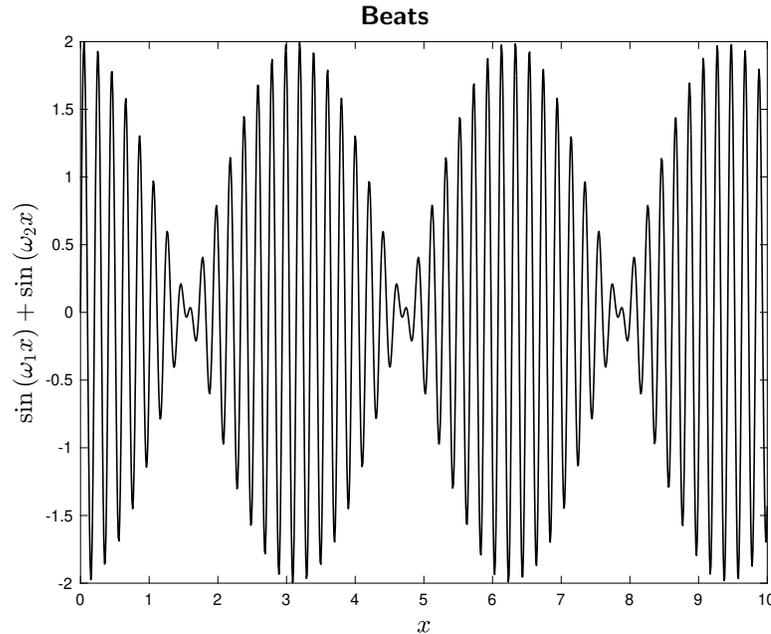


Figure 3.1 The curve $\sin \omega_1 x + \sin \omega_2 x$ for $\omega_1 = 30$ and $\omega_2 = 32$. Matlab scripts for this chapter's figures are in `Fourier_series` at github.com/kevinecahill.

for $\rho < a$ and respects the boundary condition $f(a, \theta) = h(\theta)$. \square

3.2 The interval

In section 3.1, we singled out the interval $[0, 2\pi]$, but to represent a periodic function $f(x)$ of period 2π , we could have used any interval of length 2π , such as the interval $[-\pi, \pi]$ or $[r, r + 2\pi]$

$$f_n = \int_r^{r+2\pi} e^{-inx} f(x) \frac{dx}{\sqrt{2\pi}}. \quad (3.18)$$

This integral is independent of its lower limit r when the function $f(x)$ is periodic with period 2π . The choice $r = -\pi$ is often convenient. With this choice of interval, the coefficient f_n is the integral (3.3) shifted by $-\pi$

$$f_n = \int_{-\pi}^{\pi} e^{-inx} f(x) \frac{dx}{\sqrt{2\pi}}. \quad (3.19)$$

But if the function $f(x)$ is not periodic with period 2π , then the Fourier coefficients (3.18) do depend upon the choice r of interval.

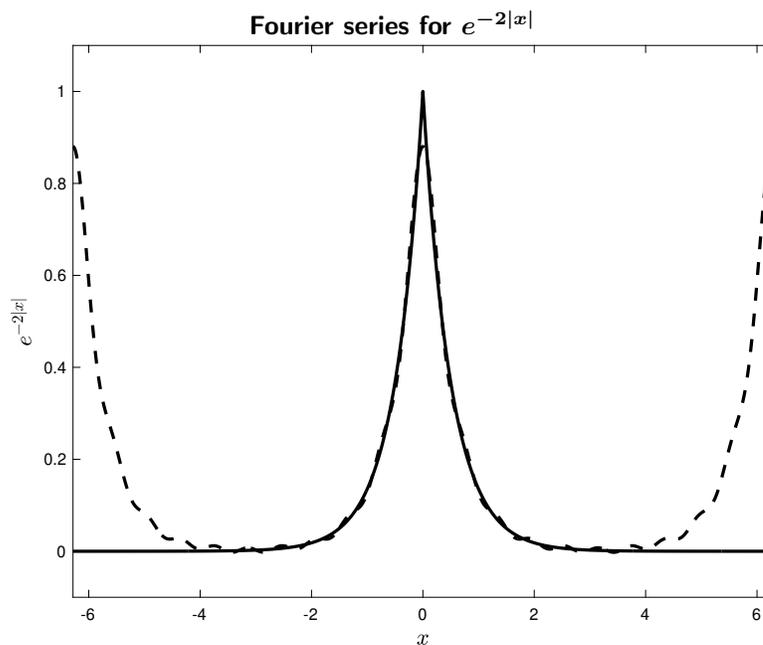


Figure 3.2 The 10-term (dashes) Fourier series (3.24) for the function $\exp(-2|x|)$ on the interval $(-\pi, \pi)$ is plotted from -2π to 2π . All Fourier series are periodic, but the function $\exp(-2|x|)$ (solid) is not.

3.3 Where to Put the 2Pi's

In sections 3.1–3.2, we used the orthonormal functions $\exp(inx)/\sqrt{2\pi}$, and so we had factors of $1/\sqrt{2\pi}$ in the Fourier equations (3.2, 3.3, 3.7, and 3.8). One can avoid these square roots by setting $d_n = f_n/\sqrt{2\pi}$ and writing the Fourier series (3.2) and the orthonormality relation (3.3) as

$$f(x) = \sum_{n=-\infty}^{\infty} d_n e^{inx} \quad \text{and} \quad d_n = \frac{1}{2\pi} \int_0^{2\pi} dx e^{-inx} f(x) \quad (3.20)$$

or by setting $c_n = \sqrt{2\pi} f_n$ and using the rules

$$f(x) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} c_n e^{inx} \quad \text{and} \quad c_n = \int_{-\pi}^{\pi} f(x) e^{-inx} dx. \quad (3.21)$$

The cost of these asymmetrical notations is that factors of 2π pop up (exercise 3.3) in equations (3.9 and 3.10) for the inner products $\langle g|f \rangle$ and $\langle f|f \rangle$.

Example 3.4 (Fourier Series for $\exp(-m|x|)$) Let's compute the Fourier

series for the real function $f(x) = \exp(-m|x|)$ on the interval $(-\pi, \pi)$. Using the shifted interval (3.19) and the 2π -placement convention (3.20), we find that the coefficient d_n is the integral

$$d_n = \int_{-\pi}^{\pi} \frac{dx}{2\pi} e^{-inx} e^{-m|x|} \quad (3.22)$$

which we may do as two simpler integrals

$$\begin{aligned} d_n &= \int_{-\pi}^0 \frac{dx}{2\pi} e^{(m-in)x} + \int_0^{\pi} \frac{dx}{2\pi} e^{-(m+in)x} \\ &= \frac{1}{\pi} \frac{m}{m^2 + n^2} [1 - (-1)^n e^{-\pi m}] \end{aligned} \quad (3.23)$$

which shows that $d_n = d_{-n}$. Since m is real, the coefficients d_n also are real, $d_n = d_n^*$. They therefore satisfy the condition (3.13) that holds for real functions, $d_n = d_{-n}^*$, and give the Fourier series for $\exp(-m|x|)$ as

$$\begin{aligned} e^{-m|x|} &= \sum_{n=-\infty}^{\infty} d_n e^{inx} = \sum_{n=-\infty}^{\infty} \frac{1}{\pi} \frac{m}{m^2 + n^2} [1 - (-1)^n e^{-\pi m}] e^{inx} \\ &= \frac{(1 - e^{-\pi m})}{m\pi} + \sum_{n=1}^{\infty} \frac{2}{\pi} \frac{m}{m^2 + n^2} [1 - (-1)^n e^{-\pi m}] \cos(nx). \end{aligned} \quad (3.24)$$

In Fig. 3.2, the 10-term (dashes) Fourier series for $m = 2$ is plotted from $x = -2\pi$ to $x = 2\pi$. The function $\exp(-2|x|)$ itself is represented by a solid line. Although $\exp(-2|x|)$ is not periodic, its Fourier series is periodic with period 2π . The 10-term Fourier series represents the function $\exp(-2|x|)$ quite well within the interval $[-\pi, \pi]$.

In what follows, we usually won't bother to use different letters to distinguish between the symmetric (3.2 and 3.3) and asymmetric conventions (3.20 or 3.21) on the placement of the 2π 's. \square

3.4 Real Fourier series for real functions

The rules (3.1–3.3 and 3.18–3.21) for Fourier series are simple and apply to functions that are continuous and periodic whether complex or real. If a function $f(x)$ is real, then its Fourier coefficients obey the rule (3.13) that holds for real functions, $d_{-n} = d_n^*$. Thus d_0 is real, $d_0 = d_0^*$, and we may

write the Fourier series (3.20) for a real function $f(x)$ as

$$\begin{aligned}
 f(x) &= d_0 + \sum_{n=1}^{\infty} d_n e^{inx} + \sum_{n=-\infty}^{-1} d_n e^{inx} \\
 &= d_0 + \sum_{n=1}^{\infty} [d_n e^{inx} + d_{-n} e^{-inx}] = d_0 + \sum_{n=1}^{\infty} [d_n e^{inx} + d_n^* e^{-inx}] \\
 &= d_0 + \sum_{n=1}^{\infty} d_n (\cos nx + i \sin nx) + d_n^* (\cos nx - i \sin nx) \\
 &= d_0 + \sum_{n=1}^{\infty} (d_n + d_n^*) \cos nx + i(d_n - d_n^*) \sin nx. \tag{3.25}
 \end{aligned}$$

In terms of the real coefficients

$$a_n = d_n + d_n^* \quad \text{and} \quad b_n = i(d_n - d_n^*), \tag{3.26}$$

the Fourier series (3.25) of a real function $f(x)$ is

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + b_n \sin nx. \tag{3.27}$$

Using the formulas (3.26) for a_n and (3.20) for d_n as well as the reality of the function $f(x)$, we find that a_n is

$$a_n = \int_0^{2\pi} [e^{-inx} f(x) + e^{inx} f^*(x)] \frac{dx}{2\pi} = \int_0^{2\pi} \frac{(e^{-inx} + e^{inx})}{2} f(x) \frac{dx}{\pi}. \tag{3.28}$$

So the coefficient a_n of $\cos nx$ in (3.27) is the cosine integral of $f(x)$

$$a_n = \int_0^{2\pi} \cos nx f(x) \frac{dx}{\pi}. \tag{3.29}$$

Similarly, equations (3.20 and 3.26) and the reality of $f(x)$ imply that the coefficient b_n is the sine integral of $f(x)$

$$b_n = \int_0^{2\pi} i \frac{(e^{-inx} - e^{inx})}{2} f(x) \frac{dx}{\pi} = \int_0^{2\pi} \sin nx f(x) \frac{dx}{\pi}. \tag{3.30}$$

The real Fourier series (3.27) and the cosine (3.29) and sine (3.30) integrals

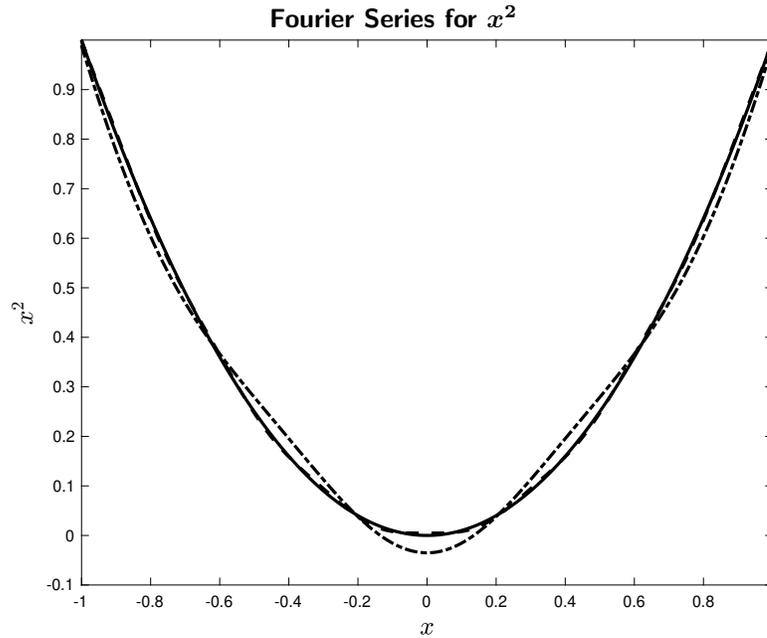


Figure 3.3 The function x^2 (solid) and its Fourier series of 7 terms (dot dash) and 20 terms (dashes). The Fourier series (3.37) for x^2 quickly converges well inside the interval $(-\pi, \pi)$.

for the coefficients a_n and b_n also follow from the orthogonality relations

$$\int_0^{2\pi} \sin mx \sin nx \, dx = \begin{cases} \pi & \text{if } n = m \neq 0 \\ 0 & \text{otherwise,} \end{cases} \quad (3.31)$$

$$\int_0^{2\pi} \cos mx \cos nx \, dx = \begin{cases} \pi & \text{if } n = m \neq 0 \\ 2\pi & \text{if } n = m = 0 \\ 0 & \text{otherwise, and} \end{cases} \quad (3.32)$$

$$\int_0^{2\pi} \sin mx \cos nx \, dx = 0 \quad (3.33)$$

which hold for integer values of n and m .

If the function $f(x)$ is periodic with period 2π , then instead of the interval $[0, 2\pi]$, one may choose any interval of length 2π such as $[-\pi, \pi]$.

What if a function $f(x)$ is not periodic? The Fourier series for an aperiodic function is itself strictly periodic, is sensitive to its interval $(r, r + 2\pi)$ of definition, may differ somewhat from the function near the ends of the interval, and usually differs markedly from it outside the interval.

Example 3.5 (Fourier series for x^2) The function x^2 is even and so the

integrals (3.30) for its sine Fourier coefficients b_n all vanish. Its cosine coefficients a_n are given by (3.29)

$$a_n = \int_{-\pi}^{\pi} \cos nx f(x) \frac{dx}{\pi} = \int_{-\pi}^{\pi} \cos nx x^2 \frac{dx}{\pi}. \quad (3.34)$$

Integrating twice by parts, we find for $n \neq 0$

$$a_n = -\frac{2}{n} \int_{-\pi}^{\pi} x \sin nx \frac{dx}{\pi} = \left[\frac{2x \cos nx}{\pi n^2} \right]_{-\pi}^{\pi} = (-1)^n \frac{4}{n^2} \quad (3.35)$$

and

$$a_0 = \int_{-\pi}^{\pi} x^2 \frac{dx}{\pi} = \frac{2\pi^2}{3}. \quad (3.36)$$

Equation (3.27) now gives for x^2 the cosine Fourier series

$$x^2 = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx = \frac{\pi^2}{3} + 4 \sum_{n=1}^{\infty} (-1)^n \frac{\cos nx}{n^2}. \quad (3.37)$$

This series rapidly converges within the interval $[-1, 1]$ as shown in Fig. 3.3, but not near the endpoints $\pm\pi$. \square

Example 3.6 (Gibbs overshoot) The function $f(x) = x$ on the interval $[-\pi, \pi]$ is not periodic. So we expect trouble if we represent it as a Fourier series. Since x is an odd function, equation (3.29) tells us that the coefficients a_n all vanish. By (3.30), the b_n 's are

$$b_n = \int_{-\pi}^{\pi} \frac{dx}{\pi} x \sin nx = 2(-1)^{n+1} \frac{1}{n}. \quad (3.38)$$

As shown in Fig. 3.4, the series

$$\sum_{n=1}^{\infty} 2(-1)^{n+1} \frac{1}{n} \sin nx \quad (3.39)$$

differs by about 2π from the function $f(x) = x$ for $-3\pi < x < -\pi$ and for $\pi < x < 3\pi$ because the series is periodic while the function x isn't.

Within the interval $(-\pi, \pi)$, the series with 100 terms is very accurate except for $x \gtrsim -\pi$ and $x \lesssim \pi$, where it overshoots by about 9% of the 2π discontinuity, a defect called a **Gibbs overshoot** (J. Willard Gibbs 1839–1903. Incidentally, Gibbs's father helped defend the Africans of the schooner *La Amistad*). Any time we use a Fourier series to represent an aperiodic function, a Gibbs overshoot will occur near the endpoints of the interval. \square

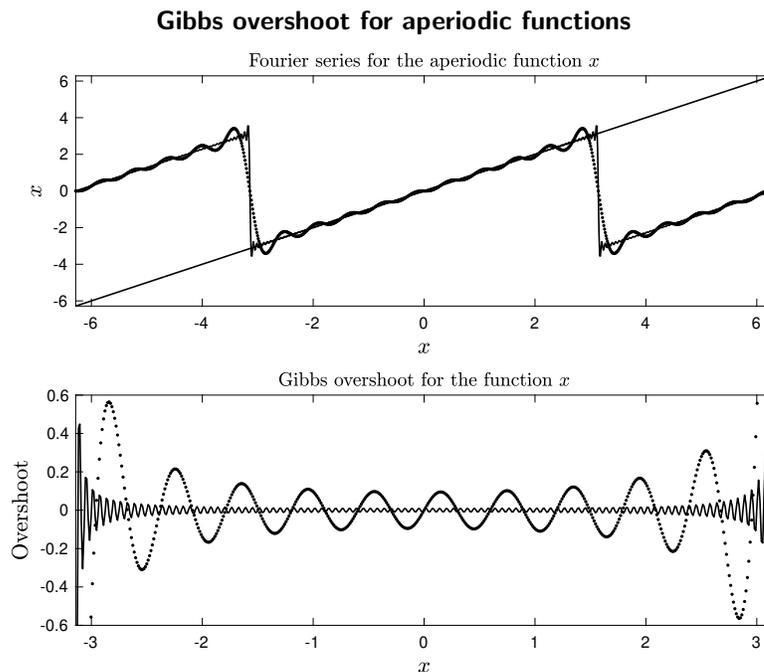


Figure 3.4 (top) The Fourier series (3.39) for the function x (solid line) with 10 terms (dots) and 100 terms (solid curve) for $-2\pi < x < 2\pi$. The Fourier series is periodic, but the function x is not. (bottom) The differences between x and the 10-term (dots) and the 100-term (solid curve) series on $(-\pi, \pi)$ exhibit a Gibbs overshoot of about 9% at $x \gtrsim -\pi$ and at $x \lesssim \pi$.

3.5 Stretched intervals

If the interval of periodicity is of length L instead of 2π , then we may use the phases $\exp(i2\pi nx/\sqrt{L})$ which are orthonormal on the interval $[0, L]$

$$\int_0^L dx \left(\frac{e^{i2\pi nx/L}}{\sqrt{L}} \right)^* \frac{e^{i2\pi mx/L}}{\sqrt{L}} = \delta_{nm}. \quad (3.40)$$

The Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad (3.41)$$

is periodic with period L . The coefficient f_n is the integral

$$f_n = \int_0^L \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) dx \quad (3.42)$$

and the sum of the squares $|f_n|^2$ is the integral of $|f(x)|^2$

$$\sum_{n=-\infty}^{\infty} |f_n|^2 = \int_0^L |f(x)|^2 dx. \quad (3.43)$$

These relations (3.40–3.43) generalize to the interval $[0, L]$ our earlier formulas of section 3.1 for the interval $[0, 2\pi]$.

