

Luca Guido Molinari

MATHEMATICAL METHODS FOR PHYSICS



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Preface

It is not completely obvious what a course named “Mathematical Methods for Physics” should include. Of course an introduction to complex analysis, series expansions, linear operators, Fourier integral, ... the list continues but time is limited, and the rest is inevitably a matter of choice.

In the former quadrennial system, which I attended as a physics student, the course in Milan was centred on the theory of linear operators. Then system and programs changed: the course is a year earlier and the duration has halved.

Admittedly, the notes were originally intended for myself, in the challenge to efficiently present different topics, partly self-taught. In 15 years they evolved, with the wish of presenting them with sufficient rigour, methodological examples and interesting applications. I also grew in awareness of their beauty, true gems of intellectual achievement, and the giants who made them.

Some chapters and sections, marked with an asterisk, are beyond the teaching program and time: they should invite the student to explore new directions and applications, and the textbooks of the masters.

I thank my colleague Mario Raciti for useful comments on the early editions, and the students: it is because of their participation and interest that the notes improved in the years, and are now collected in this volume.

Lastly, I thank the editors and referees of the Milano University Press for the opportunity of the present online edition.

Milano, 1 september 2025.

Luca Guido Molinari

Part 1

COMPLEX ANALYSIS

Chapter 1

Complex Numbers*

1.1 Cubic equation and imaginary numbers.

Imaginary numbers appeared in algebra during the Renaissance, with the solution of the cubic equation¹². The problem of solving the quadratic equation $x^2 + 1 = 0$ was considered meaningless, while a real cubic equation always has a real solution. However, the available method eventually provided the solution as a sum of terms with imaginary numbers.

The priority for the algebraic solution of the cubic equation is uncertain: it was probably known to Scipione del Ferro, a professor in Bologna, and Nicolò Fontana (Tartaglia). The solution³ was published in the book *Ars Magna* (1545) by Gerolamo Cardano (Pavia 1501, Rome 1576). It is based on the algebraic identity

$$(t - u)^3 + 3tu(t - u) = t^3 - u^3$$

which he obtained by geometric construction⁴. After setting $x = t - u$, the identity becomes

¹ Before the modern era, the solution was obtained by geometric means; the Persian poet and scientist Omar Khayyam (IX cent.) discussed it as the intersection of a parabola and a hyperbola, by methods that foreran Cartesian geometry.

² Refs: Jacques Sesiano, *An Introduction to the History of Algebra*, Mathematical World 27, AMS; Morris Kline, *Mathematical Thought from Ancient to Modern Times*, 3 voll, Oxford University Press 1972; Carl B. Boyer, *A History of Mathematics*, Princeton University Press 1985. A source of historical news and pictures is the *Mathematics Genealogy Project* (<https://www.genealogy.ams.org>).

³ The use of letters to denote parameters of equations was introduced by Francois Viète few years later; Cardano solved examples of cubic equations.

⁴ Consider a cube with edge length t . If three concurring edges are partitioned in segments of lengths u and $t - u$, the cube is cut into two cubes and four parallelepipeds. The volume is $t^3 = u^3 + (t - u)^3 + 2tu(t - u) + u^2(t - u) + u(t - u)^2$; simple algebra gives the identity (W. Dunham, *Journey through Genius, the Great Theorems of Mathematics*, Wiley Science Ed. 1990).

the reduced cubic equation

$$x^3 + 3px + q = 0 \quad (1.1)$$

with $tu = p$ and $t^3 - u^3 = -q$. Therefore, the solution $x = t - u$ of (1.1) is obtained by solving the quadratic equations for t^3 and u^3 , in terms of p and q .

Raffaello Bombelli (Bologna 1526, Rome? 1573) in his treatise *Algebra* was the first to regard imaginary numbers as a necessary detour to produce real solutions of real cubic equations. He studied the equation $x^3 - 15x - 4 = 0$, with real solution $x = 4$. Cardano's method works as follows: from $tu = -5$ and $t^3 - u^3 = 4$ obtain $t^6 - 4t^3 + 125 = 0$ with solutions $t^3 = 2 \pm \sqrt{-121}$. Bombelli showed that $2 \pm \sqrt{-121} = (2 \pm \sqrt{-1})^3$ so that $t_{\pm} = 2 \pm \sqrt{-1}$. With any choice of sign, a root is $x_1 = t_{\pm} + 5/t_{\pm} = 4$. The other two are then found $x_{2,3} = -2 \pm \sqrt{3}$.

Exercise 1.1.1. Show that any cubic equation can be brought to the form $z^3 \pm 3z + q = 0$ by a linear transformation⁵. For q real, find the roots through the substitution $z = s \mp (1/s)$.

1.2 The quartic equation.

The *Ars Magna* also contained the solution of the quartic equation, by Cardano's disciple Ludovico Ferrari (1522, 1565). In modern language, a linear change of the variable puts the equation in the form $x^4 = ax^2 + bx + c$. The smart idea is the introduction of an auxiliary parameter y in the equation:

$$(x^2 + y)^2 = (a + 2y)x^2 + bx + (y^2 + c).$$

The parameter is then chosen to make the right hand side (r.h.s.) of the equation the square of a binomial in x , so that square roots of both sides are then taken. The condition is the cubic equation for y , $0 = b^2 - 4(a + 2y)(y^2 + c)$, which may be solved by Cardano's formula. The value of y is entered in the quartic equation, $(x^2 + y)^2 = (a + 2y)[x + b/2(a + 2y)]^2$, and a square root brings it to a couple of quadratic equations in x .

Example 1.2.1. To solve the quartic equation $x^4 - 3x^2 - 2x + 5 = 0$, rewrite it as $(x^2 + y)^2 = (3 + 2y)x^2 + 2x - 5 + y^2$. Choose y such that r.h.s. is a perfect square in x , i.e. $2y^3 + 3y^2 - 10y - 16 = 0$ with a solution $y = -2$. Then the equation is $(x^2 - 2)^2 = -(x - 1)^2$, i.e. $x^2 - 2 = \pm i(x - 1)$. The two quadratic equations give the four solutions of the quartic.

In the effort to solve higher order equations, Vandermonde and especially Giuseppe Lagrange (Torino 1736, Paris 1813) emphasized the role of the permutation group and of

⁵ The equation $y^3 - 3y + 1 = 0$ can be solved with the aid of trigonometric tables: put $y = 2\cos x$ and obtain $0 = 2\cos(3x) + 1$; then $3x = \frac{2}{3}\pi$ and $3x = \frac{4}{3}\pi$ i.e. $y_1 = 2\cos(\frac{2}{3}\pi)$ and $y_2 = 2\cos(\frac{4}{3}\pi)$; the other solution is $y_3 = -y_1 - y_2$.

symmetric functions. In 1770 Lagrange obtained a new method of solution of the quartic equation,

$$z^4 + a_1 z^3 + a_2 z^2 + a_3 z + a_4 = 0.$$

Since it is instructive, we give a brief description of it. The coefficients of the equation are symmetric functions of the roots,

$$a_1 = -\sum_i z_i, \quad a_2 = \sum_{i<j} z_i z_j, \quad a_3 = -\sum_{i<j<k} z_i z_j z_k, \quad a_4 = z_1 z_2 z_3 z_4.$$

Any other symmetric function of the roots is expressible through them. The combination $s_1 = z_1 z_2 + z_3 z_4$ is not symmetric under all 4! permutations. In doing them, only two new combinations appear: $s_2 = z_1 z_3 + z_2 z_4$ and $s_3 = z_1 z_4 + z_2 z_3$. The three quantities $A_1 = s_1 + s_2 + s_3$, $A_2 = s_1 s_2 + s_1 s_3 + s_2 s_3$ and $A_3 = s_1 s_2 s_3$ are symmetric in s_1, s_2, s_3 , and are invariant under permutations of the roots z_i . As such, they may be expressed in terms of the coefficients a_i : $A_1 = a_2$, $A_2 = a_1 a_3 - 4a_4$, and $A_3 = a_3^2 + a_1^2 a_4 - 4a_2 a_4$. The s_i are the roots of the cubic equation $s^3 - A_1 s^2 + A_2 s - A_3 = 0$, and are evaluated by Cardano's method. Next, the four roots z_i are found.

1.3 Beyond the quartic.

For the fifth-order equation Lagrange eagerly tried to guess a polynomial combination of the roots that, under the 5! permutations, could produce at most 4 combinations s_1, \dots, s_4 that would solve a quartic equation. Paolo Ruffini (Modena 1765, 1822) showed that such a polynomial should be invariant under $5!/4$ permutations of the roots z_i , and does not exist.

The Norwegian mathematician Niels Henrik Abel (1802, 1829) put the last word in the memoir *On the algebraic resolution of equations* published in 1824. He proved that no rational solution involving radicals and algebraic expressions of the coefficients exists for general equations of order higher than four. The identification of the special equations that can be solved by radicals was done by Evariste Galois (1811, 1832), by methods of group theory to which he much contributed⁶.

In 1786 E. S. Bring, by exploiting an earlier method by Tschirnhausen (1683), showed that any equation of fifth degree can be brought to the amazingly simple form $z^5 + q_4 z + q_5 = 0$, and then to $z^5 + 5z + a = 0$ if $q_4 \neq 0$ (in general, an equation $x^n + a_1 x^{n-1} + \dots + a_n = 0$ can be reduced to $y^n + q_4 y^{n-4} + \dots + q_n = 0$ by means of the variable change $y = p_0 + p_1 x + \dots + p_4 x^4$ and solving equations of degree 2 and 3).

⁶ His last memoir was written in the tragical night before the duel that ended his short life. For a presentation of Galois theory see e.g. V.V.Prasolov, *Polynomials*, Springer (2004).



Figure 1.1 Leonhard Euler (1707, 1783) belongs to an impressive genealogy of mathematicians, rooted in Leibnitz and the Bernoullis. Euler spent many years in St. Petersburg, at the dawn of the Russian mathematical school. He discovered several important formulae for complex functions, and established much of the modern notation. His student Joseph Lagrange was the advisor of Fourier and Poisson. Poisson's students Dirichlet and Liouville mentored illustrious mathematicians that contributed to the advancement of complex analysis in Paris (on the side of Dirichlet: Darboux, and then Borel, Cartan, Goursat, Picard, and then Hadamard, Julia, Painlevé ...; on the side of Liouville: Catalan and then Hermite, Poincaré, Padé, Stieltjes ...).