If the function $f(x)$ is periodic with period L , that is if $f(x + nL) = f(x)$ for any integer n , then we may shift the domain of integration by any real number r

$$f_n = \int_r^{L+r} \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) dx \quad (3.44)$$

without changing the coefficients f_n . An obvious choice is $r = -L/2$ for which (3.41) and (3.42) give

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad \text{and} \quad f_n = \int_{-L/2}^{L/2} \frac{e^{-i2\pi nx/L}}{\sqrt{L}} f(x) dx. \quad (3.45)$$

If the function $f(x)$ is real, then on the interval $[0, L]$ in place of Eqs.(3.27), (3.29), and (3.30), one has

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{L}\right) + b_n \sin\left(\frac{2\pi nx}{L}\right), \quad (3.46)$$

$$a_n = \frac{2}{L} \int_0^L dx \cos\left(\frac{2\pi nx}{L}\right) f(x), \quad (3.47)$$

and

$$b_n = \frac{2}{L} \int_0^L dx \sin\left(\frac{2\pi nx}{L}\right) f(x). \quad (3.48)$$

The corresponding orthogonality relations, which follow from Eqs.(3.31), (3.32), & (3.33), are:

$$\int_0^L dx \sin\left(\frac{2\pi mx}{L}\right) \sin\left(\frac{2\pi nx}{L}\right) = \begin{cases} L/2 & \text{if } n = m \neq 0 \\ 0 & \text{otherwise,} \end{cases} \quad (3.49)$$

$$\int_0^L dx \cos\left(\frac{2\pi mx}{L}\right) \cos\left(\frac{2\pi nx}{L}\right) = \begin{cases} L/2 & \text{if } n = m \neq 0 \\ L & \text{if } n = m = 0 \\ 0 & \text{otherwise, and} \end{cases} \quad (3.50)$$

$$\int_0^L dx \sin\left(\frac{2\pi mx}{L}\right) \cos\left(\frac{2\pi nx}{L}\right) = 0. \quad (3.51)$$

They hold for integer values of n and m , and they imply Eqs.(3.46)–3.48).

3.6 Fourier Series of Functions of Several Variables

On an interval $[0, L]$, the Fourier-series formulas (3.41 & 3.42) are

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad \text{and} \quad f_n = \int_0^L \frac{e^{-2i\pi nx/L}}{\sqrt{L}} f(x) dx. \quad (3.52)$$

We may generalize these equations from one variable to m variables $x = (x_1, \dots, x_m)$ and $n = (n_1, \dots, n_m)$ with $n \cdot x = n_1 x_1 + \dots + n_m x_m$

$$\begin{aligned} f(x) &= \sum_{n_1=-\infty}^{\infty} \cdots \sum_{n_m=-\infty}^{\infty} f_n \frac{e^{i2\pi n \cdot x/L}}{L^{m/2}} \\ f_n &= \int_0^L dx_1 \cdots \int_0^L dx_m \frac{e^{-2i\pi n \cdot x/L}}{L^{m/2}} f(x). \end{aligned} \quad (3.53)$$

3.7 Integration and Differentiation of Fourier Series

What happens to the convergence of a Fourier series if we integrate or differentiate term by term? If we integrate the series

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad (3.54)$$

then we get a series

$$F(x) = \int_0^x dx' f(x') = \frac{f_0}{\sqrt{L}} x - i \frac{\sqrt{L}}{2\pi} \sum_{n=-\infty}^{\infty} \frac{f_n}{n} \left(e^{i2\pi nx/L} - 1 \right) \quad (3.55)$$

that converges **better** because of the extra factor of $1/n$. An integrated function $f(x)$ is smoother which makes its Fourier series converges better.

But if we differentiate the same series, then we get a series

$$f'(x) = i \frac{2\pi}{L^{3/2}} \sum_{n=-\infty}^{\infty} n f_n e^{i2\pi nx/L} \quad (3.56)$$

that converges **less well** because of the extra factor of n . A differentiated function is rougher, and so its Fourier series converges less well.

3.8 How Fourier series converge

A Fourier series represents a function $f(x)$ as the limit of a sequence of functions $f_N(x)$ given by

$$f_N(x) = \sum_{n=-N}^N f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} \quad \text{in which} \quad f_n = \int_0^L f(x) e^{-i2\pi nx/L} \frac{dx}{\sqrt{L}}. \quad (3.57)$$

Since the exponentials are periodic with period L , a Fourier series always is periodic. So if a function $f(x)$ is not periodic, then its Fourier series will be its **periodic extension** f_p defined by

$$f_p(x + nL) = f(x) \quad (3.58)$$

for all integers n and for $0 \leq x \leq L$.

A sequence of functions $f_N(x)$ **converges** to a function $f(x)$ on a **closed** interval $[a, b]$ if for every $\epsilon > 0$ and each point $a \leq x \leq b$, there exists an integer $N(\epsilon, x)$ such that

$$|f(x) - f_N(x)| < \epsilon \quad \text{for all} \quad N > N(\epsilon, x). \quad (3.59)$$

If this holds for an $N(\epsilon, x) = N(\epsilon)$ that is independent of $x \in [a, b]$, then the sequence of functions $f_N(x)$ **converges uniformly** to $f(x)$ on the interval $[a, b]$.

A function $f(x)$ is **continuous** on an **open** interval (a, b) if for every point $a < x < b$ the two limits

$$f(x-0) \equiv \lim_{0 < \epsilon \rightarrow 0} f(x-\epsilon) \quad \text{and} \quad f(x+0) \equiv \lim_{0 < \epsilon \rightarrow 0} f(x+\epsilon) \quad (3.60)$$

agree. If $f(x)$ also has the limits $f(a+0) = f(a)$ and $f(b-0) = f(b)$, then f is continuous on the **closed** interval $[a, b]$. A function continuous on a closed interval $[a, b]$ is bounded and integrable on that interval.

If a sequence of continuous functions $f_N(x)$ converges uniformly to a function $f(x)$ on a closed interval $a \leq x \leq b$, then $|f_N(x) - f(x)| < \epsilon$ for $N > N(\epsilon)$, and so for $N > N(\epsilon)$

$$\left| \int_a^b f_N(x) dx - \int_a^b f(x) dx \right| \leq \int_a^b |f_N(x) - f(x)| dx < (b-a)\epsilon. \quad (3.61)$$

Thus one may integrate a uniformly convergent sequence of continuous functions on a closed interval $[a, b]$ term by term

$$\lim_{N \rightarrow \infty} \int_a^b f_N(x) dx = \int_a^b \lim_{N \rightarrow \infty} f_N(x) dx = \int_a^b f(x) dx. \quad (3.62)$$

So if a Fourier series (3.2) converges uniformly, then the term-by-term integration implicit in the formula (3.3) for f_n is permitted.

A function is **piecewise continuous** on $[a, b]$ if it is continuous there except for finite jumps from $f(x-0)$ to $f(x+0)$ at a finite number of points x . At such jumps, we *define* the periodically extended function f_p to be the mean $f_p(x) = [f(x-0) + f(x+0)]/2$.

Fourier's convergence theorem (Courant, 1937, p. 439): The Fourier series of a function $f(x)$ that is piecewise continuous with a piecewise continuous first derivative converges to its periodic extension $f_p(x)$. This convergence is uniform on every closed interval on which the function $f(x)$ is continuous (and absolute if the function $f(x)$ has no discontinuities). Examples 3.12 and 3.13 illustrate this result.

A function whose k th derivative is continuous is in **class C^k** . On the interval $[-\pi, \pi]$, its Fourier coefficients (3.21) are

$$f_n = \int_{-\pi}^{\pi} f(x) e^{-inx} dx. \quad (3.63)$$

If f is both periodic and in C^k , then one integration by parts gives

$$f_n = \int_{-\pi}^{\pi} \left\{ \frac{d}{dx} \left[f(x) \frac{e^{-inx}}{-in} \right] - f'(x) \frac{e^{-inx}}{-in} \right\} dx = \int_{-\pi}^{\pi} f'(x) \frac{e^{-inx}}{in} dx$$

since the boundary terms cancel by periodicity, and k integrations by parts give

$$f_n = \int_{-\pi}^{\pi} f^{(k)}(x) \frac{e^{-inx}}{(in)^k} dx \quad (3.64)$$

since the derivatives $f^{(\ell)}(x)$ of a C^k periodic function also are periodic. Moreover if $f^{(k+1)}$ is piecewise continuous, then

$$\begin{aligned} f_n &= \int_{-\pi}^{\pi} \left\{ \frac{d}{dx} \left[f^{(k)}(x) \frac{e^{-inx}}{-(in)^{k+1}} \right] - f^{(k+1)}(x) \frac{e^{-inx}}{-(in)^{k+1}} \right\} dx \\ &= \int_{-\pi}^{\pi} f^{(k+1)}(x) \frac{e^{-inx}}{(in)^{k+1}} dx. \end{aligned} \quad (3.65)$$

Since $f^{(k+1)}(x)$ is piecewise continuous on the closed interval $[-\pi, \pi]$, it is bounded there in absolute value by, let us say, M . So the Fourier coefficients of a C^k periodic function with $f^{(k+1)}$ piecewise continuous are bounded by

$$|f_n| \leq \frac{1}{n^{k+1}} \int_{-\pi}^{\pi} |f^{(k+1)}(x)| dx \leq \frac{2\pi M}{n^{k+1}}. \quad (3.66)$$

We often can carry this derivation one step further. In most simple examples, the piecewise continuous periodic function $f^{(k+1)}(x)$ actually is piecewise continuously differentiable between its successive jumps at x_j . In this case, the derivative $f^{(k+2)}(x)$ is a piecewise continuous function plus a sum of a finite number of delta functions with finite coefficients. Thus we can integrate once more by parts. If for instance the function $f^{(k+1)}(x)$ jumps J times between $-\pi$ and π by $\Delta f_j^{(k+1)}$, then its Fourier coefficients are

$$\begin{aligned} f_n &= \int_{-\pi}^{\pi} f^{(k+2)}(x) \frac{e^{-inx}}{(in)^{k+2}} dx \\ &= \sum_{j=1}^J \int_{x_j}^{x_{j+1}} f_{pc}^{(k+2)}(x) \frac{e^{-inx}}{(in)^{k+2}} dx + \sum_{j=1}^J \Delta f_j^{(k+1)} \frac{e^{-inx_j}}{(in)^{k+2}} \end{aligned} \quad (3.67)$$

in which the subscript pc means piecewise continuous. The Fourier coefficients (3.67) then are bounded by

$$|f_n| \leq \frac{2\pi M}{n^{k+2}} \quad (3.68)$$

in which M is related to the maximum absolute values of $f_{pc}^{(k+2)}(x)$ and of the $\Delta f_j^{(k+1)}$. The Fourier series of periodic C^k functions converge rapidly if k is big.

Example 3.7 (Fourier Series of a C^0 Function) The function defined by

$$f(x) = \begin{cases} 0 & -\pi \leq x < 0 \\ x & 0 \leq x < \pi/2 \\ \pi - x & \pi/2 \leq x \leq \pi \end{cases} \quad (3.69)$$

is continuous on the interval $[-\pi, \pi]$ and its first derivative is piecewise continuous on that interval. By (3.66), its Fourier coefficients f_n should be bounded by M/n . In fact they are (exercise 3.10) bounded by $2\sqrt{2/\pi}/n^2$ in agreement with the stronger inequality (3.68)

$$f_n = \int_{-\pi}^{\pi} f(x) e^{-inx} \frac{dx}{\sqrt{2\pi}} = \frac{(-1)^{n+1} (i^n - 1)^2}{\sqrt{2\pi} n^2}. \quad (3.70)$$

□

Example 3.8 (Fourier Series for a C^1 Function) The function defined by $f(x) = 1 + \cos 2x$ for $|x| \leq \pi/2$ and $f(x) = 0$ for $|x| \geq \pi/2$ has a periodic extension f_p that is continuous with a continuous first derivative

and a piecewise continuous second derivative. Its Fourier coefficients (3.63)

$$f_n = \int_{-\pi/2}^{\pi/2} (1 + \cos 2x) e^{-inx} \frac{dx}{\sqrt{2\pi}} = \frac{8 \sin n\pi/2}{\sqrt{2\pi}(4n - n^3)}$$

satisfy the inequalities (3.66) and (3.68) for $k = 1$. \square

Example 3.9 (Fourier Series for $\cos \mu x$) The Fourier series for the even function $f(x) = \cos \mu x$ has only cosines with coefficients (3.29)

$$\begin{aligned} a_n &= \int_{-\pi}^{\pi} \cos nx \cos \mu x \frac{dx}{\pi} = \int_0^{\pi} [\cos(\mu + n)x + \cos(\mu - n)x] \frac{dx}{\pi} \\ &= \frac{1}{\pi} \left[\frac{\sin(\mu + n)\pi}{\mu + n} + \frac{\sin(\mu - n)\pi}{\mu - n} \right] = \frac{2}{\pi} \frac{\mu(-1)^n}{\mu^2 - n^2} \sin \mu\pi \end{aligned} \quad (3.71)$$

which decrease only as $1/n^2$ because $\cos \mu x$ is not periodic on $(-\pi, \pi)$ when μ is not an integer. The series (3.27) then is

$$\cos \mu x = \frac{2\mu \sin \mu\pi}{\pi} \left(\frac{1}{2\mu^2} - \frac{\cos x}{\mu^2 - 1^2} + \frac{\cos 2x}{\mu^2 - 2^2} - \frac{\cos 3x}{\mu^2 - 3^2} + \dots \right) \quad (3.72)$$

which is continuous at $x = \pm\pi$ (Courant, 1937, chap. IX). \square

Example 3.10 (Sine as an infinite product) In our series (3.72) for $\cos \mu x$, we set $x = \pi$, divide by $\sin \mu\pi$, replace μ with x , and so find for the cotangent the expansion

$$\cot \pi x = \frac{2x}{\pi} \left(\frac{1}{2x^2} + \frac{1}{x^2 - 1^2} + \frac{1}{x^2 - 2^2} + \frac{1}{x^2 - 3^2} + \dots \right) \quad (3.73)$$

or equivalently

$$\cot \pi x - \frac{1}{\pi x} = -\frac{2x}{\pi} \left(\frac{1}{1^2 - x^2} + \frac{1}{2^2 - x^2} + \frac{1}{3^2 - x^2} + \dots \right). \quad (3.74)$$

For $0 \leq x \leq q < 1$, the absolute value of the n th term on the right is less than $2q/(\pi(n^2 - q^2))$. Thus this series converges uniformly on $[0, x]$, and so we may integrate it term by term. We find (exercise 3.13)

$$\pi \int_0^x \left(\cot \pi t - \frac{1}{\pi t} \right) dt = \ln \frac{\sin \pi x}{\pi x} = \sum_{n=1}^{\infty} \int_0^x \frac{-2t dt}{n^2 - t^2} = \sum_{n=1}^{\infty} \ln \left[1 - \frac{x^2}{n^2} \right]. \quad (3.75)$$

Exponentiating, we get the infinite-product formula

$$\frac{\sin \pi x}{\pi x} = \exp \left[\sum_{n=1}^{\infty} \ln \left(1 - \frac{x^2}{n^2} \right) \right] = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2} \right) \quad (3.76)$$

for the sine from which one can derive the infinite product (exercise 3.14)

$$\cos \pi x = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{(n - \frac{1}{2})^2} \right) \quad (3.77)$$

for the cosine (Courant, 1937, chap. IX). \square

3.9 Measure and Lebesgue integration

Suppose S is a set of points x that lie in an interval $a \leq x \leq b$ of length $b - a$. All the points of S may also lie inside several subintervals $[a_i, b_i]$, $i = 1, 2, \dots$, the sum of whose lengths is $b_1 - a_1 + b_2 - a_2 + \dots$. Now consider all possible such sets of subintervals $[a_i, b_i]$ that contain all the points of S and let m be the greatest lower bound of the sum of their lengths. We may do the same for the complementary set S' consisting of all points of $[a, b]$ that do not lie in the set S . That is, we may let m' be the greatest lower bound of the sum of the lengths of all possible sets of subintervals $[c_i, d_i]$ that contain all the points of S' . If $m + m' = b - a$, then the set S is **measurable** and m is its measure. Every countable set x_i , $i = 1, 2, \dots$, has measure zero.

Suppose now that for $a \leq x \leq b$, all the values $f(x)$ of a function f lie in some finite interval J . We partition this interval J into disjoint subintervals J_k and let S_k be the set of points of $[a, b]$ that f maps into each subinterval J_k . If for every subinterval J_k , the set S_k is measurable, then the function $f(x)$ is **measurable** or **summable** on $[a, b]$. Suppose that f is measurable on this interval and let $m(S_k)$ be the measure the set S_k . Then for each subinterval J_k , we may pick any point $x_k \in S_k$ and approximate the integral of f over the interval $[a, b]$ by the sum $f(x_1)m(S_1) + f(x_2)m(S_2) + \dots$. This sum converges (Courant and Hilbert, 1955, pp. 108–111) to the Lebesgue integral as we refine the partition of the interval J into subintervals J_k such that the length L of the longest subinterval goes to zero

$$\lim_{L \rightarrow 0} \sum_{k=1}^{\infty} f(x_k) m(S_k) = \int_a^b f(x) dx \quad (3.78)$$

(Henri Lebesgue, 1875–1941).

Lebesgue integration generalizes Riemann integration and provides a more natural basis for discussions of convergence. One important theorem resulting from measure theory is that of Riesz and Fischer (Hardy and Rogosinski, 1944, p. 16): If a sum

$$\sum_{n=-\infty}^{\infty} |f_n|^2 < \infty \quad (3.79)$$

converges, then

1. there is a function f that is square integrable in the sense of Lebesgue (f is L^2 on $[a, b]$)

$$\int_a^b |f(x)|^2 dx < \infty \quad (3.80)$$

whose Fourier coefficients are

$$f_n = \int_a^b \frac{e^{-2\pi i n x / (b-a)}}{\sqrt{b-a}} f(x) dx; \quad (3.81)$$

2. the series

$$f_N(x) = \sum_{n=-N}^N f_n \frac{e^{2\pi i n x / (b-a)}}{\sqrt{b-a}} \quad (3.82)$$

converges to $f(x)$ **in the mean**,

$$\lim_{N \rightarrow \infty} \int_a^b |f_N(x) - f(x)|^2 dx = 0; \quad (3.83)$$

3. and

$$\int_a^b |f(x)|^2 dx = \sum_{n=-\infty}^{\infty} |f_n|^2 \quad (3.84)$$

which is (3.43) for $L = b - a$.

Another version of the Riesz-Fischer theorem is that a function $f(x)$ is square integrable (3.80) on an interval $[a, b]$ if and only if its Fourier series (3.82) converges to it in the mean (3.83).

Fourier series can represent a much wider class of functions than those that are continuous.