Figure 1.2 Carl Friedrich Gauss (1777, 1855) became a celebrity after computing the orbit of the first asteroid Ceres, discovered and lost of sight by padre Piazzi in Palermo (1801). To interpolate the best orbit from observed points, Gauss devised the Least Squares method. The orbital elements placed Ceres in the region where astronomers were searching the fifth planet, that fitted in Titius and Bode's law. Gauss proved the "fundamental theorem of algebra": a polynomial of degree n has n zeros in the complex plane. He anticipated several results of complex analysis, which he did not publish. His genealogy contains venerable scientists as the astronomers Bessel and Encke, and mathematicians: Dedekind, Sophie Germain, Gudermann, and Georg Riemann. Among Gauss' "nephews" are Ernst Kummer and Karl Weierstrass.

Charles Hermite succeeded in obtaining a solution of the quintic equation, in terms of elliptic functions (1858). Soon after Leopold Kronecker and Francesco Brioschi⁷ gave alternative derivations⁸.

⁷ F. Brioschi (1824, 1897) taught mechanics in Pavia. He then founded Milan's Politecnico (1863), where he taught hydraulics. He participated in Milan's insurrection, and became member of the Parliament. Among his students (in Pavia): Giuseppe Colombo (he inaugurated in 1883 in Milan the first thermo-electric generator in continental Europe, by lighting the lamps of the Scala theatre. The cables were manufactured by the newly born Pirelli. Colombo succeeded to Brioschi in the direction of the Politecnico), Eugenio Beltrami

In 1888 the solution of the general sixth order equation was obtained by Brioschi and Maschke, in terms of hyperelliptic functions.

Of course no one would solve even a quartic by the methods described, as efficient numerical methods yield the roots with the desired accuracy.

(non Euclidean geometry, singular values of a matrix, Laplace Beltrami operator in curved space) and Luigi Cremona (painter).

⁸ A discussion of the quintic eq. is in J.V.Armitage and W.EEberlein, *Elliptic functions*, Lon. Math. Soc. Student Text 67 (2006). See also http://wapedia.mobi/en/Bring_radical, or V. Barsan, *Physical applications of a new method of solving the quintic equation*, arXiv:0910.2957v2; G. Zappa, *Storia della risoluzione delle equazioni di V e VI grado ...*, Rend. Sem. Mat. Fis. Milano (1995).

Chapter 2

The Field of Complex Numbers

Complex numbers were used in the early XVIII century by Leibnitz, Jean Bernoulli, Abraham De Moivre and by Leonhard Euler (1707, 1783) who discovered several relations involving trigonometric, exponential and logarithmic functions with imaginary argument.

The great improvement in the perception of complex numbers as well defined entities was their visualisation as vectors or points, by the Norwegian cartographer Caspar Wessel (1797) and the mathematician Jean Robert Argand (1806). It were Gauss' authority and investigations since 1799, that gave complex numbers a status in analysis.

In 1833 the Irish mathematician William R. Hamilton (1805, 1865) presented before the Irish Academy an axiomatic setting of the complex field \mathbb{C} as a formal algebra on pairs of real numbers. In 1867 Hankel proved that the algebra of complex numbers is the most general one that fulfils all fundamental laws of arithmetic.

2.1 The field \mathbb{C}

Definition 2.1.1. The field of complex numbers \mathbb{C} is the set of pairs of real numbers $z = (x, y)$ with the binary operations of sum and multiplication:

$$(x_1, y_1) + (x_2, y_2) = (x_1 + x_2, y_1 + y_2), \quad (2.1)$$

$$(x_1, y_1)(x_2, y_2) = (x_1 x_2 - y_1 y_2, x_1 y_2 + y_1 x_2) \quad (2.2)$$

The sum is commutative, associative, with neutral element (called zero) $0 \equiv (0, 0)$ and opposite $(-x, -y)$ of (x, y) .

The multiplication is commutative, associative, with unity $1 \equiv (1, 0)$, inverse element of any number $(x, y) \neq 0$

$$\left(\frac{x}{x^2 + y^2}, -\frac{y}{x^2 + y^2} \right)$$

The operations satisfy the distributive property $(z_1 + z_2)z_3 = z_1z_3 + z_2z_3$.

The subset of elements $(x, 0)$ is closed under these operations and identifies with the field of real numbers \mathbb{R} . Thus the field \mathbb{C} is an extension of the field \mathbb{R} .

If an element $(x, 0)$ is identified with x , a pair can be written as

$$(x, y) = (1, 0)(x, 0) + (0, 1)(y, 0) = 1x + iy = x + iy,$$

where i is Euler's symbol for the imaginary unit $i \equiv (0, 1)$. This is the usual representation of complex numbers. Additions and multiplications are done by regarding i as a unit with the property $i^2 = (0, 1)(0, 1) = (-1, 0) = -1$.

Proposition 2.1.2. \mathbb{C} is not an ordered field.

Proof. Suppose that \mathbb{C} is an ordered field: 1) for any pair $z \neq z'$ it is either $z < z'$ or $z > z'$; 2) $z < z' \rightarrow z + w < z' + w$; 3) $z < z'$, $w > 0 \rightarrow zw < z'w$.

Fix $i > 0$ then $i^2 > 0$ i.e. $-1 > 0$. Add 1 to get $0 > 1$, multiply by $-1 > 0$ and obtain $0 > -1$, which contradicts $-1 > 0$. \square

2.2 Complex conjugation

The complex conjugate (c.c.) of $z = x + iy$ is $\bar{z} = x - iy$.

Properties: $\bar{\bar{z}} = z$ (c.c. is an involution), $\overline{z_1 + z_2} = \bar{z}_1 + \bar{z}_2$ and $\overline{z_1 z_2} = \bar{z}_1 \bar{z}_2$.

The real numbers x and y are respectively the *real* and *imaginary* parts of z :

$$x = \operatorname{Re} z = \frac{z + \bar{z}}{2}, \quad y = \operatorname{Im} z = \frac{z - \bar{z}}{2i}.$$

2.3 Modulus

The *modulus* of a complex number is $|z| = \sqrt{x^2 + y^2}$. It is $|z|^2 = z\bar{z}$ and $|\bar{z}| = |z|$, $\operatorname{Re} z \leq |z|$ and $\operatorname{Im} z \leq |z|$. The following properties qualify the modulus as a *norm* and \mathbb{C} as a normed space:

$$|z| \geq 0, \quad |z| = 0 \text{ iff } z = 0, \tag{2.3}$$

$$|z_1 z_2| = |z_1| |z_2|, \tag{2.4}$$

$$|z_1 + z_2| \leq |z_1| + |z_2| \quad (\text{triangle inequality}) \tag{2.5}$$

Proof. The first property is obvious. The second one: use $|z_1 z_2|^2 = z_1 z_2 \bar{z}_1 \bar{z}_2$. Triangle inequality: $|z_1 + z_2|^2 = (z_1 + z_2)\overline{(z_1 + z_2)} = |z_1|^2 + |z_2|^2 + \bar{z}_1 z_2 + z_1 \bar{z}_2$; the last two terms are $2\operatorname{Re}(\bar{z}_1 z_2) \leq 2|\bar{z}_1 z_2| = 2|z_1| |z_2|$. Then $|z_1 + z_2|^2 \leq |z_1|^2 + |z_2|^2 + 2|z_1| |z_2| = (|z_1| + |z_2|)^2$. \square

If $1/z$ is the inverse of z it is $|z(1/z)| = 1$ i.e. $|1/z| = 1/|z|$.

The modulus simplifies the evaluation of the inverse of a complex number:

$$\frac{1}{z} = \frac{\bar{z}}{|z|^2} \quad \text{i.e.} \quad \frac{1}{x+iy} = \frac{x}{x^2+y^2} - i\frac{y}{x^2+y^2}$$

Remark 2.3.1. Property (2.4) has two interesting consequences:

1) The unit circle $|z| = 1$ is closed for complex multiplication.

2) For any $a, b, c, d \in \mathbb{N}$ there are integers $p = ad + bc$ and $q = |ac - bd|$ such that $(a^2 + b^2)(c^2 + d^2) = q^2 + p^2$. For example: $(1^2 + 5^2)(1^2 + 7^2) = 12^2 + 34^2$.

Exercise 2.3.2. Prove that $|z_1 + z_2|^2 + |z_1 - z_2|^2 = 2|z_1|^2 + 2|z_2|^2$ (in a parallelogram, the sum of the squares of the diagonals equals the sum of the squares of the sides).

Exercise 2.3.3. Let $|a| \neq 1$, prove that

$$\left| \frac{z-a}{1-\bar{a}z} \right| = 1 \quad \text{if and only if} \quad |z| = 1$$

Exercise 2.3.4. Prove the very useful inequalities:

$$\frac{1}{\sqrt{2}}(|x| + |y|) \leq |x + iy| \leq |x| + |y|, \quad x, y \in \mathbb{R} \quad (2.6)$$

$$\left| |z| - |w| \right| \leq |z - w|, \quad z, w \in \mathbb{C} \quad (2.7)$$

Hint: $x^2 + y^2 \geq 2|xy|$, then add $x^2 + y^2$; $|z - w|^2 = (|z| - |w|)^2 + 2|z||w| - 2\text{Re}(z\bar{w}) = (|z| - |w|)^2 + 2(|z\bar{w}| - \text{Re}\bar{z}w) \geq (|z| - |w|)^2$.

2.4 Argument

A nonzero complex number $z = x + iy$ may be represented as $z = |z|(\cos\theta + i\sin\theta)$, where $\cos\theta = x/|z|$ and $\sin\theta = y/|z|$. The number $\cos\theta + i\sin\theta$ belongs to the unit circle, where multiplication acts additively on phases:

$$(\cos\theta_1 + i\sin\theta_1)(\cos\theta_2 + i\sin\theta_2) = \cos(\theta_1 + \theta_2) + i\sin(\theta_1 + \theta_2).$$

De Moivre's formula follows:

$$(\cos\theta + i\sin\theta)^n = \cos(n\theta) + i\sin(n\theta)$$

At this stage, Euler's representation $\cos\theta + i\sin\theta = e^{i\theta}$ is introduced as a definition. It is consistent with the rule $e^{i\theta} e^{i\varphi} = e^{i(\theta+\varphi)}$.

Now this is the *polar representation* of a complex number:

$$z = |z|(\cos\theta + i \sin\theta) = |z|e^{i\theta} \quad (2.8)$$

The phase θ is the *argument* of z ($\theta = \arg z$). It is defined up to integer multiples of 2π . Note the property $\arg(z_1 z_2) = \arg z_1 + \arg z_2 \pmod{2\pi}$.

The **principal argument** $\text{Arg } z$ is the single determination

$$-\pi < \text{Arg } z \leq \pi$$

The sign of $\text{Arg } z$ is the same as $y = \text{Im } z$. The real negative semi-axis is a line of discontinuity (branch cut) of $\text{Arg } z$. By definition its points have $\text{Arg } z = \pi$.

The following simple formula evaluates the principal argument, with the determination $-\frac{\pi}{2} < \text{Arctan } \alpha \leq \frac{\pi}{2}$ (see fig.2.1):

$$\text{Arg } z = 2 \text{Arctan} \frac{y}{|z| + x} \quad (2.9)$$

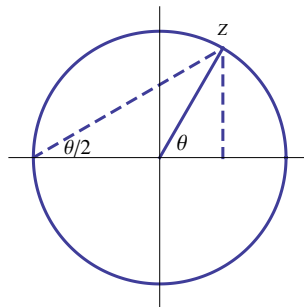


Figure 2.1 Given $z = x + iy$, the angle $\theta = \text{Arg } z$ is twice the angle at the circumference. The latter is always in $(-\frac{\pi}{2}, \frac{\pi}{2}]$, and $y = (|z| + x) \tan \frac{\theta}{2}$.

Other single determinations of the argument are possible, always having a line of discontinuity from the origin to infinity. For example, if the line is chosen as the imaginary upper half line, the range of values now is $(-\frac{3}{2}\pi, \frac{1}{2}\pi]$. The points on the cut, by definition, have argument $\frac{1}{2}\pi$; other values are: $\arg(-1+i) = -\frac{5\pi}{4}$, $\arg(-1) = -\pi$, $\arg 1 = 0$ (these points have $\text{Arg } i = \frac{\pi}{2}$, $\text{Arg}(-1+i) = \frac{3\pi}{4}$, $\text{Arg}(-1) = \pi$, $\text{Arg } 1 = 0$).

Note that the polar form $|z|\exp(i\theta)$ is insensitive to the choice of arg.

Exercise 2.4.1. In general $\text{Arg}(ab) \neq \text{Arg}(a) + \text{Arg}(b)$. Show that:

$$\text{Arg}(ab) = \text{Arg } a + \text{Arg } b + \begin{cases} -2\pi & \text{if } \pi < \text{Arg } a + \text{Arg } b \\ 0 & \text{if } -\pi < \text{Arg } a + \text{Arg } b \leq \pi \\ 2\pi & \text{if } \text{Arg } a + \text{Arg } b \leq -\pi \end{cases}$$

Exercise 2.4.2. Write the numbers $1 \pm i$ in polar form.

Exercise 2.4.3. Show that $e^{ia} + e^{ib} = 2 \cos \frac{a-b}{2} e^{\frac{i}{2}(a+b)}$, $a, b \in \mathbb{R}$

Exercise 2.4.4. Let $z = re^{i\theta}$, $r < 1$, show that $\text{Re} \frac{1+z}{1-z} > 0$.

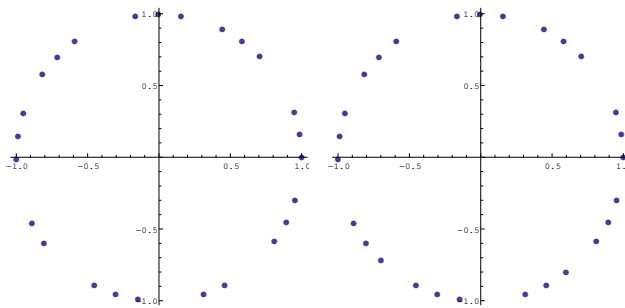


Figure 2.2 Left: the $N = 24$ points $\exp(in\sqrt{2})$, $n = 0, \dots, 23$ are separated by three gaps. For $N = 26$ (right), the new points $\exp(i24\sqrt{2})$, $\exp(i25\sqrt{2})$ modify the gaps with their neighbours, but still there are three gap-sizes.

The Three Gap Theorem (Vera T. Sós, 1957¹). This is an unexpected nice result: if $\frac{\theta}{2\pi}$ is irrational, then the N points $e^{in\theta}$, $n = 0, 1, \dots, N-1$, have at most 3 different gaps (see Fig.2.2). For $N \rightarrow \infty$ the points are uniformly distributed on the unit circle (Equidistribution Theorem, Hermann Weyl).

2.5 Exponential

The exponential of a complex number $z = x + iy$ is defined by the product

$$e^z \equiv e^x e^{iy} = e^x(\cos y + i \sin y) \tag{2.10}$$

¹ see <https://doi.org/10.48550/arXiv.2208.01680>

It exists for all z , with the fundamental property

$$\boxed{e^z e^w = e^{z+w}} \quad (2.11)$$

The exponential function is periodic, with period $2\pi i$: $e^{z+2\pi i} = e^z$ for all z . The trigonometric functions

$$\cos z = \frac{1}{2}(e^{iz} + e^{-iz}), \quad \sin z = \frac{1}{2i}(e^{iz} - e^{-iz})$$

are periodic with period 2π , and $\cos^2 z + \sin^2 z = 1$. They are unbounded on the imaginary axis. One also defines $\tan z = \sin z / \cos z$ and $\cot z = 1 / \tan z$.

The hyperbolic functions

$$\cosh z = \frac{1}{2}(e^z + e^{-z}), \quad \sinh z = \frac{1}{2}(e^z - e^{-z})$$

are periodic with period $2\pi i$, and $\cosh^2 z - \sinh^2 z = 1$. They are unbounded on the real axis. One defines $\tanh z = \sinh z / \cosh z$ and $\coth z = 1 / \tanh z$.

Exercise 2.5.1.

- 1) Show that $|e^z| = e^x$, $\overline{e^z} = e^{\bar{z}}$.
- 2) Find the zeros of $\sinh(az + b)$, $a, b \in \mathbb{R}$.
- 3) Show that $|\cosh(x + iy)| \leq \cosh x$.

Exercise 2.5.2 (Chebyshev polynomials).

Show that $\cos(n\theta)$ is a polynomial of degree n in $t = \cos\theta$. It is the Chebyshev polynomial of the first kind $T_n(t)$. Evaluate the first few polynomials.

Show that they have the following properties of recursion and "orthogonality"²:

$$T_{n+1}(t) - 2t T_n(t) + T_{n-1}(t) = 0 \quad (2.12)$$

$$\int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} T_m(t) T_n(t) = \begin{cases} 0 & n \neq m \\ \pi & n = m = 0 \\ \pi/2 & n = m \neq 0 \end{cases} \quad (2.13)$$

Prove similar properties for the Chebyshev polynomials of the second kind:

$$U_n(t) = \frac{\sin[(n+1)\theta]}{\sin\theta} \quad (t = \cos\theta). \quad (2.14)$$

Hint: $2 \cos(n\theta) = (\cos\theta + i \sin\theta)^n + c.c.$

² The meaning of this term will become clear after the introduction of Hilbert spaces.

2.6 Logarithm

The *logarithm* of a complex number z is the exponent that solves the equality $e^{\log z} = z$. Because of the periodicity of the exponential function, there are an infinite number of solutions: if $\log z$ is a solution, also $\log z + i2k\pi$ is a solution for any integer k . With $z = |z|e^{i\theta}$ one obtains

$$\log z = \log|z| + i \arg z + i2k\pi, \quad k \in \mathbb{Z} \quad (2.15)$$

Note that $\log z$ is not defined in $z = 0$.

The product rule of exponentials implies $\log(z_1 z_2) = \log z_1 + \log z_2$.

While the real part of $\log z$ is well determined as the log of a real positive number, the imaginary part reflects the same indeterminacy of the argument of a complex number.

It is natural to define the **principal logarithm** of a number as

$$\text{Log } z = \log|z| + i \text{Arg } z \quad (2.16)$$

The Log has a *cut of discontinuity* on the real negative axis: for $\epsilon \rightarrow 0^+$ and $x < 0$:

$$\text{Log}(x \pm i\epsilon) \rightarrow \log|x| \pm i\pi$$

$$\text{Log}(x) = \log|x| + i\pi$$

For example $\text{Log}(-1) = i\pi$.

By ex.2.4.1, it is $\text{Log}(ab) = \text{Log } a + \text{Log } b$ when a and \bar{b} are in sight (i.e. the segment $[a, \bar{b}]$ does not cross the negative real axis). It is $\text{Log}(a/b) = \text{Log } a - \text{Log } b$ when a and b are in sight.

In full analogy with the argument, different single-valued determinations of the log are possible and always have a line of discontinuity (*branch cut*) from 0 (*the branch point*) to ∞ . For example, $\log(-i)$ is $-i\frac{\pi}{2}$ if the Log is used; it is $i\frac{3\pi}{2}$ if the log is chosen with cut on the real positive half-line. It is $-i\frac{\pi}{2}$ if the cut is on the positive imaginary axis.

Exercise 2.6.1. Evaluate $\text{Log} \frac{1+i}{1-i}$, $\text{Log}(ie^{\frac{3}{4}i\pi})$, $\text{Log}(1 + i \tan \theta)$.

Exercise 2.6.2. What are $\text{Log}(-z)$, $\text{Log} \bar{z}$, $\text{Log}(1/z)$, and $\text{Log}(1/\bar{z})$ in terms of $\text{Log } z$?

Exercise 2.6.3. Prove for $0 < \theta < \frac{\pi}{2}$: $\text{Log}(1 - e^{i\theta}) = \log[2 \sin(\frac{1}{2}\theta)] + i\frac{1}{2}(\theta - \pi)$.

2.7 Power of a complex number

The power of a complex number is *defined* as

$$\boxed{z^{a+ib} = e^{(a+ib)\log z} = e^{(a+ib)(\log|z|+i\arg z+i2\pi k)}} \quad (2.17)$$

In general it is multi-valued (such is the log).

If the exponent is real: $z^a = |z|^a \exp(i a \arg z + i 2\pi a k)$, $k = 0, \pm 1, \pm 2, \dots$

- $a \in \mathbb{Z}$: the powers $z^{\pm n}$ are single-valued.
- $a \in \mathbb{Q}$ ($a = \pm p/q$, with p and q coprime): the powers form a periodic sequence, only q terms are distinct and are vertices of a regular polygon.
Example: $(1+i)^{2/3} = (\sqrt{2}e^{i\pi/4})^{2/3} = 2^{1/3} \exp(i\frac{\pi}{6} + i\frac{4}{3}k\pi)$, the values $k = 0, 1, 2$ give three distinct powers.
- a is irrational: the set of powers is infinite.
Example: $(1+i)^\pi = (\sqrt{2}e^{i\pi/4})^\pi = 2^{\pi/2} \exp(i\frac{\pi^2}{4} + i2\pi^2 k)$, $k = 0, \pm 1, \pm 2, \dots$

If the exponent is complex: $z^{a+ib} = [|z|^a e^{-b(\arg z + 2\pi k)}] e^{i[b \log|z| + a(\arg z + 2\pi k)]}$. Examples: $1^i = e^{i \log 1} = \{e^{i(0+2\pi k)}\}_{k \in \mathbb{Z}} = \{1, e^{\pm 2\pi}, e^{\pm 4\pi}, \dots\}$;
 $(1+i)^{1-i} = \{e^{(1-i)(\log \sqrt{2} + i\frac{\pi}{4} + 2\pi i k)}\}_{k \in \mathbb{Z}} = \{\sqrt{2}e^{\pi(\frac{1}{4} + 2k)} e^{i(\frac{\pi}{4} - \log \sqrt{2})}\}_{k \in \mathbb{Z}}$

Exercise 2.7.1. Evaluate: $8^{1/3}$, $(-1)^{1/5}$, $i^{1/4}$, $(1-i)^{1/6}$.