3.10 Quantum-mechanical examples

Suppose a particle of mass m is trapped in an infinitely deep one-dimensional square well of potential energy

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise.} \end{cases} \quad (3.85)$$

The hamiltonian operator is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x), \quad (3.86)$$

in which \hbar is Planck's constant divided by 2π . This tiny bit of action, $\hbar = 1.055 \times 10^{-34}$ Js, sets the scale below which quantum mechanics becomes important.

An eigenfunction $\psi(x)$ of the hamiltonian H with energy E satisfies the equation $H\psi(x) = E\psi(x)$ which breaks into two simple equations:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad \text{for } 0 < x < L \quad (3.87)$$

and

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \infty\psi(x) = E\psi(x) \quad \text{for } x < 0 \quad \text{and for } x > L. \quad (3.88)$$

Every solution of these equations with finite energy E must vanish outside the interval $0 < x < L$. So we must find solutions of the first equation (3.87) that satisfy the boundary conditions

$$\psi(x) = 0 \quad \text{for } x \leq 0 \quad \text{and } x \geq L. \quad (3.89)$$

For any integer $n \neq 0$, the continuous function

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \quad \text{for } x \in [0, L] \quad (3.90)$$

and $\psi_n(x) = 0$ for $x \notin (0, L)$ satisfies the boundary conditions (3.89). When inserted into equation (3.87)

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 \psi_n(x) = E_n \psi_n(x) \quad (3.91)$$

it reveals its energy to be $E_n = (n\pi\hbar/L)^2/2m$.

These eigenfunctions $\psi_n(x)$ are complete in the sense that they span the space of all functions $f(x)$ that are square-integrable on the interval $(0, L)$ and vanish at its end points. They provide for such functions the **sine Fourier series**

$$f(x) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \quad (3.92)$$

which is periodic with period $2L$ and is the Fourier series for a function that is odd $f(-x) = -f(x)$ on the interval $(-L, L)$ and zero at both ends.

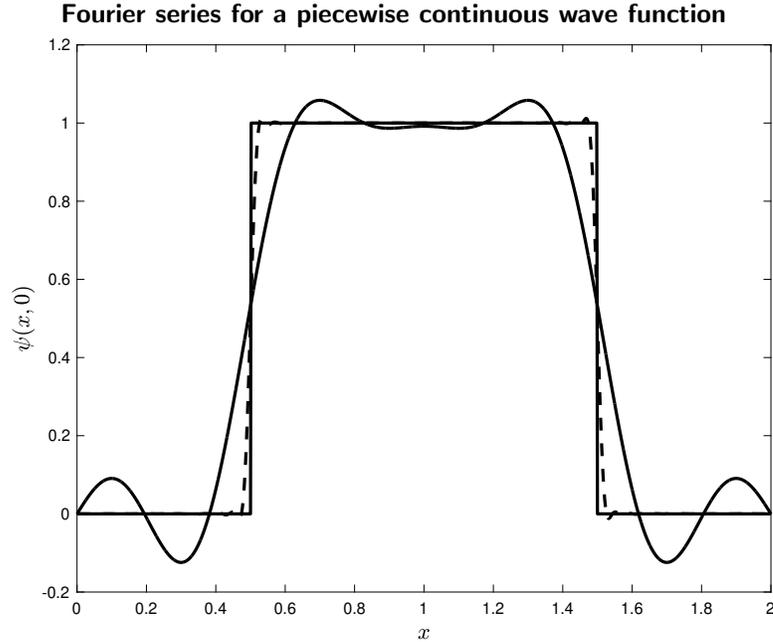


Figure 3.5 The piecewise continuous wave function $\psi(x, 0)$ for $L = 2$ (3.93, straight solid lines) and its Fourier series (3.95) with 10 terms (solid curve) and 100 terms (dashes). Gibbs overshoots occur near the discontinuities at $x = 1/2$ and $x = 3/2$.

Example 3.11 (Time Evolution of an Initially Piecewise Continuous Wave Function) Suppose now that at time $t = 0$ the particle is confined to the middle half of the well with the square wave function

$$\psi(x, 0) = \sqrt{\frac{2}{L}} \quad \text{for} \quad \frac{L}{4} < x < \frac{3L}{4} \quad (3.93)$$

and zero otherwise. This piecewise continuous C^{-1} wave function is discontinuous at $x = L/4$ and at $x = 3L/4$. Since the functions $\langle x|n\rangle = \psi_n(x)$ are orthonormal on $[0, L]$

$$\int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{\pi mx}{L}\right) = \delta_{nm} \quad (3.94)$$

the coefficients f_n in the Fourier series

$$\psi(x, 0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \quad (3.95)$$

Time evolution of $|\psi(x, t)|^2$ for a piecewise continuous wave function

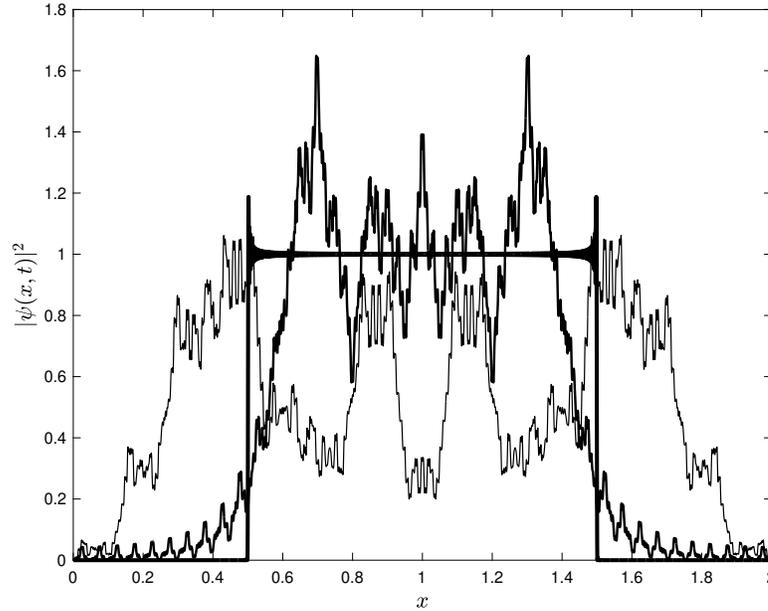


Figure 3.6 For length $L = 2$, the probability distributions $P(x, t) = |\psi(x, t)|^2$ of the 1000-term Fourier series (3.99) for the wave function $\psi(x, t)$ at $t = 0$ (thick curve), $t = 10^{-3} \tau$ (medium curve), and $\tau = 2mL^2/\hbar$ (thin curve). The jaggedness of $P(x, t)$ arises from the two discontinuities in the initial wave function $\psi(x, 0)$ (3.100) at $x = L/4$ and $x = 3L/4$. A Matlab script for the figure is in `Fourier_series` at github.com/kevinecahill.

are the inner products

$$f_n = \langle n | \psi, 0 \rangle = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) \psi(x, 0). \quad (3.96)$$

They are proportional to $1/n$ in accord with (3.68)

$$f_n = \frac{2}{L} \int_{L/4}^{3L/4} dx \sin\left(\frac{\pi n x}{L}\right) = \frac{2}{\pi n} \left[\cos\left(\frac{\pi n}{4}\right) - \cos\left(\frac{3\pi n}{4}\right) \right]. \quad (3.97)$$

Figure 3.5 plots the square wave function $\psi(x, 0)$ (3.93, straight solid lines) and its 10-term (solid curve) and 100-term (dashes) Fourier series (3.95) for an interval of length $L = 2$. Gibbs's overshoot reaches 1.093 at $x = 0.52$ for 100 terms and 1.0898 at $x = 0.502$ for 1000 terms (not shown), amounting to about 9% of the unit discontinuity at $x = 1/2$. A similar overshoot occurs at $x = 3/2$.

How does $\psi(x, 0)$ evolve with time? Since $\psi_n(x)$, the Fourier component

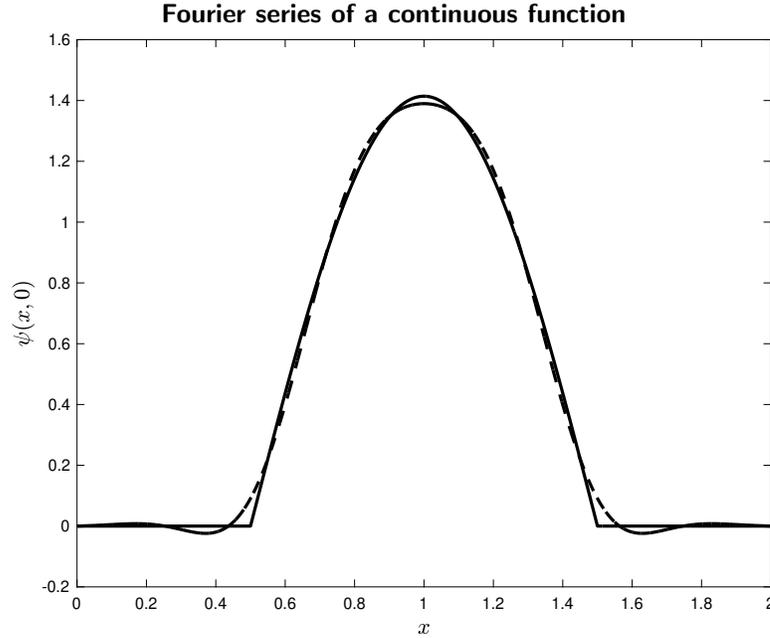


Figure 3.7 The continuous wave function $\psi(x, 0)$ (3.100, solid) and its 10-term Fourier series (3.103–3.104, dashes) are plotted for the interval $[0, 2]$.

(3.90), is an eigenfunction of H with energy E_n , the time-evolution operator $U(t) = \exp(-iHt/\hbar)$ takes $\psi(x, 0)$ into

$$\psi(x, t) = e^{-iHt/\hbar} \psi(x, 0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-iE_n t/\hbar}. \quad (3.98)$$

Because $E_n = (n\pi\hbar/L)^2/2m$, the wave function at time t is

$$\psi(x, t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-i\hbar(n\pi)^2 t/(2mL^2)}. \quad (3.99)$$

It is awkward to plot complex functions, so Fig. 3.6 displays the probability distributions $P(x, t) = |\psi(x, t)|^2$ of the 1000-term Fourier series (3.99) for the wave function $\psi(x, t)$ at $t = 0$ (thick curve), $t = 10^{-3} \tau$ (medium curve), and $\tau = 2mL^2/\hbar$ (thin curve). The discontinuities in the initial wave function $\psi(x, 0)$ cause both the Gibbs overshoots at $x = 1/2$ and $x = 3/2$ seen in the series for $\psi(x, 0)$ plotted in Fig. 3.5 and the choppiness of the probability distribution $P(x, t)$ exhibited in Fig.(3.6). \square

Example 3.12 (Time Evolution of a Continuous Function) What does the Fourier series of a continuous function look like? How does it evolve with

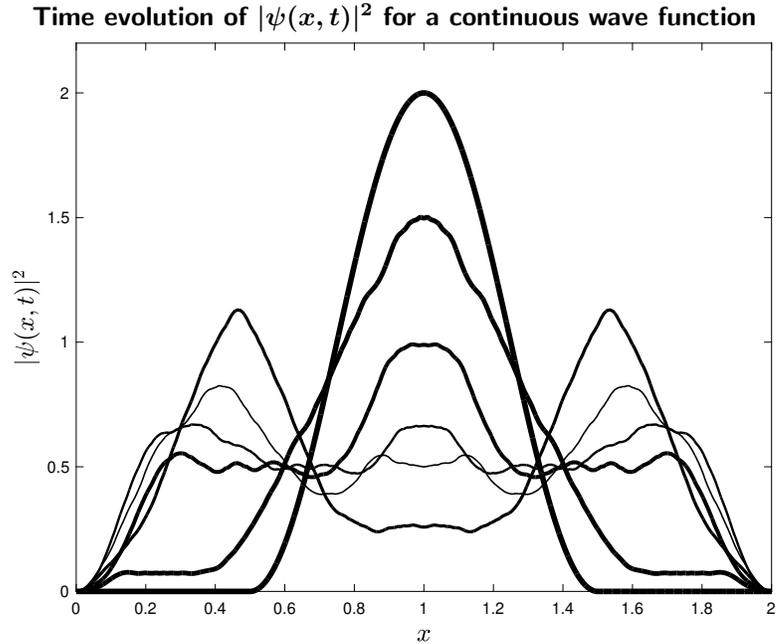


Figure 3.8 For the interval $[0, 2]$, the probability distributions $P(x, t) = |\psi(x, t)|^2$ of the 1000-term Fourier series (3.106) for the continuous wave function $\psi(x, t)$ (3.100) at $t = 0, 10^{-2}\tau, 10^{-1}\tau, \tau = 2mL^2/\hbar, 10\tau,$ and 100τ are plotted as successively thinner curves. A Matlab script for the figure is in `Fourier_series` at github.com/kevinecahill.

time? Let us take as the wave function at $t = 0$ the C^0 function

$$\psi(x, 0) = \frac{2}{\sqrt{L}} \sin\left(\frac{2\pi(x - L/4)}{L}\right) \quad \text{for } \frac{L}{4} < x < \frac{3L}{4} \quad (3.100)$$

and zero otherwise. This initial wave function is a continuous function with a piecewise continuous first derivative on the interval $[0, L]$, and it satisfies the periodic boundary condition $\psi(0, 0) = \psi(L, 0)$. It therefore satisfies the conditions of Fourier's convergence theorem (Courant, 1937, p. 439), and so its Fourier series converges uniformly (and absolutely) to $\psi(x, 0)$ on $[0, L]$.

As in Eq.(3.96), the Fourier coefficients f_n are given by the integrals

$$f_n = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nx}{L}\right) \psi(x, 0), \quad (3.101)$$

which now take the form

$$f_n = \frac{2\sqrt{2}}{L} \int_{L/4}^{3L/4} dx \sin\left(\frac{\pi nx}{L}\right) \sin\left(\frac{2\pi(x - L/4)}{L}\right). \quad (3.102)$$

Doing the integral, one finds that for $n \neq 2$

$$f_n = -\frac{\sqrt{2}}{\pi} \frac{4}{n^2 - 4} [\sin(3n\pi/4) + \sin(n\pi/4)] \quad (3.103)$$

while $f_2 = 0$. These Fourier coefficients satisfy the inequalities (3.66) and (3.68) for $k = 0$. The factor of $1/n^2$ in f_n guarantees the absolute convergence of the series

$$\psi(x, 0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) \quad (3.104)$$

because asymptotically the coefficient f_n is bounded by $|f_n| \leq A/n^2$ where A is a constant ($A = 144/(5\pi\sqrt{L})$ will do) and the sum of $1/n^2$ converges to the Riemann zeta function (5.106)

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \zeta(2) = \frac{\pi^2}{6}. \quad (3.105)$$

Figure 3.7 plots the 10-term Fourier series (3.104) for $\psi(x, 0)$ for $L = 2$. Because this series converges absolutely and uniformly on $[0, 2]$, the 100-term and 1000-term series were too close to $\psi(x, 0)$ to be seen clearly in the figure and so were omitted.

As time goes by, the wave function $\psi(x, t)$ evolves from $\psi(x, 0)$ to

$$\psi(x, t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-i\hbar(n\pi)^2 t / (2mL^2)} \quad (3.106)$$

in which the Fourier coefficients are given by (3.103). Because $\psi(x, 0)$ is continuous and periodic with a piecewise continuous first derivative, its evolution in time is much calmer than that of the piecewise continuous square wave (3.93). Figure 3.8 shows this evolution in successively thinner curves at times $t = 0, 10^{-2}\tau, 10^{-1}\tau, \tau = 2mL^2/\hbar, 10\tau,$ and 100τ . The curves at $t = 0$ and $t = 10^{-2}\tau$ are smooth, but some wobbles appear at $t = 10^{-1}\tau$ and at $t = \tau$ due to the discontinuities in the first derivative of $\psi(x, 0)$ at $x = 0.5$ and at $x = 1.5$. \square

Example 3.13 (Time Evolution of a Smooth Wave Function) Finally, let's try a wave function $\psi(x, 0)$ that is periodic and infinitely differentiable on $[0, L]$. An infinitely differentiable function is said to be **smooth** or C^∞ . The infinite square-well potential $V(x)$ of equation (3.85) imposes the periodic boundary conditions $\psi(0, 0) = \psi(L, 0) = 0$, so we try

$$\psi(x, 0) = \sqrt{\frac{2}{3L}} \left[1 - \cos\left(\frac{2\pi x}{L}\right) \right]. \quad (3.107)$$

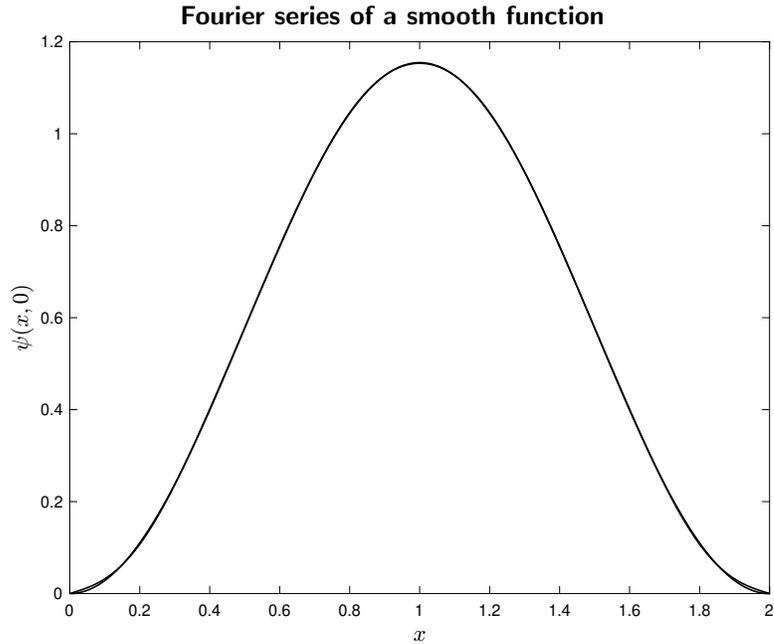


Figure 3.9 The wave function $\psi(x, 0)$ (3.107) is infinitely differentiable, and so the first 10 terms of its uniformly convergent Fourier series (3.110) offer a very good approximation to it.

Its Fourier series

$$\psi(x, 0) = \sqrt{\frac{1}{6L}} \left(2 - e^{2\pi i x/L} - e^{-2\pi i x/L} \right) \quad (3.108)$$

has coefficients that satisfy the upper bounds (3.66) by vanishing for $|n| > 1$.

The coefficients of the Fourier sine series for the wave function $\psi(x, 0)$ are given by the integrals (3.96)

$$\begin{aligned} f_n &= \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) \psi(x, 0) \\ &= \frac{2}{\sqrt{3}L} \int_0^L dx \sin\left(\frac{\pi n x}{L}\right) \left[1 - \cos\left(\frac{2\pi x}{L}\right) \right] \\ &= \frac{8[(-1)^n - 1]}{\pi\sqrt{3}n(n^2 - 4)} \end{aligned} \quad (3.109)$$

with all the even coefficients zero, $f_{2n} = 0$. The f_n 's are proportional to $1/n^3$ which is more than enough to ensure the absolute and uniform convergence

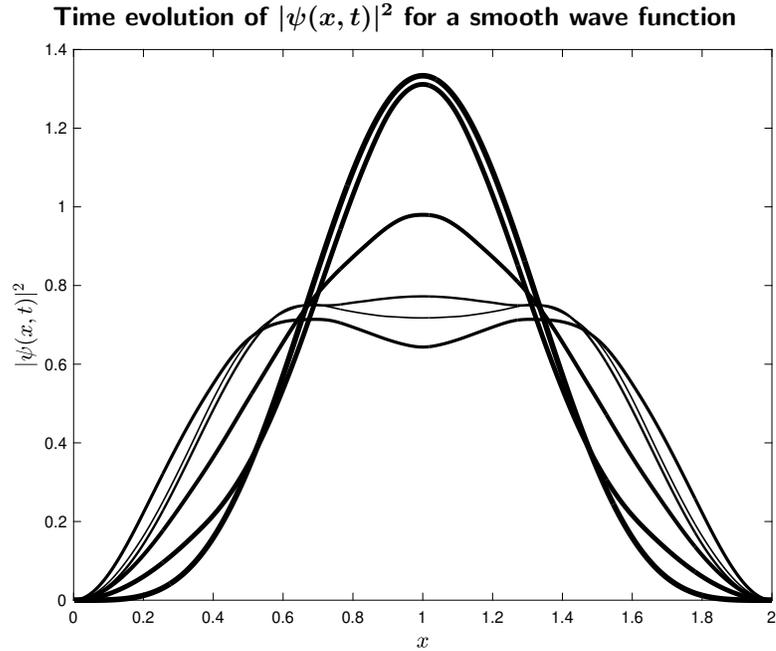


Figure 3.10 The probability distributions $P(x, t) = |\psi(x, t)|^2$ of the 1000-term Fourier series (3.111) for the wave function $\psi(x, t)$ at $t = 0, 10^{-2}\tau, 10^{-1}\tau, \tau = 2mL^2/\hbar, 10\tau,$ and 100τ are plotted as successively thinner curves. The time evolution is calm because the wave function $\psi(x, 0)$ is smooth.

of its Fourier sine series

$$\psi(x, 0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right). \quad (3.110)$$

As time goes by, it evolves to

$$\psi(x, t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-i\hbar(n\pi)^2 t / (2mL^2)} \quad (3.111)$$

and remains absolutely convergent for all times t .

The effects of the absolute and uniform convergence with $f_n \propto 1/n^3$ are obvious in the graphs. Figure 3.9 shows (for $L = 2$) that only 10 terms are required to nearly overlap the initial wave function $\psi(x, 0)$. Figure 3.10 shows that the evolution of the probability distribution $|\psi(x, t)|^2$ with time is smooth, with no sign of the jaggedness of Fig. 3.6 or the wobbles of Fig. 3.8. Because $\psi(x, 0)$ is smooth and periodic, it evolves calmly as time passes. \square

3.11 Dirac's delta function

A Dirac delta function is a (continuous, linear) map from a space of suitably well-behaved functions into the real or complex numbers. It is a **functional** that associates a number with each function in the function space. Thus $\delta(x - y)$ associates the number $f(y)$ with the function $f(x)$. We may write this association as

$$f(y) = \int f(x) \delta(x - y) dx. \quad (3.112)$$

Delta functions pop up all over physics. Multiplying the identity operator (3.5)

$$I = \int_0^{2\pi} |x\rangle\langle x| dx \quad (3.113)$$

from the right by $|f\rangle$ and from the left by $\langle y|$, we get

$$f(y) = \langle y|f\rangle = \langle y|I|f\rangle = \int_0^{2\pi} \langle y|x\rangle\langle x|f\rangle dx = \int_0^{2\pi} \langle y|x\rangle f(x) dx \quad (3.114)$$

which says that the inner product $\langle y|x\rangle$ is a **delta function**

$$\langle y|x\rangle = \langle x|y\rangle = \delta(x - y). \quad (3.115)$$

Using both Fourier-series formulas (3.2) and (3.3), we get

$$f_p(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{inx}}{\sqrt{2\pi}} = \sum_{n=-\infty}^{\infty} \int_0^{2\pi} \frac{e^{-iny}}{\sqrt{2\pi}} f(y) \frac{e^{inx}}{\sqrt{2\pi}} dy \quad (3.116)$$

in which the function f_p on the left-hand side of this equation is the periodic extension (3.58) f_p of f if f is not itself periodic with period 2π . Interchanging and rearranging, we have

$$f_p(x) = \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} \frac{e^{in(x-y)}}{2\pi} \right) f_p(y) dy. \quad (3.117)$$

But the phases e^{inx} are **periodic** with period 2π , so we also have

$$f_p(x + 2\pi\ell) = \int_0^{2\pi} \left(\sum_{n=-\infty}^{\infty} \frac{e^{in(x-y)}}{2\pi} \right) f_p(y) dy. \quad (3.118)$$

Thus we arrive at the **Dirac comb**

$$\sum_{n=-\infty}^{\infty} \frac{e^{in(x-y)}}{2\pi} = \sum_{\ell=-\infty}^{\infty} \delta(x - y - 2\pi\ell) \quad (3.119)$$

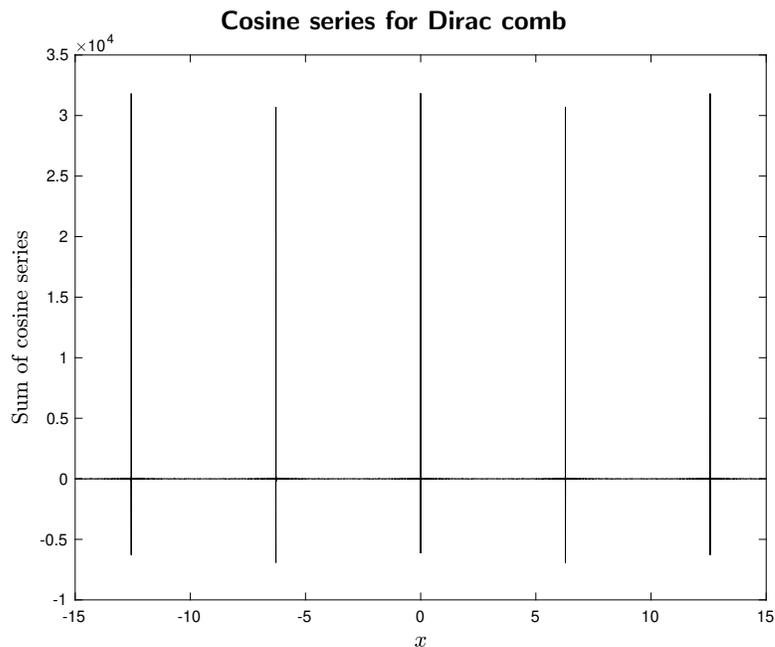


Figure 3.11 The sum of the first 100,000 terms of the series (3.120) for the Dirac comb is plotted for $-15 \leq x \leq 15$. Both Dirac spikes and Gibbs overshoots are visible.

or more simply

$$\sum_{n=-\infty}^{\infty} \frac{e^{inx}}{2\pi} = \frac{1}{2\pi} + \frac{1}{\pi} \sum_{n=1}^{\infty} \cos(nx) = \sum_{\ell=-\infty}^{\infty} \delta(x - 2\pi\ell). \quad (3.120)$$

A similar argument starting from the stretched Fourier transform (3.45) leads to the stretched Dirac comb

$$\sum_{n=-\infty}^{\infty} \frac{e^{2\pi in(x-y)/L}}{L} = \sum_{\ell=-\infty}^{\infty} \delta(x - y - L\ell). \quad (3.121)$$

Example 3.14 (Dirac's Comb) The sum of the first 100,000 terms of this cosine series (3.120) for the Dirac comb is plotted for the interval $(-15, 15)$ in Fig. 3.11. Gibbs overshoots appear at the discontinuities. The integral of the first 100,000 terms from -15 to 15 is 5.0000. \square

Example 3.15 (Parseval's Identity) Using our formula (3.42) for the Fourier coefficients of a stretched interval, we can relate a sum of products $f_n^* g_n$ of the Fourier coefficients of the functions $f(x)$ and $g(x)$ to an

integral of the product $f^*(x)g(x)$

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \sum_{n=-\infty}^{\infty} \int_0^L dx \frac{e^{i2\pi nx/L}}{\sqrt{L}} f^*(x) \int_0^L dy \frac{e^{-i2\pi ny/L}}{\sqrt{L}} g(y). \quad (3.122)$$

This sum contains Dirac's comb (3.121) and so

$$\begin{aligned} \sum_{n=-\infty}^{\infty} f_n^* g_n &= \int_0^L dx \int_0^L dy f^*(x) g(y) \frac{1}{L} \sum_{n=-\infty}^{\infty} e^{i2\pi n(x-y)/L} \\ &= \int_0^L dx \int_0^L dy f^*(x) g(y) \sum_{\ell=-\infty}^{\infty} \delta(x-y-\ell L). \end{aligned} \quad (3.123)$$

Only the $\ell = 0$ tooth of the comb contributes, and we have more simply

$$\sum_{n=-\infty}^{\infty} f_n^* g_n = \int_0^L dx \int_0^L dy f^*(x) g(y) \delta(x-y) = \int_0^L dx f^*(x) g(x). \quad (3.124)$$

In particular, if the two functions are the same, then

$$\sum_{n=-\infty}^{\infty} |f_n|^2 = \int_0^L dx |f(x)|^2 \quad (3.125)$$

which is **Parseval's identity**. Thus if a function is **square integrable** on an interval, then the sum of the squares of the absolute values of its Fourier coefficients is the integral of the square of its absolute value. \square

Example 3.16 (Derivatives of Delta Functions) Delta functions and other generalized functions or distributions map smooth functions that vanish at infinity into numbers in ways that are linear and continuous. Derivatives of delta functions are defined so as to allow integrations by parts. Thus the n th derivative of the delta function $\delta^{(n)}(x-y)$ maps the function $f(x)$ to $(-1)^n f^{(n)}(y)$

$$\int \delta^{(n)}(x-y) f(x) dx = \int \delta(x-y) (-1)^n f^{(n)}(x) dx = (-1)^n f^{(n)}(y) \quad (3.126)$$

with no surface term. \square

Example 3.17 (The Equation $xf(x) = a$) Dirac's delta function sometimes appears unexpectedly. For instance, the general solution to the equation $xf(x) = a(x)$ is $f(x) = a(x)/x + b(x)\delta(x)$ in which $b(x)$ is a constant (Dirac, 1967, sec. 15), (Waxman and Peck, 1998) or $xb(x) = 0$ at $x = 0$. Similarly, the general solution to the equation $x^2 f(x) = a(x)$ is $f(x) = a(x)/x^2 + b(x)\delta(x)/x + c(x)\delta'(x)$ in which $\delta'(x)$ is the derivative of

the delta function, $b(x)$ is continuous, $c(x)$ has a continuous first derivative, and $x b(x) = x c(x) = x^2 c'(x) = 0$ at $x = 0$. \square

3.12 Harmonic oscillators

The hamiltonian for the harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2. \quad (3.127)$$

The commutation relation $[q, p] \equiv qp - pq = i\hbar$ implies that the **lowering** and **raising** operators

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(q + \frac{ip}{m\omega} \right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(q - \frac{ip}{m\omega} \right) \quad (3.128)$$

obey the commutation relation $[a, a^\dagger] = 1$. In terms of a and a^\dagger , which also are called the **annihilation** and **creation** operators, the hamiltonian H is

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right). \quad (3.129)$$

There is a unique state $|0\rangle$ that is annihilated by the operator a , as may be seen by solving the differential equation

$$\langle q'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}} \langle q'| \left(q + \frac{ip}{m\omega} \right) |0\rangle = 0. \quad (3.130)$$

Since $\langle q'|q = q'\langle q'|$ and

$$\langle q'|p|0\rangle = \frac{\hbar}{i} \frac{d\langle q'|0\rangle}{dq'} \quad (3.131)$$

the resulting differential equation is

$$\frac{d\langle q'|0\rangle}{dq'} = -\frac{m\omega}{\hbar} q' \langle q'|0\rangle. \quad (3.132)$$

Its suitably normalized solution is the wave function for the ground state of the harmonic oscillator

$$\langle q'|0\rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega q'^2}{2\hbar} \right). \quad (3.133)$$

For $n = 0, 1, 2, \dots$, the n th eigenstate of the hamiltonian H is

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a^\dagger \right)^n |0\rangle \quad (3.134)$$

where $n! \equiv n(n-1)\dots 1$ is **n -factorial** and $0! = 1$. The commutation relation

$[a, a^\dagger] = 1$ implies that $a|n\rangle = \sqrt{n}|n-1\rangle$, that $a^\dagger|n\rangle = \sqrt{(n+1)}|n+1\rangle$, and that

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle. \quad (3.135)$$

The identity operator is

$$I = \sum_{n=0}^{\infty} |n\rangle\langle n|. \quad (3.136)$$

An arbitrary state $|\psi\rangle$ has an expansion in terms of the eigenstates $|n\rangle$

$$|\psi\rangle = I|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\psi\rangle \quad (3.137)$$

and evolves in time like a Fourier series

$$|\psi, t\rangle = e^{-iHt/\hbar}|\psi\rangle = e^{-iHt/\hbar} \sum_{n=0}^{\infty} |n\rangle\langle n|\psi\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} |n\rangle\langle n|\psi\rangle \quad (3.138)$$

with wave function

$$\psi(q, t) = \langle q|\psi, t\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-in\omega t} \langle q|n\rangle\langle n|\psi\rangle. \quad (3.139)$$

The wave functions $\langle q|n\rangle$ of the energy eigenstates are related to the Hermite polynomials (example 9.6)

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (3.140)$$

by a change of variables $x = \sqrt{m\omega/\hbar}q \equiv sq$ and a normalization factor

$$\langle q|n\rangle = \frac{\sqrt{s} e^{-(sq)^2/2}}{\sqrt{2^n n!} \sqrt{\pi}} H_n(sq) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{e^{-m\omega q^2/2\hbar}}{\sqrt{2^n n!}} H_n\left(\left(\frac{m\omega}{\hbar}\right)^{1/2} q\right). \quad (3.141)$$

For every complex number α , the **coherent state** $|\alpha\rangle$

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (3.142)$$

is an eigenstate $a|\alpha\rangle = \alpha|\alpha\rangle$ of the lowering (or annihilation) operator a with eigenvalue α . Its time evolution is simply

$$|\alpha, t\rangle = e^{-i\omega t/2} e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} |n\rangle = e^{-i\omega t/2} |\alpha e^{-i\omega t}\rangle. \quad (3.143)$$

3.13 Nonrelativistic strings

If we clamp the ends of a nonrelativistic string at $x = 0$ and $x = L$, then the amplitude $y(x, t)$ will obey the boundary conditions

$$y(0, t) = y(L, t) = 0 \quad (3.144)$$

and the wave equation

$$v^2 \frac{\partial^2 y}{\partial x^2} = \frac{\partial^2 y}{\partial t^2} \quad (3.145)$$

as long as $y(x, t)$ remains small. The functions

$$y_n(x, t) = \sin \frac{n\pi x}{L} \left(a_n \cos \frac{n\pi vt}{L} + b_n \sin \frac{n\pi vt}{L} \right) \quad (3.146)$$

satisfy this wave equation (3.145) and the boundary conditions (3.144). They represent waves traveling along the x -axis with speed v .

The space S_L of functions $f(x)$ that satisfy the boundary condition (3.144) is spanned by the functions $\sin(n\pi x/L)$. One may use the integral formula

$$\int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx = \frac{L}{2} \delta_{nm} \quad (3.147)$$

to derive for any function $f \in S_L$ the Fourier series

$$f(x) = \sum_{n=1}^{\infty} f_n \sin \frac{n\pi x}{L} \quad (3.148)$$

with coefficients

$$f_n = \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} f(x) dx \quad (3.149)$$

and the representation

$$\sum_{m=-\infty}^{\infty} \delta(x - z - 2mL) = \frac{2}{L} \sum_{n=1}^{\infty} \sin \frac{n\pi x}{L} \sin \frac{n\pi z}{L} \quad (3.150)$$

for the Dirac comb on S_L .

3.14 Periodic boundary conditions

Periodic boundary conditions often are convenient. For instance, rather than study an infinitely long one-dimensional system, we might study the same system, but of length L . The ends cause effects not present in the infinite

system. To avoid them, we imagine that the system forms a circle and impose the periodic boundary condition

$$\psi(x \pm L, t) = \psi(x, t). \quad (3.151)$$

Analogous conditions in three dimensions are

$$\psi(x + kL, y + \ell L, z + mL, t) = \psi(x, y, z, t) \quad (3.152)$$

for all integers k, ℓ , and m .

The eigenstates $|\mathbf{p}\rangle$ of the free hamiltonian $H = \mathbf{p}^2/2m$ have wave functions

$$\psi_{\mathbf{p}}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{p} \rangle = e^{i\mathbf{x}\cdot\mathbf{p}/\hbar} / (2\pi\hbar)^{3/2}. \quad (3.153)$$

The periodic boundary conditions (3.152) require that each component p_i of momentum satisfy $Lp_i/\hbar = 2\pi n_i$ or

$$\mathbf{p} = \frac{2\pi\hbar\mathbf{n}}{L} = \frac{h\mathbf{n}}{L} \quad (3.154)$$

where \mathbf{n} is a vector of integers, which may be positive or negative or zero.