Exercise 2.7.2. Show that the square roots of $z = a + ib$ are:

$$\pm \left[\sqrt{\frac{\sqrt{a^2 + b^2} + a}{2}} + i \frac{b}{2} \sqrt{\frac{2}{\sqrt{a^2 + b^2} + a}} \right]$$

Exercise 2.7.3. Show the properties: $|z^a| = |z|^a$, $z^a z^b = z^{a+b}$, $(zw)^a = z^a w^a$ (for multivalued powers, the sets in the two sides must coincide).

2.8 The fundamental theorem of algebra

The theorem states that in \mathbb{C} a polynomial of degree n with complex coefficients has precisely n zeros³. Then, a polynomial $p(z) = a_0z^n + \cdots + a_n$ has the unique factorization

$$p(z) = a_0(z - z_1)(z - z_2)\cdots(z - z_n), \quad (2.18)$$

where z_1, \dots, z_n are the zeros (or roots, that may be coincident).

A proof was found by Carl Friedrich Gauss, in his doctorate dissertation *Demonstratio nova theorematis omnem functionem algebraicam rationalem integram unius variabilis in factores reales primi vel secundi gradus resolvi posse* (1799). He showed that for any polynomial $p(z) = u(x, y) + iv(x, y)$ (with real coefficients) the curves $u(x, y) = 0$ and $v(x, y) = 0$ necessarily intersect. Before him, Girard (1629), d'Alembert (1748) and Euler (1749), proved the weaker statement that any polynomial with real coefficients factors into real linear and quadratic polynomials.

A simple proof will be given with Liouville's theorem for entire functions (see 9.2).

2.9 The cyclotomic equation

The roots of the equation $z^n = 1$ are the corners of a regular n -polygon inscribed in the unit circle:

$$\zeta_k = \cos\left(\frac{2k\pi}{n}\right) + i \sin\left(\frac{2k\pi}{n}\right), \quad k = 0, \dots, n-1.$$

The absence of intermediate powers of z in $z^n - 1 = 0$ implies the properties of the roots $\zeta_0^p + \cdots + \zeta_{n-1}^p = 0$, $p = 1, \dots, n-1$.

Given that $z^n - 1 = (z - 1)(z^{n-1} + \cdots + z + 1)$, the roots $\zeta_1, \dots, \zeta_{n-1}$ solve the *cyclotomic equation* $z^{n-1} + \cdots + z + 1 = 0$.

In 1796 Gauss, then a young student, two millennia after Euclid, announced the possibility to construct by ruler and compass the regular polygon with $n = 17$ sides. Five years later he gave a sufficient condition⁴ for a polygon to be constructible by ruler and compass: $n = 2^k p_1^{m_1} p_2^{m_2} \cdots$, where the factor 2^k accounts for repeated duplications of the number of sides of a more basic polygon. The factors p are either 1 or a Fermat number (i.e. $p = 2^{2^q} + 1$) that is also a prime number⁵.

³ This intuitive explanation is from T. Gowers, *The Princeton companion to Mathematics*, Princeton Univ. Press (2009). Let $p(z) = z^n + a_1z^{n-1} + \cdots + a_n$, with $a_n \neq 0$. For very large R the set $p(Re^{i\theta})$, $\theta \in [0, 2\pi)$, approximates a circle of radius R^n run n times, that contains the origin. For sufficiently small R , the set $p(Re^{i\theta}) \approx a_{n-1}Re^{i\theta} + a_n$ is a circle does not contain the origin. By continuity, there must be R and an angle θ such that $p(Re^{i\theta}) = 0$.

⁴ Wantzel (1836) showed that it is also necessary.

⁵ Euler showed that the Fermat number $2^{32} + 1$ ($q = 5$) is not a prime number. L. Anderson, J. S. Chahal, Jaap Top, *The last chapter of the Disquisitiones of Gauss*, <https://doi.org/10.48550/arXiv.2110.01355>.

The polygons $n = 3, 4, 5$ and duplications ($n = 6, 8, 10, \dots$) were known since Euclid's time, and correspond to the Fermat primes $p = 1, 3, 5$. The next Fermat prime number is $p = 2^{2^2} + 1 = 17$. Gauss was so proud of his discovery, that he asked for a 17-polygon to be carved on his gravestone (but the stonemason declined to do it)⁶.

Example 2.9.1. Solve the equation $z^5 = 1$ and obtain $\cos \frac{2\pi}{5} = \frac{1}{4}(\sqrt{5} - 1)$.

A: the sum of the zeros $\zeta_k = e^{i2\pi k/5}$, $k = 0, \dots, 4$, is zero (the term z^4 is missing in the equation). Then the real part of the sum is zero: $1 + 2 \cos \frac{2\pi}{5} + 2 \cos \frac{4\pi}{5} = 0$. Next use $2 \cos^2 \frac{2\pi}{5} = 1 + \cos \frac{4\pi}{5}$ and the result is found.

Exercise 2.9.2. Let $\{\zeta_k\}_{k=0}^{n-1}$ be the roots of $z^n = 1$. Show that:

$$a^n - b^n = (a - b)(a - \zeta_1 b) \cdots (a - \zeta_{n-1} b) \quad (2.19)$$

Exercise 2.9.3. Consider the polygon with corners at the n roots of unity $1, \zeta, \dots, \zeta^{n-1}$ and draw the diagonals connecting 1 to the other corners. Show⁷ that the product of their lengths is precisely n : $|1 - \zeta| \cdots |1 - \zeta^{n-1}| = n$.

Exercise 2.9.4 (Madhava Math. competition, 2013). Let $1, \zeta, \dots, \zeta^{n-1}$ be the n roots of unity. Show that the sum of squared distances $\sum_{k=0}^{n-1} |z - \zeta_k|^2$ is the same for all z on the unit circle.

Exercise 2.9.5 (Discrete Fourier transform⁸). Show that the $N \times N$ matrix

$$F_{rs} = \frac{1}{\sqrt{N}} \exp(i \frac{2\pi}{N} rs) \quad r, s = 1 \dots N$$

is unitary. Evaluate F^2 and show that $F^4 = 1$. What are the eigenvalues of F ? (Hint: you need the sum of powers of the N roots of unity).

Example 2.9.6. Evaluate the characteristic polynomial of the $n \times n$ matrix

$$H_n = \begin{bmatrix} 0 & 1 & & 0 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 0 & & 1 & 0 \end{bmatrix}.$$

⁶ The tale of the $(2^8 + 1)$ -gon is narrated in the nice book *Dr. Euler's fabulous formula* by Paul Nahin, Princeton Univ. Press (2006).

⁷ An amusing generalization to the ellipse is discussed in <https://doi.org/10.48550/arXiv.1810.00492>

⁸ M.L.Mehta, Eigenvalues and eigenvectors of the finite Fourier transform, J. Math. Phys. 28 (1987) 781.

A.: If $D_k(z) = \det[zI_k - H_k]$ then $D_{k+1}(z) = zD_k(z) - D_{k-1}(z)$ with the initial conditions $D_1(z) = z$ and $D_0(z) = 1$. The expansion can be written with a "transfer matrix" T :

$$\begin{bmatrix} D_{k+1}(z) \\ D_k(z) \end{bmatrix} = T \begin{bmatrix} D_k(z) \\ D_{k-1}(z) \end{bmatrix}, \quad T = \begin{bmatrix} z-1 \\ 1 & 0 \end{bmatrix}$$

Iteration gives the solution for any matrix size

$$\begin{bmatrix} D_{k+1}(z) \\ D_k(z) \end{bmatrix} = T^k \begin{bmatrix} z \\ 1 \end{bmatrix} = T^{k+1} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Then $D_k(z) = [T^{k+1}]_{21}$. The matrix T^{k+1} is evaluated with the Cayley-Hamilton theorem, that states that a square matrix solves its characteristic equation. In this case: $\det(\lambda I_2 - T) = \lambda^2 - \lambda z + 1$. Then $T^2 - Tz + I_2 = 0$. This implies $T^{k+1} = a_{k+1}T + b_{k+1}I_2$, with numbers a_{k+1} , b_{k+1} to be found. Since the eigenvalues of T are $\lambda_{\pm} = \frac{1}{2}[z \pm \sqrt{z^2 - 4}]$, it is $\lambda_{\pm}^{k+1} = a_{k+1}\lambda_{\pm} + b_{k+1}$. The result for $k = n$ is

$$\det(zI_n - H_n) = [T^{n+1}]_{21} = a_{n+1} = \frac{\lambda_+^{n+1} - \lambda_-^{n+1}}{\lambda_+ - \lambda_-}$$

In particular, if $z = 2 \cos \theta$ one finds $\lambda_{\pm} = e^{\pm i\theta}$:

$$\det(2 \cos \theta I_n - H_n) = \frac{\sin(n+1)\theta}{\sin \theta} = U_n(\cos \theta)$$

where U_n is a Chebyshev polynomial of the second kind, (2.14).

The eigenvalues of H_n are easily found: $\epsilon_k = 2 \cos(\frac{\pi}{n+1} k)$, $k = 1, \dots, n$.

Exercise 2.9.7. Consider the following $n \times n$ matrix:

$$S_n = \begin{bmatrix} 0 & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ 1 & & & & 0 \end{bmatrix} \tag{2.20}$$

Its action on a vector $u \in \mathbb{C}^n$ is a cyclic shift of the components: $(S_n u)_k = u_{k+1}$ and $(S_n u)_n = u_1$.

1) Show that $S_n^{n-1} = S_n^T$ (T means transposition).

2) Find the eigenvalues and the eigenvectors of S_n .

3) Find the spectrum of the periodic "Laplacian matrix" $\Delta_n = S_n + S_n^T - 2I_n$

$$\Delta_n = \begin{bmatrix} -2 & 1 & & 1 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 1 & & 1 & -2 \end{bmatrix}$$

4) Find the characteristic polynomial $\det(zI_n - \Delta_n)$.