Periodic boundary conditions naturally arise in the study of solids. The atoms of a perfect crystal are at the vertices of a **Bravais** lattice

$$\mathbf{x}_i = \mathbf{x}_0 + \sum_{i=1}^3 n_i \mathbf{a}_i \quad (3.155)$$

in which the three vectors \mathbf{a}_i are the **primitive vectors** of the lattice and the n_i are three integers. The hamiltonian of such an infinite crystal is invariant under translations in space by

$$\sum_{i=1}^3 n_i \mathbf{a}_i. \quad (3.156)$$

To keep the notation simple, let's restrict ourselves to a cubic lattice with lattice spacing a . Then since the momentum operator \mathbf{p} generates translations in space, the invariance of H under translations by $a\mathbf{n}$

$$\exp(i\mathbf{a}\mathbf{n} \cdot \mathbf{p}) H \exp(-i\mathbf{a}\mathbf{n} \cdot \mathbf{p}) = H \quad (3.157)$$

implies that $e^{i\mathbf{a}\mathbf{n}\cdot\mathbf{p}}$ and H are compatible normal operators $[e^{i\mathbf{a}\mathbf{n}\cdot\mathbf{p}}, H] = 0$. As explained in section 1.33, it follows that we may choose the eigenstates of H also to be eigenstates of $e^{i\mathbf{a}\mathbf{n}\cdot\mathbf{p}}$ with eigenvalue $e^{i\mathbf{a}\mathbf{n}\cdot\mathbf{k}}$

$$e^{i\mathbf{a}\mathbf{p}\cdot\mathbf{n}/\hbar} |\psi\rangle = e^{i\mathbf{a}\mathbf{k}\cdot\mathbf{n}} |\psi\rangle \quad (3.158)$$

which implies that

$$\psi(\mathbf{x} + a\mathbf{n}) = \langle \mathbf{x} + a\mathbf{n} | \psi \rangle = \langle \mathbf{x} | e^{iap \cdot \mathbf{n} / \hbar} | \psi \rangle = \langle \mathbf{x} | e^{iak \cdot \mathbf{n} / \hbar} | \psi \rangle = e^{iak \cdot \mathbf{n}} \psi(\mathbf{x}). \quad (3.159)$$

Setting

$$\psi(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} u(\mathbf{x}) \quad (3.160)$$

we see that condition (3.159) implies that $u(\mathbf{x})$ is periodic

$$u(\mathbf{x} + a\mathbf{n}) = u(\mathbf{x}). \quad (3.161)$$

For a general Bravais lattice, this **Born–von Karman** periodic boundary condition is

$$u\left(\mathbf{x} + \sum_{i=1}^3 n_i \mathbf{a}_i\right) = u(\mathbf{x}). \quad (3.162)$$

Equations (3.159) and (3.161) are known as **Bloch's theorem**.

Exercises

- 3.1 Show that $\sin \omega_1 x + \sin \omega_2 x$ is the same as (3.15).
- 3.2 Show that the Fourier series (3.16) obeys Laplace's equation (3.17) for $\rho < a$ and respects the boundary condition $f(a, \theta) = h(\theta)$.
- 3.3 Find the forms that equations (3.9 & 3.10) for the inner products $\langle g | f \rangle$ and $\langle f | f \rangle$ take when one uses the asymmetrical notations (3.20 & 3.21).
- 3.4 **HW2021** Find the Fourier series for the function $\exp(ax)$ on the interval $-\pi < x \leq \pi$.
- 3.5 **HW2021** Find the Fourier series for the function $(x^2 - \pi^2)^2$ on the same interval $(-\pi, \pi]$.
- 3.6 **HW2021** Find the Fourier series for the function $(1 + \cos x) \sin ax$ on the interval $(-\pi, \pi]$.
- 3.7 Show that the Fourier series for the function $x \cos x$ on the interval $[-\pi, \pi]$ is

$$x \cos x = -\frac{1}{2} \sin x + 2 \sum_{n=2}^{\infty} \frac{(-1)^n n}{n^2 - 1} \sin nx. \quad (3.163)$$

- 3.8 (a) Show that the Fourier series for the function $|x|$ on the interval $[-\pi, \pi]$ is

$$|x| = \frac{\pi}{2} - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\cos(2n+1)x}{(2n+1)^2}. \quad (3.164)$$

- (b) Use this result to find a neat formula for $\pi^2/8$. Hint: set $x = 0$.

3.9 Show that the Fourier series for the function $|\sin x|$ on the interval $[-\pi, \pi]$ is

$$|\sin x| = \frac{2}{\pi} - \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\cos 2nx}{4n^2 - 1}. \quad (3.165)$$

3.10 Show that the Fourier coefficients of the C^0 function (3.69) on the interval $[-\pi, \pi]$ are given by (3.70).

3.11 Find by inspection the Fourier series for the function $\exp[\exp(-ix)]$.

3.12 Fill in the steps in the computation (3.35) of the Fourier series for x^2 .

3.13 Do the first integral in equation (3.75). Hint: differentiate $\ln\left(\frac{\sin \pi x}{\pi x}\right)$.

3.14 Use the infinite-product formula (3.76) for the sine and the relation $\cos \pi x = \sin 2\pi x / (2 \sin \pi x)$ to derive the infinite-product formula (3.77) for the cosine. Hint:

$$\prod_{n=1}^{\infty} \left[1 - \frac{x^2}{\frac{1}{4}n^2}\right] = \prod_{n=1}^{\infty} \left[1 - \frac{x^2}{\frac{1}{4}(2n-1)^2}\right] \left[1 - \frac{x^2}{\frac{1}{4}(2n)^2}\right]. \quad (3.166)$$

3.15 What's the general solution to the equation $x^3 f(x) = a(x)$?

3.16 **HW2021** Suppose we wish to approximate the real square-integrable function $f(x)$ by the Fourier series with N terms

$$f_N(x) = \frac{a_0}{2} + \sum_{n=1}^N (a_n \cos nx + b_n \sin nx). \quad (3.167)$$

Then the error

$$E_N = \int_0^{2\pi} [f(x) - f_N(x)]^2 dx \quad (3.168)$$

will depend upon the $2N+1$ coefficients a_n and b_n . The best coefficients minimize this error and satisfy the conditions

$$\frac{\partial E_N}{\partial a_n} = \frac{\partial E_N}{\partial b_n} = 0. \quad (3.169)$$

By using these conditions, find the best coefficients.

3.17 Find the Fourier series for the function $f(x) = \theta(a^2 - x^2)$ on the interval $[-\pi, \pi]$ for the case $a^2 < \pi^2$. The **Heaviside step function** $\theta(x)$ is zero for $x < 0$, one-half for $x = 0$, and unity for $x > 0$ (Oliver Heaviside, 1850–1925). The value assigned to $\theta(0)$ seldom matters, and you need not worry about it in this problem.

3.18 Derive or infer the formula (3.121) for the stretched Dirac comb.

- 3.19 Use the commutation relation $[q, p] = i\hbar$ to show that the annihilation and creation operators (3.128) satisfy the commutation relation $[a, a^\dagger] = 1$.
- 3.20 Show that the state $|n\rangle = (a^\dagger)^n |0\rangle / \sqrt{n!}$ is an eigenstate of the hamiltonian (3.129) with energy $\hbar\omega(n + 1/2)$.
- 3.21 **HW2021** Show that the coherent state $|\alpha\rangle$ (3.142) is an eigenstate of the annihilation operator a with eigenvalue α .
- 3.22 Derive equations (3.149 & 3.150) from the expansion (3.148) and the integral formula (3.147).
- 3.23 **HW2021** Consider a string like the one described in section 3.13, which satisfies the boundary conditions (3.144) and the wave equation (3.145). The string is at rest $y(x, 0) = 0$ at time $t = 0$ and is struck precisely at $t = 0$ and $x = a$ so that its time derivative at $t = 0$ (denoted by a dot) $\dot{y}(x, 0) = Lv_0\delta(x - a)$. Find $y(x, t)$ and $\dot{y}(x, t)$.
- 3.24 Same as exercise (3.23), but now the initial conditions are

$$u(x, 0) = f(x) \quad \text{and} \quad \dot{u}(x, 0) = g(x) \quad (3.170)$$

in which $f(0) = f(L) = 0$ and $g(0) = g(L) = 0$. Find the motion of the amplitude $u(x, t)$ of the string.

- 3.25 (a) Find the Fourier series for the function $f(x) = x^2$ on the interval $[-\pi, \pi]$. (b) Use your result at $x = \pi$ to show that

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \quad (3.171)$$

which is the value of Riemann's zeta function (5.106) $\zeta(x)$ at $x = 2$.

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.

4.1 Fourier transforms

The interval $[-L/2, L/2]$ is arbitrary in the Fourier series (3.41)

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}}. \quad (4.1)$$

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

We may use the **nearest-integer function** $[p]$ to convert the coefficients f_n into a function of a continuous variable $\hat{f}(p) \equiv f_{[p]}$ such that $\hat{f}(p) = f_n$ when $|p - n| < 1/2$. In terms of this function $\hat{f}(p)$, the Fourier series (4.1) for the function $f(x)$ is

$$f(x) = \sum_{n=-\infty}^{\infty} \int_{n-1/2}^{n+1/2} \hat{f}(p) \frac{e^{i2\pi[p]x/L}}{\sqrt{L}} dp = \int_{-\infty}^{\infty} \hat{f}(p) \frac{e^{i2\pi[p]x/L}}{\sqrt{L}} dp. \quad (4.2)$$

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

$$\left| e^{i2\pi[p]x/L} - e^{i2\pi px/L} \right| = \left| e^{i2\pi([p]-p)x/L} - 1 \right| \approx \frac{\pi|x|}{L} \quad (4.3)$$

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

express $f(x)$ as

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(p) \frac{e^{i2\pi px/L}}{\sqrt{L}} dp. \quad (4.4)$$

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

$$f(x) = \int_{-\infty}^{\infty} \hat{f}\left(\frac{Lk}{2\pi}\right) \frac{e^{ikx}}{\sqrt{L}} \frac{L}{2\pi} dk = \int_{-\infty}^{\infty} \sqrt{\frac{L}{2\pi}} \hat{f}\left(\frac{Lk}{2\pi}\right) e^{ikx} \frac{dk}{\sqrt{2\pi}}. \quad (4.5)$$

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

$$\tilde{f}(k) = \sqrt{\frac{L}{2\pi}} \hat{f}\left(\frac{Lk}{2\pi}\right), \quad (4.6)$$

the integral (4.5) for $f(x)$ is the inverse Fourier transform

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} \frac{dk}{\sqrt{2\pi}}. \quad (4.7)$$

To find $\tilde{f}(k)$, we use its definition (4.6), the definition (3.42) 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 $|2\pi[Lk/2\pi]/L - k| \leq \pi/2L$ 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 $L \rightarrow \infty$

$$\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} \frac{dx}{\sqrt{2\pi}} \quad (4.8)$$

and so we have the Fourier transformations

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} \frac{dk}{\sqrt{2\pi}} \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} \frac{dx}{\sqrt{2\pi}}. \quad (4.9)$$

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 (4.9), 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

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{\pm ikx} dk \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{\mp ikx} \frac{dx}{2\pi} \quad (4.10)$$

as well as

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{\pm ikx} \frac{dk}{2\pi} \quad \text{and} \quad \tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{\mp ikx} dx. \quad (4.11)$$

One sometimes needs to relate a function's Fourier series to its Fourier transform. So let's compare the Fourier series (4.1) for the function $f(x)$ on the interval $[-L/2, L/2]$ with its Fourier transform (4.9) in the limit of large L setting $k_n = 2\pi n/L$

$$f(x) = \sum_{n=-\infty}^{\infty} f_n \frac{e^{i2\pi nx/L}}{\sqrt{L}} = \sum_{n=-\infty}^{\infty} f_n \frac{e^{ik_n x}}{\sqrt{L}} = \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} \frac{dk}{\sqrt{2\pi}}. \quad (4.12)$$

Since $f_n = \hat{f}(p) = f_{[p]}$, by using the definition (4.6) of $\tilde{f}(k)$, we have

$$f_n = f_{[n]} = f_{[p]} = \hat{f}(p) = \hat{f}\left(\frac{Lk}{2\pi}\right) = \sqrt{\frac{2\pi}{L}} \tilde{f}(k). \quad (4.13)$$

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 $\sqrt{2\pi}$

$$f(x) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} f_n e^{ik_n x} = \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} \frac{\tilde{f}(k_n)}{\sqrt{2\pi}} e^{ik_n x}. \quad (4.14)$$

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

$$f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} \frac{dk}{\sqrt{2\pi}} = \frac{L}{2\pi} \int_{-\infty}^{\infty} \frac{f_{[Lk/2\pi]}}{\sqrt{L}} e^{ikx} dk. \quad (4.15)$$

Example 4.1 (The Fourier transform of a gaussian is a gaussian) The Fourier transform of the gaussian $f(x) = \exp(-m^2 x^2)$ is

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} e^{-m^2 x^2}. \quad (4.16)$$

We complete the square in the exponent

$$\tilde{f}(k) = e^{-k^2/4m^2} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-m^2 (x+ik/2m^2)^2}. \quad (4.17)$$

As we'll see in Sec. 6.14 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

$$\tilde{f}(k) = e^{-k^2/4m^2} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-m^2 x^2} = \frac{1}{\sqrt{2} m} e^{-k^2/4m^2}. \quad (4.18)$$

Thus the Fourier transform of a gaussian is another gaussian

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} e^{-m^2 x^2} = \frac{1}{\sqrt{2} m} e^{-k^2/4m^2}. \quad (4.19)$$

But their exponents are very different. So if the gaussian $f(x) = \exp(-m^2 x^2)$ decreases slowly as $x \rightarrow \infty$ 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 $k \rightarrow \infty$ because m is small (or slowly because m is big).

Can we invert $\tilde{f}(k)$ to get $f(x)$? The inverse Fourier transform (4.7) says

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) e^{ikx} = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \frac{1}{m\sqrt{2}} e^{ikx - k^2/4m^2}. \quad (4.20)$$

By again completing the square in the exponent

$$f(x) = e^{-m^2 x^2} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \frac{1}{m\sqrt{2}} e^{-(k - i2m^2 x)^2/4m^2} \quad (4.21)$$

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

$$f(x) = e^{-m^2 x^2} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \frac{1}{m\sqrt{2}} e^{-k^2/(4m^2)} = e^{-m^2 x^2} \quad (4.22)$$

which is reassuring.

Using (4.18) for $\tilde{f}(k)$ and the connections (4.12–4.15) between Fourier series and transforms, we see that a Fourier series for this gaussian is in the limit of $L \gg x$

$$f(x) = e^{-m^2 x^2} = \frac{2\pi}{L} \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{4\pi} m} e^{-k_n^2/(4m^2)} e^{ik_n x} \quad (4.23)$$

in which $k_n = 2\pi n/L$. □

4.2 Fourier transforms of real functions

If a function $f(x)$ is real, then just as its Fourier coefficients satisfy $f_n^* = f_{-n}$ (3.13), so too the complex conjugate of its Fourier transform (4.8)

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} f(x) e^{-ikx} \quad (4.24)$$

is its Fourier transform evaluated at $-k$

$$\tilde{f}^*(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} f(x) e^{ikx} = \tilde{f}(-k). \quad (4.25)$$

It follows (exercise 4.1) that a real function $f(x)$ satisfies the relation

$$f(x) = \frac{1}{\pi} \int_0^{\infty} dk \int_{-\infty}^{\infty} f(y) \cos k(y-x) dy. \quad (4.26)$$

If $f(x)$ is both real and even, then (exercise 4.2)

$$f(x) = \frac{2}{\pi} \int_0^{\infty} \cos kx dk \int_0^{\infty} f(y) \cos ky dy, \quad (4.27)$$

while if it is real and odd, then

$$f(x) = \frac{2}{\pi} \int_0^{\infty} \sin kx dk \int_0^{\infty} f(y) \sin ky dy. \quad (4.28)$$

Example 4.2 (Dirichlet's Discontinuous Factor) Using (4.27), one may write the square wave

$$f(x) = \begin{cases} 1 & |x| < 1 \\ \frac{1}{2} & |x| = 1 \\ 0 & |x| > 1 \end{cases} \quad (4.29)$$

as Dirichlet's discontinuous factor

$$f(x) = \frac{2}{\pi} \int_0^{\infty} \frac{\sin k \cos kx}{k} dk \quad (4.30)$$

(exercise 4.3). □

Example 4.3 (Even and Odd Exponentials) By using the Fourier-transform formulas (4.27 & 4.28), one may show that the Fourier transform of the even exponential $\exp(-\beta|x|)$ is

$$e^{-\beta|x|} = \frac{2}{\pi} \int_0^{\infty} \frac{\beta \cos kx}{\beta^2 + k^2} dk \quad (4.31)$$

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

$$\frac{x}{|x|} e^{-\beta|x|} = \frac{2}{\pi} \int_0^{\infty} \frac{k \sin kx}{\beta^2 + k^2} dk \quad (4.32)$$

(exercise 4.4). □

4.3 Dirac, Parseval, and Poisson

Combining the basic equations (4.9) that define the Fourier transform, we may do something apparently useless: we may write the function $f(x)$ in terms of itself as

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) e^{ikx} = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} e^{-iky} f(y). \quad (4.33)$$

Let's compare this equation

$$f(x) = \int_{-\infty}^{\infty} dy \left(\int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp[ik(x-y)] \right) f(y) \quad (4.34)$$

with one (3.112) that describes Dirac's delta function

$$f(x) = \int_{-\infty}^{\infty} dy \delta(x-y) f(y). \quad (4.35)$$

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

$$\delta(x-y) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp[ik(x-y)]. \quad (4.36)$$

The same integral from $-N$ to N

$$\delta_N(x-y) = \int_{-N}^N \frac{dk}{2\pi} \exp[ik(x-y)] = \frac{\sin(N(x-y))}{\pi(x-y)} \quad (4.37)$$

is plotted in Fig. 4.1 for $y = 0$ and $N = 10^6$. The scales of the two axes differ by more than 10^8 .

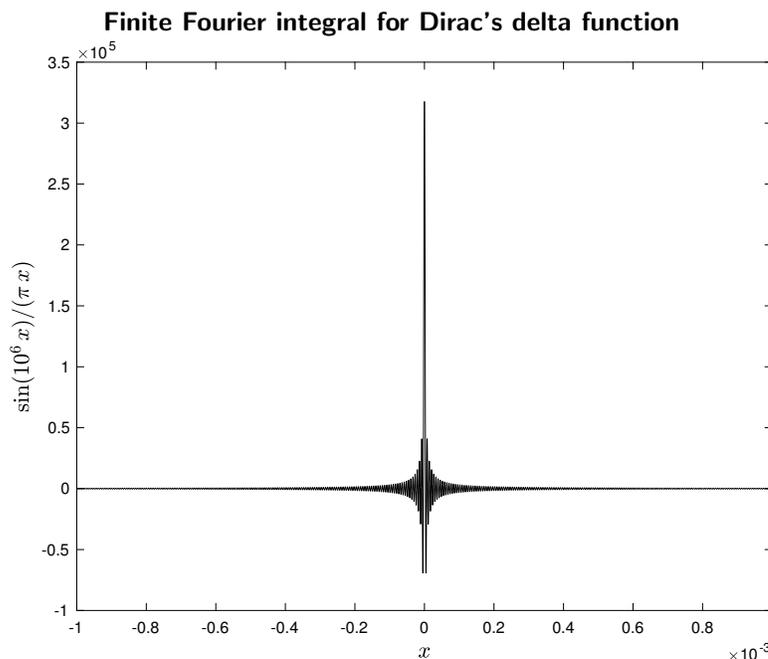


Figure 4.1 The integral (4.37) for $N = 10^6$ is plotted for $|x| \leq 0.001$. The scales of the axes differ by more than 10^8 . Matlab scripts for this chapter's figures are in `Fourier_and_Laplace.transforms` at github.com/kevinecahill.