Exercise 2.9.8. A matrix $A = a_0 I_n + a_1 S_n + \dots + a_{n-1} S_n^{n-1}$, where S_n is the shift matrix (2.20), is named “circulant”. Find the eigenvalues and eigenvectors for the case $n = 4$:

$$A = \begin{bmatrix} a_0 & a_1 & a_2 & a_3 \\ a_3 & a_0 & a_1 & a_2 \\ a_2 & a_3 & a_0 & a_1 \\ a_1 & a_2 & a_3 & a_0 \end{bmatrix}$$

Hint: A commutes with S, whose eigenvectors and eigenvalues are known.

(The eigenvalues of A are: $\lambda_0 = a_0 + a_1 + a_2 + a_3$, $\lambda_1 = a_0 + i a_1 - a_2 - i a_3$, $\lambda_2 = a_0 - a_1 + a_2 - a_3$, $\lambda_3 = a_0 - i a_1 - a_2 + i a_3$).

Chapter 3

The Complex Plane

The modulus defines the Euclidean distance of two points $z = (x, y)$ and $z' = (x', y')$ in the complex plane:

$$d(z, z') = |z - z'| = \sqrt{(x - x')^2 + (y - y')^2} \quad (3.1)$$

Results of Cartesian geometry of \mathbb{R}^2 can be transposed to \mathbb{C} . Disks, circles and lines are important in complex analysis; let's review them in complex notation.

3.1 Straight lines and circles

Given two points a and b in \mathbb{C} , the oriented straight line ab has parametric equation $z(t) = (1 - t)a + tb$, $t \in \mathbb{R}$. The restriction $0 \leq t \leq 1$ traces the closed oriented segment $[a, b]$ from a to b .

Exercise 3.1.1.

- 1) Find the corners of the squares and of the equilateral triangles having one side on the segment $[0, a]$.
- 2) Describe the sets: $\text{Arg} z = \frac{\pi}{3}$, $\text{Arg}(z - i) = \frac{\pi}{3}$, $|\text{Arg}(z - i)| < \frac{\pi}{3}$.
- 3) Give the conditions for a point z to be inside the triangle with vertices a, b, c . Answer: $z = \alpha a + \beta b + \gamma c$, where $\alpha + \beta + \gamma = 1$ and $0 \leq \alpha, \beta, \gamma \leq 1$.

A circle with center a and radius r has equation $|z - a| = r$. The parametrization

$$z(\theta) = a + r e^{i\theta}, \quad 0 \leq \theta < 2\pi \quad (3.2)$$

endows the circle with the standard anticlockwise orientation.

Exercise 3.1.2.

1) Show that the locus $|z - a|^2 + |z - b|^2 = |a - b|^2$ is a circle with diameter $[a, b]$. Find the parametric equation of the circle.

2) Show that the locus $|z - a| = \lambda|z - b|$, $\lambda > 0$ is a circle (Apollonius of Perga).

The circle has radius $\frac{\lambda}{|1 - \lambda^2|}|a - b|$ and center $\frac{a - \lambda^2 b}{1 - \lambda^2}$. The value $\lambda = 1$ is the limit case of a line (axis of segment $[a, b]$).

3) Show that the circle through z_1, z_2, z_3 has equation

$$\det \begin{bmatrix} |z|^2 & z & \bar{z} & 1 \\ |z_1|^2 & z_1 & \bar{z}_1 & 1 \\ |z_2|^2 & z_2 & \bar{z}_2 & 1 \\ |z_3|^2 & z_3 & \bar{z}_3 & 1 \end{bmatrix} = 0$$

Exercise 3.1.3.

1) Find the equation of the ellipse with foci z_1 and z_2 , major semiaxis length a .

2) Study the family of Cassini ovals¹ $|z^2 - 1| = r^2$ as r changes. It is a single closed line for $r \geq 1$.

3.2 The stereographic projection

It is useful to introduce the **extended complex plane** $\bar{\mathbb{C}} = \mathbb{C} \cup \infty$.

The point at infinity is subject to the rules $z + \infty = \infty + z = \infty$ and $z\infty = \infty z = \infty$ ($z \neq 0$). Moreover, one puts the conventions $z/\infty = 0$ ($z \neq \infty$), and $z/0 = \infty$ ($z \neq 0$). The point at infinity is better appreciated in the stereographic projection, a bijection among the points of the extended complex plane and the points of the surface S_2 of the *Riemann sphere*.

The Riemann sphere that is here considered has unit diameter and is tangent to the complex plane in its south pole².

In a Cartesian frame XYZ the equation of the surface is $X^2 + Y^2 + (Z - \frac{1}{2})^2 = \frac{1}{4}$. The plane $Z = 0$ is the complex plane z . A segment from the north pole $(0, 0, 1)$ to a point z intersects the spherical surface at the point P with coordinates

$$X = \frac{1}{2} \frac{z + \bar{z}}{|z|^2 + 1}, \quad Y = \frac{1}{2i} \frac{z - \bar{z}}{|z|^2 + 1}, \quad Z = \frac{|z|^2}{|z|^2 + 1} \quad (3.3)$$

The north pole corresponds to the point ∞ of the extended plane.

¹ A Cassini oval is the planar locus of points whose distances from two points have constant product: $|z - a| \cdot |z - b| = C^2$.

² The sphere is often fixed to have unit radius and center in the origin; other choices are possible.

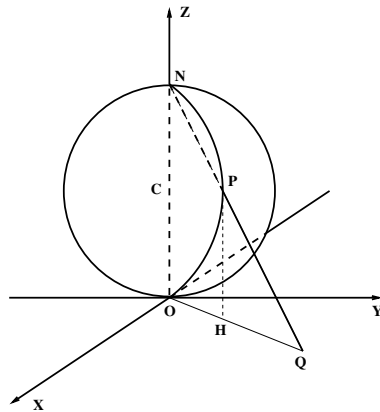


Figure 3.1 The stereographic projection maps a point $Q = z = x + iy$ in \mathbb{C} to a point $P = (X, Y, Z)$ of the Riemann sphere. The correspondence among coordinates is obtained through similitudes. First find OH : let K be the projection of P on the axis and consider CPK : $OH = PK$ and $OH^2 = CP^2 - CK^2 = \frac{1}{4} - (Z - \frac{1}{2})^2$. Now it is: $1 : Z = |z| : (|z| - OH)$. This gives Z . Next: $X : x = OH : |z|$ and $Y : y = OH : z$.

The Euclidean distance $\|P - P'\|$ in \mathbb{R}^3 between two points of the sphere S_2 defines the **chordal distance** between the two corresponding points in \mathbb{C} :

$$d_c(z, z') = \frac{|z - z'|}{\sqrt{1 + |z|^2} \sqrt{1 + |z'|^2}} \tag{3.4}$$

The chordal distance has limit value 1, the diameter of the sphere, and is also the distance of $(0, \infty)$.

Exercise 3.2.1. Show that $d_c(z, z') = 1$ only for pairs $(z, -1/\bar{z})$. Show that a pair correspond to antipodal points of the sphere.

Proposition 3.2.2. The stereographic projection maps circles in S_2 to circles in \mathbb{C} . The circles through the north pole are mapped to straight lines.

Proof. The locus of points of S_2 with Euclidean distance R from a point $C \in S_2$ is a circle. Its image in \mathbb{C} is the locus $d_c(z, z_C) = R$, or

$$|z - z_C|^2 = [R^2(1 + |z_C|^2)](1 + |z|^2)$$

This is the equation of a circle. If the circle in S_2 goes through the north pole, the image in \mathbb{C} contains $z = \infty$. Thus it must be $R^2(1 + |z_C|^2) = 1$ to balance infinities. The equation $|z - z_C|^2 = 1 + |z|^2$ is linear in z (a straight line). □

Proposition 3.2.3. The stereographic projection is conformal (angle-preserving).

Proof. A triangle in \mathbb{C} has vertices z , $z + \epsilon$ and $z + \eta$ and side lengths $|\epsilon|$, $|\eta|$ and $|\eta - \epsilon|$. The angle in z is given by Carnot's formula:

$$\cos \alpha = \frac{|\epsilon|^2 + |\eta|^2 - |\eta - \epsilon|^2}{2|\epsilon||\eta|} = \frac{\bar{\epsilon}\eta + \epsilon\bar{\eta}}{2|\epsilon||\eta|}$$

The corresponding points on the Riemann's sphere form a triangle with side-lengths given by the chordal distances. The angle corresponding to α is

$$\begin{aligned} \cos \alpha' &= \frac{d_c(z, z + \epsilon)^2 + d_c(z, z + \eta)^2 - d_c(z + \epsilon, z + \eta)^2}{2d_c(z, z + \epsilon)d_c(z, z + \eta)} \\ &= \frac{|\epsilon|^2(1 + |z + \eta|^2) + |\eta|^2(1 + |z + \epsilon|^2) - |\epsilon - \eta|^2(1 + |z|^2)}{2|\epsilon||\eta|\sqrt{(1 + |z + \epsilon|^2)(1 + |z + \eta|^2)}} \end{aligned}$$

For $|\epsilon|, |\eta| \rightarrow 0$, the angle α' identifies with the spherical angle and $\alpha' \rightarrow \alpha$. □

3.3 Simple maps

In this section we study simple maps $w = F(z)$, where $F : \mathbb{C} \rightarrow \mathbb{C}$. The subject is of considerable interest and will be fully appreciated after the discussion of analytic functions.

3.3.1 The linear map

The linear map $w = az + b$ has one fixed point $z^* = b/(1 - a)$. By writing $w - z^* = a(z - z^*)$ one obtains

$$|w - z^*| = |a||z - z^*|, \quad \arg(w - z^*) = \arg a + \arg(z - z^*)$$

Therefore the map is a *dilation* by a factor $|a|$ of all segments originating from z^* and a *rotation* of the plane by $\arg a$ around the fixed point.

Equivalently, the map can be viewed as a rotation by $\arg a$ around the origin and a dilation centred in the origin ($z' = az$), followed by a shift ($w = z' + b$).

Exercise 3.3.1. Show that a linear map takes circles to circles and straight lines to straight lines.

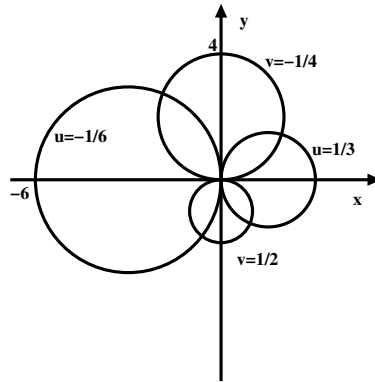


Figure 3.2 *Inversion map. The circles through the origin of the z plane with centers on the real or the imaginary axis are mapped to lines of constant u or v in the w plane. As the lines form an orthogonal grid in the w plane, also the circles cross at right angles.*

3.3.2 The inversion map

The map $w = 1/z$ transforms a circle $|z| = r$ centred in the origin into the circle $|w| = 1/r$. It maps 0 to infinity and vice versa. The interior of the unit circle is exchanged with the exterior.

By regarding straight lines as circles with a point at infinity, the inversion takes circles to circles (prove it). Then, a straight line that does not contain the origin is mapped to a circle through the origin (because of the point at infinity). Only straight lines through the origin (containing both 0 and ∞) are mapped to straight lines through the origin. Conversely, circles through the origin are mapped to straight lines, and circles not through the origin are mapped to circles.

Set $w = u + iv$, the image of $x + iy$ has Cartesian coordinates

$$u = \frac{x}{x^2 + y^2}, \quad v = -\frac{y}{x^2 + y^2}$$

A line $u(x, y) = U$ in w -plane is the image of a circle through the origin $z = 0$ with center $(\frac{1}{2U}, 0)$. A line $v(x, y) = V$ is the image of a circle again through the origin with center $(0, -\frac{1}{2V})$. All these circles, that are mapped to the orthogonal grid of $u - v$ lines, are orthogonal to each other (we'll give a general proof of this fact).

Exercise 3.3.2. *For the inversion map:*

- 1) Find the image of the circle $|z - i| = 1$.
- 2) Show that the circle $|z - z_0| = |z_0|$ is mapped to the axis of $[0, 1/z_0]$.
- 3) Obtain the image of the line $|z - a| = |z - b|$, where $a, b \in \mathbb{C}$.

3.3.3 The Möbius maps

A Möbius map $w = M(z)$ is a linear fractional transformation

$$M(z) = \frac{az + b}{cz + d}, \quad ad - bc \neq 0 \quad (3.5)$$

The map is unchanged if the complex parameters a, b, c, d are multiplied by the same nonzero value. It has at most two fixed points $z^* = M(z^*)$. If $c \neq 0$ $M(-d/c) = \infty$, and $M(\infty) = a/c$.

This is easily checked:

Proposition 3.3.3. *Möbius maps form a group.*

To the Möbius map (3.5) there corresponds an invertible matrix

$$L = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \det L \neq 0. \quad (3.6)$$

Such matrices form the linear group $GL(2, \mathbb{C})$ of invertible complex 2×2 matrices. If $M_L(z)$ is the Möbius map with parameters specified by the matrix L , the composition of two Möbius maps is $M_{L'}(M_L(z)) = M_{L'L}(z)$.

The linear map and the inversion map are Möbius maps with matrices

$$\begin{bmatrix} a & b \\ 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (3.7)$$

If $c \neq 0$ put it equal to 1; the factorization

$$\begin{bmatrix} a & b \\ 1 & d \end{bmatrix} = \begin{bmatrix} -ad + b & a \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & d \\ 0 & 1 \end{bmatrix}. \quad (3.8)$$

shows that a Möbius map is a composition of two linear maps with an inversion between (the case $c = 0$ is a linear map). As a consequence:

1) circles are mapped to circles (where a straight line is a circle with point at ∞). More precisely, M takes every line and circle passing through $-d/c$ to a line, and every other line or circle to a circle.

2) Möbius maps are bijections from $\bar{\mathbb{C}}$ to $\bar{\mathbb{C}}$ (actually, they are the most general bijections of the extended complex plane).

Example 3.3.4. The Möbius maps of the upper half-plane $\mathbb{H} = \{z : \text{Im} z > 0\}$ to the unit disk $\mathbb{D} = \{w : |w| < 1\}$, are

$$w = e^{i\theta} \frac{z - z_0}{z - \bar{z}_0} \quad (3.9)$$

where z_0 is the point with $\text{Im} z_0 > 0$ that is mapped to $w = 0$, and the prefactor is a rotation of the disk.

Proof. Let $w(z)$ have the form (3.5), with $c = 1$. Since a boundary is mapped to a boundary, the image of the real axis must be the unit circle. Then $|ax + b| = |x + d|$ for all real x . The limit cases $x \rightarrow \infty$ and $x = 0$ imply $|a| = 1$, $|b| = |d|$ i.e. $a = e^{i\theta}$, $b = -e^{i\theta} z_0$, $|d| = |z_0|$. Then $|x - z_0| = |x - d|$ for all x i.e.: $x^2 + |z_0|^2 - 2x\text{Re} z_0 = x^2 + |z_0|^2 - 2x\text{Re} d$. The equation is solved by $d = \bar{z}_0$. \square

Exercise 3.3.5. Show that the Möbius maps of the upper-half plane \mathbb{H} on itself are represented by real matrices $\text{GL}(2, \mathbb{R})$ with positive determinant.

A Möbius map can be specified by requiring that three points (z_1, z_2, z_3) are mapped (in the order) to prescribed points (w_1, w_2, w_3) . The choice $(0, 1, \infty)$ for the image points gives the Möbius map

$$M(z) = \frac{z - z_1}{z - z_3} \frac{z_2 - z_3}{z_2 - z_1}. \quad (3.10)$$

It maps the circle through z_1, z_2 and z_3 to the real axis (the circle that contains $0, 1$ and ∞).

Exercise 3.3.6. Show that for any Möbius map $z' = M(z)$ the cross-ratio with 4 points is invariant:

$$\frac{z'_1 - z'_3}{z'_1 - z'_4} \frac{z'_2 - z'_4}{z'_2 - z'_3} = \frac{z_1 - z_3}{z_1 - z_4} \frac{z_2 - z_4}{z_2 - z_3}$$

Example 3.3.7. The Möbius map $w(z) = \frac{2iz}{z+i}$ has fixed points 0 and i . The point $-i$ is mapped to infinity: any circle or line through it is mapped to a line.

We know a priori that the parallel lines $\text{Im} z = Y$ ($z = x + iY$) are mapped to circles parameterized by x . Elimination of x brings to the familiar expression:

$$w = \frac{-2Y + 2ix}{x + i(1 + Y)} \Rightarrow \left| w - i \frac{2Y + 1}{Y + 1} \right| = \frac{1}{|Y + 1|}$$

The real axis $Y = 0$ is mapped to the circle $|w - i| = 1$. The line $Y = -1$ ($z = x - i$) through the special point $-i$ is mapped to the line $w = (2/x) + 2i$ (not shown in fig.3.3). The lines with $Y > 0$ are mapped as circles in the disk $|w - i| < 1$ (the image of the upper half z -plane). The

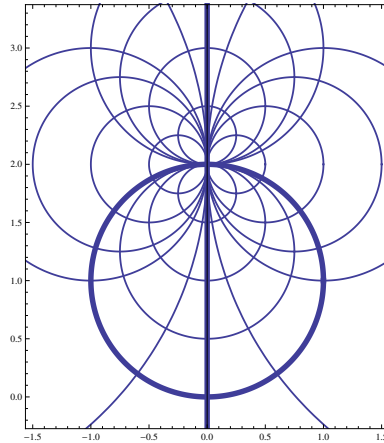


Figure 3.3 The Möbius map of example 3.3.7. The x and y axes are mapped to the thick circle and the v axis of the w -plane; 0 and i are fixed points. The circles with center on v axis are images of horizontal lines, while the others are images of vertical lines. The upper half plane is mapped to the interior of the thick circle.

lines with $Y < 0$ are outside the disk. In any case the circles are tangent at $2i$. The lines $Re z = X$ are mapped to circles through $w = 2i$, orthogonal to the previous circles (see fig.3.3).

Exercise 3.3.8.

- 1) Find the images of $|z - 1| = 1$ and $|z - 1| = 2$ for the map $2 + (1/z)$.
- 2) Evaluate the Möbius map that takes $(0, 1, i)$ to (w_1, w_2, w_3) .
- 3) Let 0 and 1 be the fixed points of a Möbius map $M(z)$. Write the general equation of circles through the two points, and evaluate their images under $M(z)$.

3.3.4 Rigid motions of the Riemann sphere*

Consider the Möbius maps that preserve the chordal distance:

$$d_c(M(z), M(z')) = d_c(z, z'), \quad \forall z, z' \in \mathbb{C}$$

They map a pair $(z, -1/\bar{z})$ with chordal distance 1 to a pair with chordal distance 1, i.e. $M(-1/\bar{z}) = -1/\overline{M(z)}$:

$$\frac{a - b\bar{z}}{c - d\bar{z}} = -\frac{\bar{c}\bar{z} + \bar{d}}{\bar{a}\bar{z} + \bar{b}}, \quad \forall z$$

The equality gives: $|a|^2 + |c|^2 = |b|^2 + |d|^2$ and $\bar{a}b = -\bar{c}d$. They imply $|a| = |d|$ and $|b| = |c|$ and a condition on the phases ($a = |a|e^{i\alpha}$ etc.): $-\alpha + \beta = -\gamma + \delta \pm \pi$. Since the parameters of

the Möbius map can be divided by a common factor, we divide them by $\sqrt{|a|^2 + |b|^2}$. The resulting matrix is (with a redefinition of the parameters):

$$U = e^{i\theta} \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}, \quad |a|^2 + |b|^2 = 1 \quad (3.11)$$

The matrices are unitary, $UU^\dagger = 1$, and form the Unitary Group $U(2)$. They preserve the norm of vectors in \mathbb{C}^2 .

The subgroup with $\det U = 1$ is the special unitary group $SU(2)$. It is characterized by three independent real parameters that identify a point of the spherical surface $|a|^2 + |b|^2 = 1$ in \mathbb{R}^4 .

Via the stereographic map, the Möbius map associated to a $SU(2)$ matrix induces a rotation of the Riemann sphere with center $(0, 0, 1/2)$. Matrices U and $-U$ correspond to the same Möbius map and hence to the same rotation.

- Rotation of the sphere around the Z axis:

$$\begin{bmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{bmatrix} \Rightarrow z' = e^{2i\alpha} z \Rightarrow \begin{cases} X' = X \cos(2\alpha) - Y \sin(2\alpha) \\ Y' = X \sin(2\alpha) + X \cos(2\alpha) \\ Z' = Z \end{cases}$$

- Rotation of the sphere around the X axis through $(0, 0, \frac{1}{2})$:

$$\begin{bmatrix} \cos \alpha & i \sin \alpha \\ i \sin \alpha & \cos \alpha \end{bmatrix} \Rightarrow z' = \frac{z \cos \alpha + i \sin \alpha}{iz \sin \alpha + \cos \alpha} \Rightarrow \begin{cases} X' = X \\ Y' = Y \cos(2\alpha) + (Z - \frac{1}{2}) \sin(2\alpha) \\ Z' - \frac{1}{2} = -Y \sin(2\alpha) + (Z - \frac{1}{2}) \cos(2\alpha) \end{cases}$$

- Rotation of the sphere around the Y axis through $(0, 0, \frac{1}{2})$:

$$\begin{bmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix} \Rightarrow z' = \frac{z \cos \alpha + \sin \alpha}{-z \sin \alpha + \cos \alpha} \Rightarrow \begin{cases} X' = X \cos(2\alpha) + (Z - \frac{1}{2}) \sin(2\alpha) \\ Y' = Y \\ Z' - \frac{1}{2} = -X \sin(2\alpha) + (Z - \frac{1}{2}) \cos(2\alpha) \end{cases}$$

Note the doubling of the angular parameter of the $SU(2)$ matrix while performing the rotation of the sphere.