If we multiply Dirac's delta function (4.36) by the function $f(y)$ and integrate over y , then we get back the Fourier-transform relation (4.33)

$$f(x) = \int dy \delta(x-y) f(y) = \int dy \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-y)} f(y) = \int \frac{dk}{\sqrt{2\pi}} e^{ikx} \tilde{f}(k). \quad (4.38)$$

The inner product (f, g) or $\langle f|g \rangle$ of two functions $f(x)$ and $g(x)$ is

$$\langle f|g \rangle = (f, g) = \int_{-\infty}^{\infty} dx f^*(x) g(x). \quad (4.39)$$

In terms of the Fourier transforms (4.8) $\tilde{f}(k)$ and $\tilde{g}(k)$, this inner product is

$$\begin{aligned} (f, g) &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \left(\tilde{f}(k) e^{ikx} \right)^* \int_{-\infty}^{\infty} \frac{dk'}{\sqrt{2\pi}} \tilde{g}(k') e^{ik'x} \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix(k'-k)} \tilde{f}^*(k) \tilde{g}(k') \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \delta(k' - k) \tilde{f}^*(k) \tilde{g}(k') = \int_{-\infty}^{\infty} dk \tilde{f}^*(k) \tilde{g}(k). \end{aligned} \quad (4.40)$$

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

$$(f, g) = \int_{-\infty}^{\infty} dx f^*(x) g(x) = \int_{-\infty}^{\infty} dk \tilde{f}^*(k) \tilde{g}(k) = (\tilde{f}, \tilde{g}) \quad (4.41)$$

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

$$\langle f|f \rangle = (f, f) = \int_{-\infty}^{\infty} dx |f(x)|^2 = \int_{-\infty}^{\infty} dk |\tilde{f}(k)|^2 \quad (4.42)$$

(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 (4.36) 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

$$J = \int \delta(g(x)) f(x) dx. \quad (4.43)$$

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

$$J = f(x_0) \int \delta(g(x)) dx. \quad (4.44)$$

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

$$J = f(x_0) \int \delta(g'(x_0)(x - x_0)) dx. \quad (4.45)$$

Since the delta function is nonnegative, we can write

$$\begin{aligned} J &= \frac{f(x_0)}{|g'(x_0)|} \int \delta(g'(x_0)(x - x_0)) |g'(x_0)| dx \\ &= \frac{f(x_0)}{|g'(x_0)|} \int \delta(g - g_0) dg = \frac{f(x_0)}{|g'(x_0)|}. \end{aligned} \quad (4.46)$$

Thus for a function $g(x)$ that has a single zero at $x = x_0$, we have

$$\int \delta(g(x)) f(x) dx = \frac{f(x_0)}{|g'(x_0)|} \quad \text{or} \quad \delta(g(x)) = \frac{\delta(x - x_0)}{|g'(x_0)|}. \quad (4.47)$$

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

$$\int \delta(g(x)) f(x) dx = \sum_k \frac{f(x_{0k})}{|g'(x_{0k})|} \quad \text{or} \quad \delta(g(x)) = \sum_k \frac{\delta(x - x_{0k})}{|g'(x_{0k})|}. \quad (4.48)$$

Example 4.4 (Delta function of a function whose derivative vanishes) The integral (4.43) 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 (4.47)

$$\begin{aligned} J &= \int \delta(g(x)) f(x) dx = \int \delta\left(\frac{1}{2}(x - x_0)^2 g''(x_0)\right) (x - x_0) f'(x_0) dx \\ &= \int \delta(y g''(x_0)) f'(x_0) dy = \frac{f'(x_0)}{|g''(x_0)|}. \end{aligned} \quad (4.49)$$

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

$$\delta(g(x)) = -\frac{\delta'(x - x_0)}{|g''(x_0)|} \quad (4.50)$$

works in an integral like (4.43 or 4.49) if $f \in C^1$ and $f(x_0) = 0$. \square

Our Dirac-comb formula (3.120) with $y = 0$ is

$$\sum_{n=-\infty}^{\infty} \frac{e^{-inx}}{2\pi} = \sum_{\ell=-\infty}^{\infty} \delta(x - 2\pi\ell). \quad (4.51)$$

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

$$\sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{-inx}}{2\pi} f(x) dx = \sum_{\ell=-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x - 2\pi\ell) f(x) dx. \quad (4.52)$$

Our formula (4.9) 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 $\tilde{f}(n)$

$$\frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \tilde{f}(n) = \sum_{\ell=-\infty}^{\infty} f(2\pi\ell) \quad (4.53)$$

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

$$\frac{\sqrt{2\pi}}{L} \sum_{n=-\infty}^{\infty} \tilde{f}(2\pi n/L) = \sum_{\ell=-\infty}^{\infty} f(\ell L). \quad (4.54)$$

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

Example 4.5 (Poisson Summation Formula) In example 4.1, 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 (4.53) gives

$$\frac{1}{2\sqrt{\pi}m} \sum_{k=-\infty}^{\infty} e^{-k^2/4m^2} = \sum_{\ell=-\infty}^{\infty} e^{-(2\pi\ell m)^2}. \quad (4.55)$$

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. \square

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).

4.4 Derivatives and integrals of Fourier transforms

By differentiating the inverse Fourier-transform relation (4.7)

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) e^{ikx} \quad (4.56)$$

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

$$f'(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} ik \tilde{f}(k) e^{ikx}. \quad (4.57)$$

Differentiation with respect to x corresponds to multiplication by ik .

We may repeat the process and express the second derivative as

$$f''(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} (-k^2) \tilde{f}(k) e^{ikx} \quad (4.58)$$

and the n th derivative as

$$f^{(n)}(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} (ik)^n \tilde{f}(k) e^{ikx}. \quad (4.59)$$

The indefinite integral of the inverse Fourier transform (4.56) is

$$\int f(x) \equiv \int^x dx_1 f(x_1) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) \frac{e^{ikx}}{ik} \quad (4.60)$$

and the n th indefinite integral is

$${}^{(n)}f(x) \equiv \int^x dx_1 \dots \int^{x_{n-1}} dx_n f(x_n) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \tilde{f}(k) \frac{e^{ikx}}{(ik)^n}. \quad (4.61)$$

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 $|k| \rightarrow \infty$.

Example 4.6 (Momentum and Momentum Space) Let's write the inverse Fourier transform (4.7) with ψ instead of f and with the wave number k replaced by $k = p/\hbar$

$$\psi(x) = \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx} \frac{dk}{\sqrt{2\pi}} = \int_{-\infty}^{\infty} \frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}} e^{ipx/\hbar} \frac{dp}{\sqrt{2\pi\hbar}}. \quad (4.62)$$

For a normalized wave function $\psi(x)$, Parseval's relation (4.42) implies

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} |\tilde{\psi}(k)|^2 dk = \int_{-\infty}^{\infty} \left| \frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}} \right|^2 dp. \quad (4.63)$$

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

$$\begin{aligned} 1 &= \langle \psi|\psi\rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \langle \psi|x\rangle \langle x|\psi\rangle dx \\ &= \int_{-\infty}^{\infty} \langle \psi|p\rangle \langle p|\psi\rangle dp = \int_{-\infty}^{\infty} |\varphi(p)|^2 dp. \end{aligned} \quad (4.64)$$

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

$$\begin{aligned}\langle\psi|\phi\rangle &= \int_{-\infty}^{\infty} \psi^*(x)\phi(x) dx = \int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|\phi\rangle dx \\ &= \int_{-\infty}^{\infty} \psi^*(p)\phi(p) dp = \int_{-\infty}^{\infty} \langle\psi|p\rangle\langle p|\phi\rangle dp\end{aligned}\quad (4.65)$$

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

$$I = \int_{-\infty}^{\infty} dx |x\rangle\langle x| = \int_{-\infty}^{\infty} dp |p\rangle\langle p|. \quad (4.66)$$

The Fourier transform (4.62) relating the wave function in momentum space to that in position space is

$$\psi(x) = \int_{-\infty}^{\infty} e^{ipx/\hbar} \varphi(p) \frac{dp}{\sqrt{2\pi\hbar}} \quad (4.67)$$

and the inverse Fourier transform is

$$\varphi(p) = \int_{-\infty}^{\infty} e^{-ipx/\hbar} \psi(x) \frac{dx}{\sqrt{2\pi\hbar}}. \quad (4.68)$$

In Dirac notation, the first equation (4.67) of this pair is

$$\psi(x) = \langle x|\psi\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle dp = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \varphi(p) dp \quad (4.69)$$

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

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \quad (4.70)$$

which in turn is consistent with the delta-function relation (4.36)

$$\begin{aligned}\delta(x-y) &= \langle x|y\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|y\rangle dp = \int_{-\infty}^{\infty} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{-ipy/\hbar}}{\sqrt{2\pi\hbar}} dp \\ &= \int_{-\infty}^{\infty} \frac{e^{ip(x-y)/\hbar}}{2\pi\hbar} dp = \int_{-\infty}^{\infty} e^{ik(x-y)} \frac{dk}{2\pi}.\end{aligned}\quad (4.71)$$

If we differentiate $\psi(x)$ as given by (4.69), then we find as in (4.57)

$$\frac{\hbar}{i} \frac{d}{dx} \psi(x) = \int_{-\infty}^{\infty} p \varphi(p) e^{ipx/\hbar} \frac{dp}{\sqrt{2\pi\hbar}} \quad (4.72)$$

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. \square

Example 4.7 (Uncertainty principle) Let's first normalize the gaussian $\psi(x) = N \exp(-(x/a)^2)$ to unity over the real axis

$$1 = N^2 \int_{-\infty}^{\infty} e^{-2(x/a)^2} dx = \sqrt{\frac{\pi}{2}} a N^2 \quad (4.73)$$

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

$$\psi(x) \equiv \langle x|\psi\rangle = \left(\frac{2}{\pi}\right)^{1/4} \frac{1}{\sqrt{a}} e^{-(x/a)^2}. \quad (4.74)$$

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

$$\langle A \rangle \equiv \langle \psi|A|\psi\rangle. \quad (4.75)$$

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

$$\langle A \rangle \equiv \text{Tr}(\rho A). \quad (4.76)$$

Since the gaussian (4.74) is an even function of x (that is, $\psi(-x) = \psi(x)$), the mean value of the position operator x in the state (4.74) vanishes

$$\langle x \rangle = \langle \psi|x|\psi\rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = 0. \quad (4.77)$$

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 $A - \langle A \rangle$

$$(\Delta A)^2 \equiv \langle \psi|(A - \langle A \rangle)^2|\psi\rangle. \quad (4.78)$$

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

$$(\Delta A)^2 \equiv \text{Tr}[\rho(A - \langle A \rangle)^2]. \quad (4.79)$$

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

$$\begin{aligned} (\Delta x)^2 &= \langle \psi|(x - \langle x \rangle)^2|\psi\rangle = \langle \psi|x^2|\psi\rangle \\ &= \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \frac{a^2}{4}. \end{aligned} \quad (4.80)$$

We can use the Fourier transform to find the variance of the momentum operator. By (4.68), the wave function $\varphi(p)$ in momentum space is

$$\varphi(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle \langle x|\psi\rangle dx. \quad (4.81)$$

By (4.70), the inner product $\langle p|x\rangle = \langle x|p\rangle^*$ is $\langle p|x\rangle = e^{-ipx/\hbar}/\sqrt{2\pi\hbar}$, so

$$\varphi(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \langle x|\psi\rangle. \quad (4.82)$$

Thus by (4.73 & 4.74), $\varphi(p)$ is the Fourier transform

$$\varphi(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \left(\frac{2}{\pi}\right)^{1/4} \frac{1}{\sqrt{a}} e^{-(x/a)^2}. \quad (4.83)$$

Using our formula (4.19) for the Fourier transform of a gaussian, we get

$$\varphi(p) = \sqrt{\frac{a}{2\hbar}} \left(\frac{2}{\pi}\right)^{1/4} e^{-(ap)^2/(2\hbar)^2}. \quad (4.84)$$

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

$$\begin{aligned} (\Delta p)^2 &= \langle \psi|(p - \langle p\rangle)^2|\psi\rangle = \langle \psi|p^2|\psi\rangle = \int_{-\infty}^{\infty} p^2 |\varphi(p)|^2 dp \\ &= \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} p^2 \frac{a}{2\hbar} e^{-(ap)^2/2\hbar^2} dp = \frac{\hbar^2}{a^2}. \end{aligned} \quad (4.85)$$

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

$$(\Delta x)^2 (\Delta p)^2 = \frac{a^2 \hbar^2}{4 a^2} = \frac{\hbar^2}{4} \quad (4.86)$$

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

$$\Delta x \Delta p \geq \frac{\hbar}{2} \quad (4.87)$$

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

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

$$|\psi, 0\rangle = \int_{-\infty}^{\infty} |p\rangle \langle p|\psi\rangle dp = \int_{-\infty}^{\infty} |p\rangle \varphi(p) dp \quad (4.88)$$

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

$$e^{-iHt/\hbar} |\psi, 0\rangle = \int_{-\infty}^{\infty} e^{-iHt/\hbar} |p\rangle \varphi(p) dp = \int_{-\infty}^{\infty} e^{-ip^2 t/(2\hbar m)} |p\rangle \varphi(p) dp \quad (4.89)$$

at time t . □

Example 4.8 (Characteristic function) If $P(x)$ is a **probability distribution** normalized to unity over the range of x

$$\int P(x) dx = 1 \quad (4.90)$$

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

$$\chi(k) = \tilde{P}(k) = \int e^{ikx} P(x) dx. \quad (4.91)$$

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

$$E[f(x)] = \int f(x) P(x) dx. \quad (4.92)$$

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

$$E[x^n] = \int x^n P(x) dx = (-i)^n \left. \frac{d^n \chi(k)}{dk^n} \right|_{k=0}. \quad (4.93)$$

We'll pick up this thread again in section 15.16. □

4.5 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

$$\tilde{f}(k_1, k_2) = \int_{-\infty}^{\infty} \frac{dx_1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dx_2}{\sqrt{2\pi}} e^{-ik_1 x_1 - ik_2 x_2} f(x_1, x_2). \quad (4.94)$$

By twice using the Fourier representation (4.36) of Dirac's delta function, we may invert this double Fourier transformation

$$\begin{aligned} & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi} e^{i(k_1 x_1 + k_2 x_2)} \tilde{f}(k_1, k_2) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dx'_1 dx'_2}{2\pi} e^{ik_1(x_1 - x'_1) + ik_2(x_2 - x'_2)} f(x'_1, x'_2) \\ &= \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'_1 dx'_2 e^{ik_2(x_2 - x'_2)} \delta(x_1 - x'_1) f(x'_1, x'_2) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'_1 dx'_2 \delta(x_1 - x'_1) \delta(x_2 - x'_2) f(x'_1, x'_2) = f(x_1, x_2). \end{aligned} \quad (4.95)$$

That is

$$f(x_1, x_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dk_1 dk_2}{2\pi} e^{i(k_1 x_1 + k_2 x_2)} \tilde{f}(k_1, k_2). \quad (4.96)$$

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

$$\tilde{f}(k_1, \dots, k_n) = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \frac{dx_1 \dots dx_n}{(2\pi)^{n/2}} e^{-i(k_1 x_1 + \dots + k_n x_n)} f(x_1, \dots, x_n) \quad (4.97)$$

and its inverse is

$$f(x_1, \dots, x_n) = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \frac{dk_1 \dots dk_n}{(2\pi)^{n/2}} e^{i(k_1 x_1 + \dots + k_n x_n)} \tilde{f}(k_1, \dots, k_n) \quad (4.98)$$

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

If we generalize the relations (4.12–4.15) between Fourier series and transforms from one to n dimensions, then we find that the Fourier series corresponding to the Fourier transform (4.98) is

$$f(x_1, \dots, x_n) = \left(\frac{2\pi}{L}\right)^n \sum_{j_1=-\infty}^{\infty} \dots \sum_{j_n=-\infty}^{\infty} e^{i(k_{j_1} x_1 + \dots + k_{j_n} x_n)} \frac{\tilde{f}(k_{j_1}, \dots, k_{j_n})}{(2\pi)^{n/2}} \quad (4.99)$$

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

$$f(\mathbf{x}) = \frac{(2\pi)^3}{V} \sum_{j_1=-\infty}^{\infty} \sum_{j_2=-\infty}^{\infty} \sum_{j_3=-\infty}^{\infty} e^{i\mathbf{k}_j \cdot \mathbf{x}} \frac{\tilde{f}(\mathbf{k}_j)}{(2\pi)^{3/2}} \quad (4.100)$$

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

Example 4.9 (Helmholtz decomposition) Using the Levi-Civita formula (2.73) that expresses every 3-vector $\mathbf{V}(\mathbf{x})$ in terms of any nonzero 3-vector \mathbf{k} , we can write the Fourier transform $\mathbf{V}(\mathbf{k})$ of any square-integrable 3-vector field $\mathbf{V}(\mathbf{x})$ as

$$\begin{aligned} \mathbf{V}(\mathbf{x}) &= \int \mathbf{V}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} d^3x = \int \left(\frac{\mathbf{k}(\mathbf{k} \cdot \mathbf{V}(\mathbf{k}))}{\mathbf{k}^2} - \frac{\mathbf{k} \times (\mathbf{k} \times \mathbf{V}(\mathbf{k}))}{\mathbf{k}^2} \right) e^{i\mathbf{k} \cdot \mathbf{x}} d^3x \\ &= \nabla \int \frac{-i\mathbf{k} \cdot \mathbf{V}(\mathbf{k})}{\mathbf{k}^2} e^{i\mathbf{k} \cdot \mathbf{x}} d^3x + \nabla \times \int \frac{i\mathbf{k} \times \mathbf{V}(\mathbf{k})}{\mathbf{k}^2} e^{i\mathbf{k} \cdot \mathbf{x}} d^3x \end{aligned} \quad (4.101)$$

which is the sum of the gradient of a scalar field plus the curl of a vector field. \square

Example 4.10 (Feynman propagator) For a spinless quantum field of

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

$$\Delta_F(x) = \int \frac{\exp(ik \cdot x)}{k^2 + m^2 - i\epsilon} \frac{d^4k}{(2\pi)^4} \quad (4.102)$$

where $k \cdot x = \mathbf{k} \cdot \mathbf{x} - k^0 x^0$, all physical quantities are in **natural units** ($c = \hbar = 1$), and $x^0 = ct = t$. The tiny imaginary term $-i\epsilon$ makes $\Delta_F(x-y)$ 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 6.46)

$$\begin{aligned} -i \Delta_F(x-y) &= \langle 0 | \mathcal{T} [\phi(x)\phi(y)] | 0 \rangle \\ &\equiv \theta(x^0 - y^0) \langle 0 | \phi(x)\phi(y) | 0 \rangle + \theta(y^0 - x^0) \langle 0 | \phi(y)\phi(x) | 0 \rangle \end{aligned} \quad (4.103)$$

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

4.6 Convolutions

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

$$f * g(x) = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} f(x-y) g(y). \quad (4.104)$$

The convolution product is symmetric

$$f * g(x) = g * f(x) \quad (4.105)$$

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

$$\begin{aligned} f * g(x) &= \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} f(x-y) g(y) = - \int_{\infty}^{-\infty} \frac{dz}{\sqrt{2\pi}} f(z) g(x-z) \\ &= \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} g(x-z) f(z) = g * f(x). \end{aligned} \quad (4.106)$$

Convolutions often occur in physics in the three-dimensional form

$$F(\mathbf{x}) = \int G(\mathbf{x} - \mathbf{x}') S(\mathbf{x}') d^3\mathbf{x}' \quad (4.107)$$

in which G is a Green's function and S is a source.