More on $SU(2)$ matrices is in sect.22.4.1, where we introduce the mathematical description of the angular momentum. In particular, $SU(2)$ matrices are ‘rotation’ matrices acting on complex vectors in \mathbb{C}^2 (spinors), that describe the spin state of particles such as the electron, the proton.

Chapter 4

Sequences and Series

4.1 Topology

The modulus endows \mathbb{C} with the structure of normed space¹ and defines a distance between points, $d(z, z') = |z - z'|$. Therefore (\mathbb{C}, d) is also a metric space. At every point z_0 one may introduce a *basis of neighbourhoods*, which makes \mathbb{C} a topological space. The elements of the basis are the disks centred in z_0 with radii $r > 0$:

$$D(z_0, r) = \{z : |z - z_0| < r\}.$$

The following definitions and statements are important and used thoroughly:

- A set S in \mathbb{C} is *open* if for every point $z \in S$ there is a disk $D(z, r)$ wholly in S . The union of any collection of open sets is an open set; the intersection of two open sets is open.
- A point $z \in \mathbb{C}$ is an *accumulation point* of a set S if every disk $D(z, r)$ contains a point in S different from z .
- A *boundary point* of S is a point z such that every disk $D(z, r)$ contains points in S and points not in S . The boundary of S is the set ∂S of boundary points of S .
- A set is *closed* if it contains all its boundary points. The *closure* of a set S is the set $\bar{S} = S \cup \partial S$.
- A set S is disconnected if there are two disjoint *open* sets A and B such that $S \subseteq A \cup B$ but S is not a subset of A or B alone. A set is *connected* if it is not disconnected.

Recall that a set S is closed if and only if \mathbb{C}/S is open.

Definition 4.1.1. A **domain** is a set both open and connected.

¹ Normed, metric and topological spaces are general structures that will be defined later.

Proposition 4.1.2. Any two points in a domain can be joined by a continuous polygonal line in the domain (see Bak & Newman, *Complex Analysis*, Springer).

4.2 Sequences

Complex sequences are maps $\mathbb{N} \rightarrow \mathbb{C}$. They arise in analysis, approximation theory, iteration of maps. Infinite series and infinite products are limits of sequences of partial sums and partial products. General statements about sequences are now presented.

Definition 4.2.1. A sequence z_n converges to z ($z_n \rightarrow z$) if $|z_n - z| \rightarrow 0$ i.e.

$$\forall \epsilon \quad \exists N_\epsilon \quad \text{such that} \quad |z_n - z| < \epsilon, \quad \forall n > N_\epsilon. \quad (4.1)$$

Exercise 4.2.2. Show that:

- 1) if $z_n \rightarrow z$ and $w_n \rightarrow w$ then: $z_n + w_n \rightarrow z + w$, $z_n w_n \rightarrow zw$, $z_n/w_n \rightarrow z/w$ if $w_n \neq 0$ and $w \neq 0$.
- 2) z_n is convergent in \mathbb{C} if and only if $\text{Re } z_n$ and $\text{Im } z_n$ are convergent in \mathbb{R} .
- 3) if $z_n \rightarrow z$, then $\bar{z}_n \rightarrow \bar{z}$ and $|z_n| \rightarrow |z|$. Hint: use inequality (2.7).

Definition 4.2.3. A sequence z_n is a *Cauchy sequence* if

$$\forall \epsilon > 0 \quad \exists N_\epsilon \quad \text{such that:} \quad |z_n - z_m| < \epsilon, \quad \forall m, n > N_\epsilon. \quad (4.2)$$

All convergent sequences are Cauchy sequences, but the converse may not be true. When every Cauchy sequence is convergent to an element in the space, the space is *complete*. The Cauchy criterion is then extremely useful to predict convergence without the need to identify the limit.

Proposition 4.2.4. \mathbb{C} is complete

Proof. The inequalities (2.6) imply that $\{x_n + iy_n\}$ is a Cauchy sequence if and only if both $\{x_n\}$ and $\{y_n\}$ are Cauchy sequences. Since \mathbb{R} is complete, they both converge. Let x and y be their limits, then $|(x_n + iy_n) - (x + iy)| = |(x_n - x) + i(y_n - y)| \leq |x_n - x| + |y_n - y| \rightarrow 0$. \square

4.2.1 Quadratic maps*

The iteration of a map $z' = F(z)$, with a function $F: \mathbb{C} \rightarrow \mathbb{C}$ and initial value z_0 , generates a sequence: $z_{k+1} = F(z_k)$. The sequence depends on the initial value, and this dependence may be surprisingly interesting. The problem was studied by Pierre Fatou and Gaston Julia in the early 1900.

The simplest non-trivial function is the quadratic map $F(z) = z^2 + c$, $c \in \mathbb{C}$. It has two fixed points, $z^* = z^{*2} + c$. Near a fixed point $F(z) \approx z^* + 2z^*(z - z^*)$. According to $2|z^*|$ being

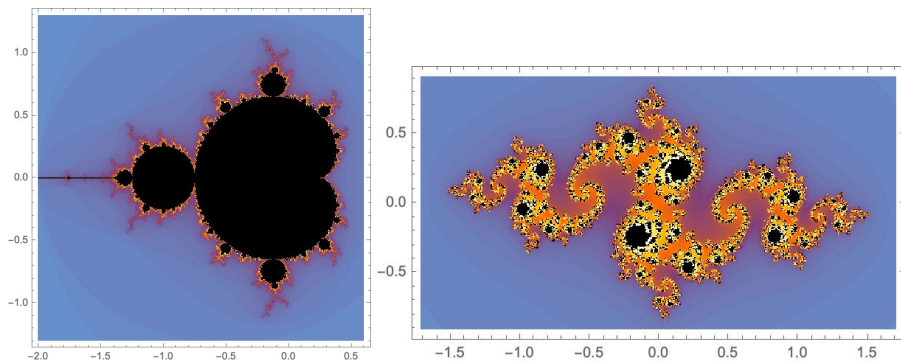


Figure 4.1 Left: The Mandelbrot set: it is the locus of parameters c such that the sequence $z_{n+1} = z_n^2 + c$, $z_0 = 0$ remains bounded. Right: the Filled Julia set for $c = -0.8 + i0.16$; any point in it generates a bounded sequence. Shapes change a lot as c moves from the interior to the boundary of the Mandelbrot set (pictures are built in functions of Mathematica 13)

greater, less or equal to one, the linearized map in z^* is expanding, contracting or indifferent, i.e. the distance $|F(z) - z^*|$ is greater, less or equal to the distance $|z - z^*|$. Period-2 points are the fixed points of $F^2(z) = (z^2 + c)^2 + c$ (the previous two period-1 points, and two new ones that map to each other), and so on.

The sequences that escape to ∞ define a set of initial points $A_c(\infty)$ called the *attraction basin* of ∞ . Of course, if $z \in A_c(\infty)$ also $F(z)$ and the whole sequence belong to it. It was proven that it is an open and connected set.

The complementary set K_c is the *filled Julia set*. It contains the initial points of bounded sequences and it is a closed and bounded (i.e. compact) set. The boundary is the *Julia set* J_c .

The three sets are left invariant by the action of the map.² Fatou and Julia proved the theorem: *If the sequence $0, c, F(c), F(F(c)), \dots$ diverges to ∞ , i.e. $0 \in A_c(\infty)$, then J_c is totally disconnected, whereas if $0 \in K_c$, then J_c is connected.*

While at IBM, in 1980, Benoit Mandelbrot (1924-2010) studied with the aid of a computer the properties of invariant Julia sets of the quadratic map and more complex ones, and disclosed the beauty of their fractal structures³. The *Mandelbrot set* (1980) is the set of parameters $c \in \mathbb{C}$ such that J_c is connected. Again, it is a wonderful fractal⁴.

² For $c = 0$ the sets are easily identified. Clearly $A_0(\infty)$ is the set $|z| > 1$, K_0 is the set $|z| \leq 1$ (the filled Julia set) and J_0 (the Julia set) is the unit circle $|z| = 1$. The action of $z \rightarrow z^2$ on the points $e^{i2\pi\theta} \in J_0$ ($\theta \in [0, 1]$), is the map $\theta_{n+1} = 2\theta_n \pmod{1}$. A point θ_0 after k iterations of the map is again θ_0 if $(2^k - 1)\theta_0$ is an integer. Then the initial point θ_0 generates a periodic sequence (*periodic orbit* of the map) of period k . Only rational angles give rise to periodic orbits. The irrational ones spread on the unit circle and the map is chaotic.

³ See the book by L. Carleson and Th.W. Gamelin, *Complex dynamics* (Springer UniversiText 1995), and Wikipedia for wonderful pictures.

⁴ The boundary is the “Mandelbrot lemniscate”. It is the limit of a sequence of level curves (lemniscates) $M_n = \{z \in \mathbb{C} : |p_n(z)| = 2\}$, where $p_n(z)$ is the sequence of polynomials: $p_1(z) = z$, $p_{n+1}(z) = p_n(z)^2 + z$.

Exercise 4.2.5. Consider the linear map $z_{n+1} = az_n + b$. Write the general expression of z_n in terms of z_0 . When is the sequence bounded?

Exercise 4.2.6. Study the fixed points z^* of the exponential map $z' = e^z$. The map is chaotic⁵.

4.3 Series

Infinite sums were studied long before sequences. The oldest known ones were obtained by Madhava (1350, 1425), the founder of the Kerala school of astronomy and mathematics. He developed series for trigonometric functions, including an error term. The one for arctan enabled him to evaluate π up to 11 digits. His work may have influenced European mathematics through transmission by the Jesuits. The same series were rediscovered by Gregory two centuries later.

Oresme in XIV century, Jakob & Johann Bernoulli (*Tractatus de seriebus infinitis*, 1689), and Pietro Mengoli (1625, 1686), discovered and rediscovered the divergence of the *Harmonic series* $1 + \frac{1}{2} + \frac{1}{3} + \dots$. In the *Tractatus*, the convergence of $\sum_k 1/k^2$ was also proven, but the sum (the Basel problem) was evaluated later (1734) by Johann's prodigious student Leonhard Euler. Euler also proved that the sum of the reciprocals of prime numbers is divergent⁶.