Example 4.11 (Gauss's law and the potential for static electric fields) The divergence of the electric field \mathbf{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, $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$. This constraint is known as Gauss's law. If the charges and fields are independent of time, then the electric field \mathbf{E} is the gradient of a

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

$$-\nabla^2\phi = \frac{\rho}{\epsilon_0}. \quad (4.108)$$

We may solve this equation by using Fourier transforms as described in Section 4.14. If $\tilde{\phi}(\mathbf{k})$ and $\tilde{\rho}(\mathbf{k})$ respectively are the Fourier transforms of $\phi(\mathbf{x})$ and $\rho(\mathbf{x})$, then Poisson's differential equation (4.108) gives

$$\begin{aligned} -\nabla^2\phi(\mathbf{x}) &= -\nabla^2 \int e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\phi}(\mathbf{k}) d^3\mathbf{k} = \int \mathbf{k}^2 e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\phi}(\mathbf{k}) d^3\mathbf{k} \\ &= \frac{\rho(\mathbf{x})}{\epsilon_0} = \int e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\tilde{\rho}(\mathbf{k})}{\epsilon_0} d^3\mathbf{k} \end{aligned} \quad (4.109)$$

which implies the algebraic equation $\tilde{\phi}(\mathbf{k}) = \tilde{\rho}(\mathbf{k})/\epsilon_0\mathbf{k}^2$ which gives $\tilde{\phi}(\mathbf{k})$ as a product of the Fourier transforms $\tilde{\rho}(\mathbf{k})$ and $1/\mathbf{k}^2$ (and is an instance of (4.175)). The inverse Fourier transform of $\tilde{\phi}(\mathbf{k})$ is the scalar potential

$$\begin{aligned} \phi(\mathbf{x}) &= \int e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\phi}(\mathbf{k}) d^3\mathbf{k} = \int e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\tilde{\rho}(\mathbf{k})}{\epsilon_0\mathbf{k}^2} d^3\mathbf{k} \\ &= \int e^{i\mathbf{k}\cdot\mathbf{x}} \frac{1}{\mathbf{k}^2} \int e^{-i\mathbf{k}\cdot\mathbf{x}'} \frac{\rho(\mathbf{x}')}{\epsilon_0} \frac{d^3\mathbf{x}' d^3\mathbf{k}}{(2\pi)^3} = \int G(\mathbf{x} - \mathbf{x}') \frac{\rho(\mathbf{x}')}{\epsilon_0} d^3\mathbf{x}' \end{aligned} \quad (4.110)$$

in which

$$G(\mathbf{x} - \mathbf{x}') = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\mathbf{k}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}. \quad (4.111)$$

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

$$-\nabla^2 G(\mathbf{x} - \mathbf{x}') = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (4.112)$$

We may think of G as the inverse of the operator $-\nabla^2$. The Green's function $G(\mathbf{x} - \mathbf{x}')$ ensures that $\phi(\mathbf{x})$ as given by (4.110) satisfies Poisson's equation (4.108). To integrate (4.111) and compute $G(\mathbf{x} - \mathbf{x}')$, we use spherical coordinates with the z -axis parallel to the vector $\mathbf{x} - \mathbf{x}'$

$$\begin{aligned} G(\mathbf{x} - \mathbf{x}') &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\mathbf{k}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} = \int_0^\infty \frac{dk}{(2\pi)^2} \int_{-1}^1 d\cos\theta e^{ik|\mathbf{x}-\mathbf{x}'|\cos\theta} \\ &= \int_0^\infty \frac{dk}{(2\pi)^2} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|} - e^{-ik|\mathbf{x}-\mathbf{x}'|}}{ik|\mathbf{x}-\mathbf{x}'|} \\ &= \frac{1}{2\pi^2|\mathbf{x}-\mathbf{x}'|} \int_0^\infty \frac{\sin k|\mathbf{x}-\mathbf{x}'| dk}{k} = \frac{1}{2\pi^2|\mathbf{x}-\mathbf{x}'|} \int_0^\infty \frac{\sin k dk}{k}. \end{aligned} \quad (4.113)$$

In example 6.47 of section 6.46 on Cauchy's principal value, we'll show that

$$\int_0^\infty \frac{\sin k}{k} dk = \frac{\pi}{2}. \quad (4.114)$$

Using this result, we have

$$\int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{\mathbf{k}^2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} = G(\mathbf{x} - \mathbf{x}') = \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}. \quad (4.115)$$

Finally by substituting this formula for $G(\mathbf{x} - \mathbf{x}')$ into Eq. (4.110), we find that the Fourier transform $\phi(\mathbf{x})$ of the product $\tilde{\rho}(\mathbf{k})/\mathbf{k}^2$ of the functions $\tilde{\rho}(\mathbf{k})$ and $1/\mathbf{k}^2$ is the convolution

$$\phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3 \mathbf{x}' \quad (4.116)$$

of their Fourier transforms $1/|\mathbf{x} - \mathbf{x}'|$ and $\rho(\mathbf{x}')$. 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) \square

Example 4.12 (Static magnetic vector potential) By Gauss's law for magnetism (2.30) the magnetic induction \mathbf{B} has zero divergence and so by the Helmholtz decomposition (2.8) may be written as the curl $\mathbf{B} = \nabla \times \mathbf{A}$ of a vector potential \mathbf{A} . For static currents, Ampère's law is $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$ in which $\mu_0 = 1/(\epsilon_0 c^2) = 4\pi \times 10^{-7} \text{ N A}^{-2}$ is the permeability of the vacuum. It then follows from the curl identity (2.51) that in Coulomb's gauge $\nabla \cdot \mathbf{A} = 0$, the magnetostatic vector potential \mathbf{A} satisfies the equation

$$\nabla \times \mathbf{B} = \nabla \times (\nabla \times \mathbf{A}) = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = -\nabla^2 \mathbf{A} = \mu_0 \mathbf{J}. \quad (4.117)$$

Applying the Fourier-transform technique (4.108–4.116), we find that the Fourier transforms of \mathbf{A} and \mathbf{J} satisfy the algebraic equation

$$\tilde{\mathbf{A}}(\mathbf{k}) = \mu_0 \frac{\tilde{\mathbf{J}}(\mathbf{k})}{\mathbf{k}^2} \quad (4.118)$$

which is an instance of (4.175). Performing the inverse Fourier transform, we see that \mathbf{A} is the convolution

$$\mathbf{A}(\mathbf{x}) = \frac{\mu_0}{4\pi} \int d^3 \mathbf{x}' \frac{\mathbf{J}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}. \quad (4.119)$$

If in the solution (4.116) of Poisson's equation, $\rho(\mathbf{x})$ is translated by \mathbf{a} , then so is $\phi(\mathbf{x})$. That is, if $\rho'(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{a})$ then $\phi'(\mathbf{x}) = \phi(\mathbf{x} + \mathbf{a})$. Similarly, if the current $\mathbf{J}(\mathbf{x})$ in (4.119) is translated by \mathbf{a} , then so is the potential $\mathbf{A}(\mathbf{x})$.

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

4.7 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} :

$$\widetilde{f * g}(k) = \tilde{f}(k) \tilde{g}(k). \quad (4.120)$$

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

$$\begin{aligned} \widetilde{f * g}(k) &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} f * g(x) \\ &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} f(x-y) g(y). \end{aligned} \quad (4.121)$$

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

$$\widetilde{f * g}(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} \tilde{f}(p) e^{ip(x-y)} \int_{-\infty}^{\infty} \frac{dq}{\sqrt{2\pi}} \tilde{g}(q) e^{iqy} \quad (4.122)$$

and use the representation (4.36) of Dirac's delta function twice to get

$$\begin{aligned} \widetilde{f * g}(k) &= \int_{-\infty}^{\infty} \frac{dy}{2\pi} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq \delta(p-k) \tilde{f}(p) \tilde{g}(q) e^{i(q-p)y} \\ &= \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dq \delta(p-k) \delta(q-p) \tilde{f}(p) \tilde{g}(q) \\ &= \int_{-\infty}^{\infty} dp \delta(p-k) \tilde{f}(p) \tilde{g}(p) = \tilde{f}(k) \tilde{g}(k) \end{aligned} \quad (4.123)$$

which is (4.120). Examples 4.11 and 4.12 illustrate this result.

4.8 Fourier transforms and Green's functions

The Green's function $G_P(x)$ of a differential operator P is the inverse of P in the sense that $P G_P(x) = \delta(x)$. If the differential operator is a polynomial $P(\partial) \equiv P(\partial_1, \dots, \partial_n)$ in the derivatives $\partial_1, \dots, \partial_n$ with constant coefficients, then a suitable Green's function $G_P(x) \equiv G_P(x_1, \dots, x_n)$ will satisfy

$$P(\partial)G_P(x) = \delta^{(n)}(x). \quad (4.124)$$

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

$$\begin{aligned} P(\partial)G_P(x) &= P(\partial) \int d^n k e^{ik \cdot x} \tilde{G}_P(k) = \int d^n k P(ik) e^{ik \cdot x} \tilde{G}_P(k) \\ &= \delta^{(n)}(x) = \int \frac{d^n k}{(2\pi)^n} e^{ik \cdot x} \end{aligned} \quad (4.125)$$

which gives us the algebraic equation

$$\tilde{G}_P(k) = \frac{1}{(2\pi)^n P(ik)}. \quad (4.126)$$

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

$$G_P(x) = \int \frac{d^n k}{(2\pi)^n} \frac{e^{ik \cdot x}}{P(ik)}. \quad (4.127)$$

Example 4.13 (Green and Yukawa) In 1935, Hideki Yukawa (1907–1981) proposed the partial differential equation

$$P_Y(\partial)G_Y(\mathbf{x}) \equiv (-\Delta + m^2)G_Y(\mathbf{x}) = (-\nabla^2 + m^2)G_Y(\mathbf{x}) = \delta(\mathbf{x}). \quad (4.128)$$

Our (4.127) gives as the Green's function for $P_Y(\partial)$ the Yukawa potential

$$G_Y(x) = \int \frac{d^3 k}{(2\pi)^3} \frac{e^{ik \cdot x}}{P_Y(ik)} = \int \frac{d^3 k}{(2\pi)^3} \frac{e^{ik \cdot x}}{\mathbf{k}^2 + m^2} = \frac{e^{-mr}}{4\pi r} \quad (4.129)$$

an integration done in example 6.28. \square

4.9 Laplace transforms

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

$$f(s) = \int_0^\infty dt e^{-st} F(t). \quad (4.130)$$

Because the integration is over positive values of t , the exponential $\exp(-st)$ falls off rapidly for $\text{Re } s > 0$. As $\text{Re } s$ increases, the Laplace transform $f(s)$ becomes smoother and smaller. For $\text{Re } s > 0$, 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

$$f(s) = \int_0^\infty dt e^{-st} F(t) = \int_0^\infty dt e^{-st} = \frac{1}{s} \quad (4.131)$$

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

$$f(s) = \int_0^\infty dt e^{-st} F(t) = \int_0^\infty dt e^{-(s-k)t} = \frac{1}{s-k} \quad (4.132)$$

is well defined for $\operatorname{Re} s > k$ with a simple pole at $s = k$ (section 6.10) and is square integrable for $\operatorname{Re} s > k + \epsilon$.

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

$$f(s) = \int_0^\infty dt e^{-st} \cosh kt = \frac{1}{2} \int_0^\infty dt e^{-st} (e^{kt} + e^{-kt}) = \frac{s}{s^2 - k^2} \quad (4.133)$$

and

$$f(s) = \int_0^\infty dt e^{-st} \sinh kt = \frac{1}{2} \int_0^\infty dt e^{-st} (e^{kt} - e^{-kt}) = \frac{k}{s^2 - k^2}. \quad (4.134)$$

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

$$f(s) = \int_0^\infty dt e^{-st} \cos \omega t = \frac{1}{2} \int_0^\infty dt e^{-st} (e^{i\omega t} + e^{-i\omega t}) = \frac{s}{s^2 + \omega^2} \quad (4.135)$$

and that of $\sin \omega t$ is

$$f(s) = \int_0^\infty dt e^{-st} \sin \omega t = \frac{1}{2i} \int_0^\infty dt e^{-st} (e^{i\omega t} - e^{-i\omega t}) = \frac{\omega}{s^2 + \omega^2}. \quad (4.136)$$

Example 4.14 The Laplace transform of t^{z-1} is related to the gamma function (5.58)

$$s^{-z} \Gamma(z) = \int_0^\infty dt s^{-st} t^{z-1}. \quad (4.137)$$

□

Example 4.15 (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

$$P(t, t') = \tau^{-1} e^{-(t-t')/\tau} \theta(t - t') \quad (4.138)$$

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 $\sin \omega t$

$$\begin{aligned} L(t) &= \int_{-\infty}^{\infty} P(t, t') \sin(\omega t') dt' = \int_{-\infty}^{\infty} \tau^{-1} e^{-(t-t')/\tau} \theta(t-t') \sin(\omega t') dt' \\ &= \int_{-\infty}^t \tau^{-1} e^{-(t-t')/\tau} \sin(\omega t') dt'. \end{aligned} \quad (4.139)$$

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

$$\sin(a - b) = \sin a \cos b - \cos a \sin b \quad (4.140)$$

we may relate this integral to the Laplace transforms of a sine (4.136) and a cosine (4.135)

$$\begin{aligned} L(t) &= -\tau^{-1} \int_0^{\infty} e^{-u/\tau} \sin \omega(u - t) du \\ &= -\tau^{-1} \int_0^{\infty} e^{-u/\tau} (\sin \omega u \cos \omega t - \cos \omega u \sin \omega t) du \\ &= \frac{\sin(\omega t) - \omega \tau \cos(\omega t)}{1 + (\omega \tau)^2}. \end{aligned} \quad (4.141)$$

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

$$L(t) = \frac{1}{\sqrt{1 + (\omega \tau)^2}} (\sin \omega t \cos \phi - \cos \omega t \sin \phi) = \frac{1}{\sqrt{1 + (\omega \tau)^2}} \sin(\omega t - \phi). \quad (4.142)$$

The phase-shift ϕ then is given by

$$\phi = \arctan(\omega \tau) \leq \frac{\pi}{2} \quad (4.143)$$

and the lifetime of the fluorophore in terms of the phase-shift ϕ

$$\tau = (1/\omega) \tan \phi \quad (4.144)$$

which is much easier to measure than the lifetime τ . \square

4.10 Inversion of Laplace transforms

How do we invert the Laplace transform

$$f(s) = \int_0^{\infty} dt e^{-st} F(t)? \quad (4.145)$$

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

$$f(s + iu) = \int_0^{\infty} dt e^{-(s+iu)t} F(t) \quad (4.146)$$

and choose s to be sufficiently positive that $f(s + iu)$ is suitably smooth and bounded. Then we apply the delta-function formula (4.36) to the integral

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{du}{2\pi} e^{iut} f(s + iu) &= \int_{-\infty}^{\infty} \frac{du}{2\pi} \int_0^{\infty} dt' e^{iut} e^{-(s+iu)t'} F(t') \\ &= \int_0^{\infty} dt' e^{-st'} F(t') \int_{-\infty}^{\infty} \frac{du}{2\pi} e^{iu(t-t')} \\ &= \int_0^{\infty} dt' e^{-st'} F(t') \delta(t - t') = e^{-st} F(t). \end{aligned} \quad (4.147)$$

So our inversion formula is

$$F(t) = e^{st} \int_{-\infty}^{\infty} \frac{du}{2\pi} e^{iut} f(s + iu) \quad (4.148)$$

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

Example 4.16 (Inverting a Laplace transform) To find the inverse Laplace transform of $f(s) = 1/(s - k)$, we use the inversion formula (4.148)

$$F(t) = e^{st} \int_{-\infty}^{\infty} \frac{du}{2\pi} e^{iut} f(s + iu) = \frac{e^{st}}{2\pi} \int_{-\infty}^{\infty} du \frac{e^{iut}}{s + iu - k} = e^{kt}. \quad (4.149)$$

We'll learn how to do such integrals in Section 6.14. \square

4.11 Volterra's Convolution

Volterra introduced a convolution

$$F \star G(x) = \int_0^x F(y)G(x - y) dy \quad (4.150)$$

that is well suited to the Laplace transform.

Example 4.17 (Laplace transform of Volterra's Convolution) The Laplace transform of Volterra's convolution (4.150) of F and G is.

$$\begin{aligned} \int_0^{\infty} e^{-sx} F \star G(x) dx &= \int_0^{\infty} dx \int_0^x dy e^{-sx} F(y)G(x - y) \\ &= \int_0^{\infty} dy \int_y^{\infty} dx e^{-sx} F(y)G(x - y) \\ &= \int_0^{\infty} dy \int_0^{\infty} dz e^{-s(y+z)} F(y)G(z) = f(s)g(s) \end{aligned} \quad (4.151)$$

the product fg of the Laplace transforms of F and G . \square

4.12 Derivatives and integrals of Laplace transforms

The derivatives of a Laplace transform $f(s)$ are by its definition (4.130)

$$\frac{d^n f(s)}{ds^n} = \int_0^\infty dt (-t)^n e^{-st} F(t). \quad (4.152)$$

They usually are well defined if $f(s)$ is well defined. For instance, if we differentiate the Laplace transform (4.131) of the function $F(t) = 1$ which is $f(s) = 1/s$, then we get

$$(-1)^n \frac{d^n s^{-1}}{ds^n} = \frac{n!}{s^{n+1}} = \int_0^\infty dt e^{-st} t^n \quad (4.153)$$

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 $F'(t)$

$$\begin{aligned} \int_0^\infty dt e^{-st} F'(t) &= \int_0^\infty dt \left\{ \frac{d}{dt} [e^{-st} F(t)] - F(t) \frac{d}{dt} e^{-st} \right\} \\ &= -F(0) + \int_0^\infty dt F(t) s e^{-st} \\ &= -F(0) + s f(s) \end{aligned} \quad (4.154)$$

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

The indefinite integral of the Laplace transform (4.130) is

$$\int f(s) \equiv \int ds_1 f(s_1) = \int_0^\infty dt \frac{e^{-st}}{(-t)} F(t) \quad (4.155)$$

and its n th indefinite integral is

$${}^{(n)}f(s) \equiv \int ds_n \dots \int ds_1 f(s_1) = \int_0^\infty dt \frac{e^{-st}}{(-t)^n} F(t). \quad (4.156)$$

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

4.13 Laplace transforms and differential equations

Suppose we wish to solve the differential equation

$$P(d/ds) f(s) = j(s). \quad (4.157)$$

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

$$f(s) = \int_0^\infty e^{-st} F(t) dt \quad \text{and} \quad j(s) = \int_0^\infty e^{-st} J(t) dt. \quad (4.158)$$

and using the formula (4.152) for the n th derivative of a Laplace transform, we see that the differential equation (4.157) amounts to

$$P(d/ds) f(s) = \int_0^\infty e^{-st} P(-t) F(t) dt = \int_0^\infty e^{-st} J(t) dt. \quad (4.159)$$

which is equivalent to the algebraic equation

$$F(t) = \frac{J(t)}{P(-t)}. \quad (4.160)$$

A particular solution to the inhomogeneous differential equation (4.157) is then the Laplace transform of this ratio

$$f(s) = \int_0^\infty e^{-st} \frac{J(t)}{P(-t)} dt. \quad (4.161)$$

A fairly general solution of the associated homogeneous equation

$$P(d/ds) f(s) = 0 \quad (4.162)$$

is the Laplace transform

$$f(s) = \int_0^\infty e^{-st} \delta(P(-t)) H(t) dt \quad (4.163)$$

because

$$P(d/ds) f(s) = \int_0^\infty e^{-st} P(-t) \delta(P(-t)) H(t) dt = 0 \quad (4.164)$$

as long as the function $H(t)$ is suitably smooth. Thus our solution of the inhomogeneous equation (4.157) is the sum of the two

$$f(s) = \int_0^\infty e^{-st} \frac{J(t)}{P(-t)} dt + \int_0^\infty e^{-st} \delta(P(-t)) H(t) dt. \quad (4.165)$$

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 $j(s)$.

Example 4.18 One solution to the differential equation

$$\left(\frac{d^2}{ds^2} - 1 \right) f(s) = j(s) = \int_0^\infty dt e^{-st} J(t) \quad (4.166)$$

in which $P(d/ds) = d^2/ds^2 - 1$ is

$$f(s) = \int_0^\infty dt e^{-st} \frac{J(t)}{t^2 - 1}. \quad (4.167)$$

A more general solution is

$$\begin{aligned} f(s) &= \int_0^\infty dt e^{-st} \frac{J(t)}{t^2 - 1} + \int_0^\infty dt e^{-st} \delta(t^2 - 1) H(t) \\ &= \int_0^\infty dt e^{-st} \frac{J(t)}{t^2 - 1} + \alpha e^{-s} \end{aligned} \quad (4.168)$$

in which α is an arbitrary constant. \square

4.14 Applications to Differential Equations

Let us consider a linear partial differential equation in n variables

$$P(\partial_1, \dots, \partial_n) f(x_1, \dots, x_n) = g(x_1, \dots, x_n) \quad (4.169)$$

in which P is a polynomial in the derivatives

$$\partial_j \equiv \frac{\partial}{\partial x_j} \quad (4.170)$$

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

$$\begin{aligned} f(x_1, \dots, x_n) &= \int \tilde{f}(k_1, \dots, k_n) e^{i(k_1 x_1 + \dots + k_n x_n)} d^n k \\ g(x_1, \dots, x_n) &= \int \tilde{g}(k_1, \dots, k_n) e^{i(k_1 x_1 + \dots + k_n x_n)} d^n k \end{aligned} \quad (4.171)$$

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

$$\partial_j^m f(x_1, \dots, x_n) = \int \tilde{f}(k_1, \dots, k_n) (ik_j)^m e^{i(k_1 x_1 + \dots + k_n x_n)} d^n k. \quad (4.172)$$

If we abbreviate $f(x_1, \dots, x_n)$ by $f(x)$ and do the same for g , then we may write our partial differential equation (4.169) as

$$\begin{aligned} P(\partial_1, \dots, \partial_n) f(x) &= \int \tilde{f}(k) P(ik_1, \dots, ik_n) e^{i(k_1 x_1 + \dots + k_n x_n)} d^n k \\ &= \int \tilde{g}(k) e^{i(k_1 x_1 + \dots + k_n x_n)} d^n k. \end{aligned} \quad (4.173)$$

Thus the inhomogeneous partial differential equation

$$P(\partial_1, \dots, \partial_n) f_i(x_1, \dots, x_n) = g(x_1, \dots, x_n) \quad (4.174)$$

becomes an algebraic equation in k -space

$$P(ik_1, \dots, ik_n) \tilde{f}_i(k_1, \dots, k_n) = \tilde{g}(k_1, \dots, k_n) \quad (4.175)$$

where $\tilde{g}(k_1, \dots, k_n)$ is the mixed Fourier-Laplace transform of $g(x_1, \dots, x_n)$. So one solution of the inhomogeneous differential equation (4.169) is

$$f_i(x_1, \dots, x_n) = \int e^{i(k_1 x_1 + \dots + k_n x_n)} \frac{\tilde{g}(k_1, \dots, k_n)}{P(ik_1, \dots, ik_n)} d^n k. \quad (4.176)$$

The space of solutions to the **homogeneous** form of equation (4.169)

$$P(\partial_1, \dots, \partial_n) f_h(x_1, \dots, x_n) = 0 \quad (4.177)$$

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

$$P(ik_1, \dots, ik_n) \tilde{f}_h(k_1, \dots, k_n) = 0 \quad (4.178)$$

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

$$\tilde{f}_h(k_1, \dots, k_n) = \delta(P(ik_1, \dots, ik_n)) h(k_1, \dots, k_n) \quad (4.179)$$

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

$$f_h(x) = \int e^{i(k_1 x_1 + \dots + k_n x_n)} \delta(P(ik_1, \dots, ik_n)) h(k) d^n k. \quad (4.180)$$

Our solution to the differential equation (4.169) then is a sum of a particular solution (4.176) of the inhomogeneous equation (4.175) and our solution (4.180) of the associated homogeneous equation (4.177)

$$f(x_1, \dots, x_n) = \int e^{i(k_1 x_1 + \dots + k_n x_n)} \left[\frac{\tilde{g}(k_1, \dots, k_n)}{P(ik_1, \dots, ik_n)} + \delta(P(ik_1, \dots, ik_n)) h(k_1, \dots, k_n) \right] d^n k \quad (4.181)$$

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

$$f(x) = \int e^{ik \cdot x} \left[\frac{\tilde{g}(k)}{P(ik)} + \delta(P(ik)) h(k) \right] d^n k. \quad (4.182)$$

Example 4.19 (Wave equation for a scalar field)

A free scalar field $\phi(x)$ of mass m in flat spacetime obeys the wave equation

$$(\nabla^2 - \partial_t^2 - m^2) \phi(x) = 0 \quad (4.183)$$

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

$$\phi(x) = \int e^{ik \cdot x} \tilde{\phi}(k) \frac{d^4 k}{(2\pi)^2} \quad (4.184)$$

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

The homogeneous wave equation (4.183) then says

$$(\nabla^2 - \partial_t^2 - m^2) \phi(x) = \int (-\mathbf{k}^2 + (k^0)^2 - m^2) e^{ik \cdot x} \tilde{\phi}(k) \frac{d^4 k}{(2\pi)^2} = 0 \quad (4.185)$$

which implies the algebraic equation

$$(-\mathbf{k}^2 + (k^0)^2 - m^2) \tilde{\phi}(k) = 0 \quad (4.186)$$

an instance of (4.178). Our solution (4.180) is

$$\phi(x) = \int \delta(-\mathbf{k}^2 + (k^0)^2 - m^2) e^{ik \cdot x} h(k) \frac{d^4 k}{(2\pi)^2} \quad (4.187)$$

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

$$P(ik) = (k^0)^2 - \mathbf{k}^2 - m^2 = (k^0 - \sqrt{\mathbf{k}^2 + m^2}) (k^0 + \sqrt{\mathbf{k}^2 + m^2}) \quad (4.188)$$

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

$$\left| \frac{dP(\pm \omega_k)}{dk^0} \right| = 2\omega_k. \quad (4.189)$$

So using our formula (4.48) for integrals involving delta functions of functions, we have

$$\phi(x) = \int \left[e^{i(\mathbf{k} \cdot \mathbf{x} - \omega_k t)} h_+(\mathbf{k}) + e^{i(\mathbf{k} \cdot \mathbf{x} + \omega_k t)} h_-(\mathbf{k}) \right] \frac{d^3 k}{(2\pi)^2 2\omega_k} \quad (4.190)$$

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

$$\phi(x) = \int \left[e^{i(\mathbf{k} \cdot \mathbf{x} - \omega_k t)} h_+(\mathbf{k}) + e^{-i(\mathbf{k} \cdot \mathbf{x} - \omega_k t)} h_-(-\mathbf{k}) \right] \frac{d^3 k}{(2\pi)^2 2\omega_k}. \quad (4.191)$$

If $\phi(x) = \phi(\mathbf{x}, t)$ is a real-valued classical field, then its Fourier transform $h(\mathbf{k})$ must obey the relation (4.25) which says that $h_-(-\mathbf{k}) = h_+(\mathbf{k})^*$. If ϕ

is a hermitian quantum field, then $h_-(-\mathbf{k}) = h_+^\dagger(\mathbf{k})$. In terms of the **annihilation** operator $a(\mathbf{k}) \equiv h_+(\mathbf{k})/\sqrt{4\pi\omega_k}$ and its adjoint $a^\dagger(\mathbf{k})$, a creation operator, the field $\phi(x)$ is the integral

$$\phi(x) = \int \left[e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} a(\mathbf{k}) + e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} a^\dagger(\mathbf{k}) \right] \frac{d^3k}{\sqrt{(2\pi)^3 2\omega_k}}. \quad (4.192)$$

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

$$\pi(x) = -i \int \left[e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} a(\mathbf{k}) - e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} a^\dagger(\mathbf{k}) \right] \sqrt{\frac{\omega_k}{2(2\pi)^3}} d^3k. \quad (4.193)$$

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

$$[a(\mathbf{k}), a^\dagger(\mathbf{k}')] = \delta(\mathbf{k} - \mathbf{k}') \quad \text{and} \quad [a(\mathbf{k}), a(\mathbf{k}')] = [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')] = 0 \quad (4.194)$$

then the field $\phi(\mathbf{x}, t)$ and its conjugate momentum $\pi(\mathbf{y}, t)$ satisfy (exercise 4.17) the equal-time commutation relations

$$[\phi(\mathbf{x}, t), \pi(\mathbf{y}, t)] = i\delta(\mathbf{x} - \mathbf{y}) \quad \text{and} \quad [\phi(\mathbf{x}, t), \phi(\mathbf{y}, t)] = [\pi(\mathbf{x}, t), \pi(\mathbf{y}, t)] = 0 \quad (4.195)$$

which generalize the commutation relations of quantum mechanics

$$[q_j, p_\ell] = i\hbar\delta_{j,\ell} \quad \text{and} \quad [q_j, q_\ell] = [p_j, p_\ell] = 0 \quad (4.196)$$

for a set of coordinates q_j and conjugate momenta p_ℓ . \square

Example 4.20 (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 3.14) 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 (4.100) between Fourier-transform and Fourier-series representations in 3 dimensions, we expect the Fourier series representation for the field (4.192) to be

$$\begin{aligned} \phi(x) &= \frac{(2\pi)^3}{V} \sum_{\mathbf{k}} \frac{1}{\sqrt{(2\pi)^3 2\omega_k}} \left[a(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} + a^\dagger(\mathbf{k}) e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} \right] \\ &= \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_k V}} \sqrt{\frac{(2\pi)^3}{V}} \left[a(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} + a^\dagger(\mathbf{k}) e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_k t)} \right] \end{aligned} \quad (4.197)$$

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

$$a_{\mathbf{k}} \equiv \sqrt{\frac{(2\pi)^3}{V}} a(\mathbf{k}) \quad (4.198)$$

and write the field as

$$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_{\mathbf{k}}V}} \left[a_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_{\mathbf{k}}t)} + a_{\mathbf{k}}^{\dagger} e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_{\mathbf{k}}t)} \right]. \quad (4.199)$$

The commutator of Fourier-series annihilation and creation operators is by (4.36, 4.194 & 4.198)

$$\begin{aligned} [a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] &= \frac{(2\pi)^3}{V} [a(\mathbf{k}), a^{\dagger}(\mathbf{k}')] = \frac{(2\pi)^3}{V} \delta(\mathbf{k} - \mathbf{k}') \\ &= \frac{(2\pi)^3}{V} \int e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \frac{d^3x}{(2\pi)^3} = \frac{(2\pi)^3}{V} \frac{V}{(2\pi)^3} \delta_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \end{aligned} \quad (4.200)$$

in which the Kronecker delta $\delta_{\mathbf{k},\mathbf{k}'}$ is $\delta_{\ell,\ell'}\delta_{n,n'}\delta_{m,m'}$. The two formulas for $\phi(x)$ (4.192 and 4.199) and the relation (4.198) between $a(k)$ and a_k implies that our sums and integrals over momentum are related by

$$\frac{(2\pi)^3}{V} \sum_{\mathbf{k}} \sim \int d^3k. \quad (4.201)$$

□

Example 4.21 (Diffusion) The flow rate \mathbf{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 $\rho(\mathbf{x}, t)$

$$\mathbf{J}(\mathbf{x}, t) = -D \nabla \rho(\mathbf{x}, t) \quad (4.202)$$

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 $J = (\rho, \mathbf{J})$ obeys the conservation law

$$\frac{\partial}{\partial t} \int \rho(\mathbf{x}, t) d^3\mathbf{x} = - \oint \mathbf{J}(\mathbf{x}, t) \cdot d\mathbf{a} = - \int \nabla \cdot \mathbf{J}(\mathbf{x}, t) d^3\mathbf{x} \quad (4.203)$$

which with Fick's law (4.202) gives the **diffusion equation**

$$\dot{\rho}(\mathbf{x}, t) = -\nabla \cdot \mathbf{J}(\mathbf{x}, t) = D \nabla^2 \rho(\mathbf{x}, t) \quad \text{or} \quad (D \nabla^2 - \partial_t) \rho(\mathbf{x}, t) = 0. \quad (4.204)$$

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

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

$$\rho(\mathbf{x}, t) = \int e^{i\mathbf{k}\cdot\mathbf{x}+i\omega t} \tilde{\rho}(\mathbf{k}, \omega) d^3\mathbf{k}d\omega \quad (4.205)$$

then the diffusion equation becomes

$$(D\nabla^2 - \partial_t) \rho(\mathbf{x}, t) = \int e^{i\mathbf{k}\cdot\mathbf{x}+i\omega t} (-D\mathbf{k}^2 - i\omega) \tilde{\rho}(\mathbf{k}, \omega) d^3\mathbf{k} d\omega = 0 \quad (4.206)$$

which implies the algebraic equation

$$(D\mathbf{k}^2 + i\omega) \tilde{\rho}(\mathbf{k}, \omega) = 0. \quad (4.207)$$

Our solution (4.180) of this homogeneous equation is

$$\rho(\mathbf{x}, t) = \int e^{i\mathbf{k}\cdot\mathbf{x}+i\omega t} \delta(-D\mathbf{k}^2 - i\omega) h(\mathbf{k}, \omega) d^3\mathbf{k} d\omega \quad (4.208)$$

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

$$\rho(\mathbf{x}, t) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}-D\mathbf{k}^2 t} \tilde{\rho}(\mathbf{k}) d^3\mathbf{k} \quad (4.209)$$

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

$$\rho(\mathbf{x}, 0) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{\rho}(\mathbf{k}) d^3\mathbf{k}. \quad (4.210)$$

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

$$\rho(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{y}) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{d^3\mathbf{k}}{(2\pi)^3} \quad (4.211)$$

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

$$\tilde{\rho}(\mathbf{k}) = \frac{e^{-i\mathbf{k}\cdot\mathbf{y}}}{(2\pi)^3} \quad (4.212)$$

and at later times the density $\rho(\mathbf{x}, t)$ is given by (4.209) as

$$\rho(\mathbf{x}, t) = \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-D\mathbf{k}^2 t} \frac{d^3\mathbf{k}}{(2\pi)^3}. \quad (4.213)$$

Using our formula (4.19) for the Fourier transform of a gaussian, we find

$$\rho(\mathbf{x}, t) = \frac{1}{(4\pi Dt)^{3/2}} e^{-(\mathbf{x}-\mathbf{y})^2/(4Dt)}. \quad (4.214)$$

Since the diffusion equation is linear, it follows (exercise 4.18) that an arbitrary initial distribution $\rho(\mathbf{y}, 0)$ evolves to the convolution (section 4.6)

$$\rho(\mathbf{x}, t) = \frac{1}{(4\pi Dt)^{3/2}} \int e^{-(\mathbf{x}-\mathbf{y})^2/(4Dt)} \rho(\mathbf{y}, 0) d^3\mathbf{y}. \quad (4.215)$$

□

Exercises

- 4.1 Show that the Fourier integral formula (4.26) for real functions follows from (4.9) and (4.25).
- 4.2 Show that the Fourier integral formula (4.26) for real functions implies (4.27) if f is even and (4.28) if it is odd.
- 4.3 Derive the formula (4.30) for the square wave (4.29).
- 4.4 By using the Fourier-transform formulas (4.27 & 4.28), derive the formulas (4.31) and (4.32) for the even and odd extensions of the exponential $\exp(-\beta|x|)$.
- 4.5 For the state $|\psi, t\rangle$ given by Eqs. (4.84 & 4.89), 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?
- 4.6 At time $t = 0$, a particle of mass m is in a gaussian superposition of momentum eigenstates centered at $p = \hbar K$

$$\psi(x, 0) = N \int_{-\infty}^{\infty} e^{ikx} e^{-L^2(k-K)^2} dk. \quad (4.216)$$

- (a) Complete the square in the exponent and then shift k by an appropriate amount so as to 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 $ikx - i\hbar k^2 t/2m$. Complete the square in the new exponent and then shift k by an appropriate amount so as to do the integral. Where is the particle most likely to be found? (c) Does the wave packet spread out like t or like \sqrt{t} as in classical diffusion (15.157)?
- 4.7 Express a probability distribution $P(x)$ as the Fourier transform of its characteristic function (4.91).
- 4.8 Express the characteristic function (4.91) of a probability distribution as a power series in its moments (4.93).
- 4.9 Find the characteristic function (4.91) of the gaussian probability distribution

$$P_G(x, \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \quad (4.217)$$

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

- 4.11 Derive (4.117) from $\mathbf{B} = \nabla \times \mathbf{A}$ and Ampère's law $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$.
4.12 Derive (4.118) from (4.117).
4.13 Derive (4.119) from (4.118).
4.14 Use the Green's function relations (4.112) and (4.113) to show that (4.119) satisfies (4.117).
4.15 Show that the Laplace transform of t^{z-1} is the gamma function (5.58) divided by s^z

$$f(s) = \int_0^\infty e^{-st} t^{z-1} dt = s^{-z} \Gamma(z). \quad (4.218)$$

- 4.16 Compute the Laplace transform of $1/\sqrt{t}$. Hint: let $t = u^2$.
4.17 Show that the commutation relations (4.194) of the annihilation and creation operators imply the equal-time commutation relations (4.195) for the field ϕ and its conjugate momentum π .
4.18 Use the linearity of the diffusion equation and equations (4.211–4.214) to derive the general solution (4.215) of the diffusion equation.