Christian Huygens asked his student Leibnitz to evaluate the sum of reciprocals of triangular numbers⁷. The result (the sum is 2) was obtained after noting that $\frac{2}{k(k+1)} = \frac{2}{k} - \frac{2}{k+1}$ (the sum is a *telescopic series*).

Series gained rigour after Cauchy, who defined convergence in terms of the sequence of partial sums.

Given a sequence of complex numbers a_k one constructs the partial sums $A_n = \sum_{k=0}^n a_k$. If the sequence A_n converges to a finite limit A , the limit is the *sum of the series*

$$A = \sum_{k=0}^{\infty} a_k.$$

If $\sum_k^{\infty} a_k$ and $\sum_k^{\infty} b_k$ both converge with finite limits A and B , then the series $\sum_k^{\infty} (a_k \pm b_k)$ is convergent and the sum is $A \pm B$.

⁵ <https://doi.org/10.48550/arXiv.1408.1129>

⁶ For nice accounts see P. Pollack, *Euler and the partial sums of the prime harmonic series*, <http://pollack.uga.edu/eulerprime.pdf>; M. Villarino, *Mertens Proof of Mertens Theorem*, arXiv:math/0504289.

⁷ The triangular numbers are $n_1 = 1$, $n_{k+1} = 1 + 2 + \dots + k = \frac{(k+1)k}{2}$.

Completeness of \mathbb{C} implies that the necessary and sufficient condition for a series to converge is that the sequence of partial sums is a Cauchy sequence:

$$\forall \epsilon > 0 \quad \exists N_\epsilon \quad \text{such that} \quad \forall m > N_\epsilon \text{ and } \forall n > 0: \quad \left| \sum_{k=m+1}^{m+n} a_k \right| < \epsilon. \quad (4.3)$$

- For $n = 1$ it is $|a_{m+1}| < \epsilon$. A necessary condition for convergence is $|a_k| \rightarrow 0$.
- The inequality $|\sum_{m+1}^{m+n} a_k| \leq \sum_{m+1}^{m+n} |a_k|$ implies

$$\sum_{k=1}^{\infty} |a_k| \text{ converges} \implies \sum_{k=1}^{\infty} a_k \text{ converges}$$

4.3.1 Absolute convergence

Definition 4.3.1. $\sum_k a_k$ is *absolutely convergent* if $\sum_k |a_k|$ is convergent.

Absolute convergence is a sufficient criterion for convergence; moreover it deals with series in \mathbb{R} . We state but not prove the important property:

Proposition 4.3.2. *The sum of an absolutely convergent series does not change if the terms of the series are permuted*⁸: $\sum_k a_k = \sum_k a_{\pi(k)}$.

Definition 4.3.3. Given an infinite set $A \subset \mathbb{R}$ bounded above, $\limsup A$ (or $\overline{\lim} A$) is the *largest* real number \bar{a} such that $\forall \epsilon$ the set $\{a \in A : a > \bar{a} + \epsilon\}$ is finite and $\{a \in A : a > \bar{a} - \epsilon\}$ is infinite.

For a sequence:

$$\overline{\lim} |a_k| = \lim_{n \rightarrow \infty} \sup_{k \geq n} |a_k|$$

These are sufficient conditions for absolute convergence of the series $\sum_k a_k$. They must hold for k greater than some finite N :

- **Comparison** (Gauss): $|a_k| < b_k$, where $\sum_k b_k < \infty$
- **Ratio** (d'Alembert): for $a_k \neq 0$ $\limsup_k \frac{|a_{k+1}|}{|a_k|} < 1$
- **Root** (Cauchy-Hadamard): $\limsup_k \sqrt[k]{|a_k|} < 1$

If the sequences $|a_k|^{1/k}$ and $\frac{|a_{k+1}|}{|a_k|}$ converge to finite limits, the limits are equal. The limit coincides with \limsup (Cesaro).

⁸ A convergent series that is not absolutely convergent is *conditionally convergent*. The series $\sum_{k=1}^{\infty} i^k/k$ is convergent as it is the sum of two convergent series $\sum_{k \geq 1} (-1)^k/(2k) + i \sum_{k \geq 0} (-1)^k/(2k+1)$, and is conditionally convergent. Riemann proved the surprising result that by rearranging terms of a conditionally convergent real series one can obtain any limit sum in \mathbb{R} .

Example 4.3.4. *The Jacobi Theta function*

$$\theta_3(z, q) = 1 + 2 \sum_{m=1}^{\infty} q^{m^2} \cos(2mz), \quad |q| < 1$$

is convergent for all z .

The series $1 + 2 \sum_{m=1}^{\infty} q^{m^2} e^{i2mz}$ is absolutely convergent for all $z = x + iy$:

$$\lim_m \sqrt[m]{|q|^{m^2} e^{-2my}} = e^{-2y} \lim_{m \rightarrow \infty} |q|^m = 0$$

As such, the series with $\cos(2mz)$ and $\sin(2mz)$ converge.

Check that: $\theta_3(z + \pi, q) = \theta_3(z, q)$ and $\theta_3(z + \tau, q) = \frac{1}{q} e^{-2iz} \theta_3(z, q)$, ($q = e^{i\pi\tau}$).

The series occurs in physics in the study of the heat equation, vortex lattices.

Lemma 4.3.5 (Abel). *Let a series be such that for all n the partial sums are bounded by the same finite M : $|\sum_{k=0}^n a_k| < M$. Then, if $b_0 \geq b_1 \geq \dots \geq b_k \rightarrow 0$ the series $\sum_{k=0}^{\infty} a_k b_k$ converges.*

4.3.2 Cauchy product of series

The Cauchy product of two series is so defined:

$$\left[\sum_{k=0}^{\infty} a_k \right] \left[\sum_{r=0}^{\infty} b_r \right] = \sum_{k=0}^{\infty} \left(\sum_{r=0}^k a_r b_{k-r} \right) \quad (4.4)$$

The definition is natural for power series, as it expresses the product of polynomials as a polynomial: $[\sum_{k=0}^{\infty} a_k z^k] [\sum_{r=0}^{\infty} b_r z^r] = \sum_{k=0}^{\infty} z^k (\sum_{r=0}^k a_r b_{k-r})$.

Proposition 4.3.6 (Franz Mertens, 1874⁹). *If a series is absolutely convergent to A and another is convergent to B , their Cauchy product is convergent to AB .*

Proposition 4.3.7. *If a series is absolutely convergent to A and another is absolutely convergent to B , their Cauchy product absolutely converges to AB .*

Proof.

$$\begin{aligned} \sum_{k=0}^n |c_k| &= \sum_{k=0}^n \left| \sum_{r=0}^k a_r b_{k-r} \right| \leq \sum_{k=0}^n \sum_{r=0}^k |a_r| |b_{k-r}| \\ &= \sum_{r=0}^n |a_r| \sum_{k=r}^n |b_{k-r}| = \sum_{r=0}^n |a_r| \sum_{k=0}^{n-r} |b_k| \leq \sum_{k=0}^{\infty} |a_k| \sum_{l=0}^{\infty} |b_l| \end{aligned}$$

⁹ see Boas, <http://www.math.tamu.edu/~boas/courses/617-2006c/sept14.pdf>

Since the sequence $\sum_{k=0}^n |c_k|$ is increasing and bounded above, it is convergent. Then $C_n = \sum_{k=0}^n c_k$ is absolutely convergent to a limit C . The limit does not depend on rearrangements of terms and is the sum of all possible products $a_r b_s$. It is $C = \lim_k (A_k B_k) = (\lim_k A_k)(\lim_k B_k) = AB$. \square

4.3.3 The geometric series

The partial sum $S_n = 1 + z + \dots + z^n$ is evaluated with the identities $S_{n+1} = S_n + z^{n+1}$ and $S_{n+1} = 1 + zS_n$:

$$\sum_{k=0}^n z^k = \frac{1 - z^{n+1}}{1 - z}, \quad z \neq 1 \quad (4.5)$$

If $|z| < 1$, it is $\lim_{n \rightarrow \infty} z^n = 0$ and $S_n(z)$ converges to the simple but fundamental geometric series

$$\sum_{n=0}^{\infty} z^n = \frac{1}{1 - z}, \quad |z| < 1 \quad (4.6)$$

The convergence is absolute in $|z| < 1$. The geometric series is useful for assessing convergence of series by the comparison test.

Exercise 4.3.8. Evaluate the sums: $1 + 2 \cos x + \dots + 2 \cos nx$ and $\sin x + \sin 2x + \dots + \sin nx$.

Exercise 4.3.9. For $a > 0$, b real, obtain the sums:

$$\sum_{k=0}^{\infty} e^{-ka} \cos kb = \frac{1}{2} + \frac{\sinh a}{2 \cosh a - 2 \cos b}, \quad \sum_{k=0}^{\infty} e^{-ka} \sin kb = \frac{\sin b}{2 \cosh a - 2 \cos b}$$

(Hint: evaluate $\sum_k e^{-k(a+ib)}$ and separate Im and Re parts).

Exercise 4.3.10. Write $(1 - z^2)^{-1}$ as a geometric series in z^2 and as the Cauchy product of two geometric series.

4.3.4 The exponential series

The sequence of partial sums $e_n(z) = 1 + z + \dots + \frac{1}{n!} z^n$ is absolutely convergent for any z . The limit is the complex exponential function:

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!}, \quad z \in \mathbb{C} \quad (4.7)$$

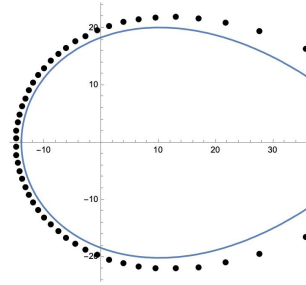


Figure 4.2 Although e^z has no zeros, its polynomial truncations $e_n(z)$ have n complex zeros. For large n they fly to infinity. Szegö (1924) proved that for $n \rightarrow \infty$ the zeros of $e_n(z)$ divided by n distribute on the curve $|ze^{1-z}| = 1$ with $|z| \leq 1$. The figure shows the zeros of e_{50} and the limit curve (rescaled).

Exercise 4.3.11. Prove that the Cauchy product of two exponential series is the exponential series $e^{z+z'} = e^z e^{z'}$. Then show that $e^{x+iy} = e^x (\cos y + i \sin y)$, in accordance with (4.7).

Exercise 4.3.12 (Madhava math. competition 2013). Show that $e_n(z)$ has no real roots if n is even, and exactly one if n is odd¹⁰.

4.3.5 Riemann's Zeta function

The following series is of greatest importance in number theory¹¹, and is often encountered in physics:

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}, \quad \operatorname{Re} z > 1 \quad (4.8)$$

Since $|n^z| = |e^{z \log n}| = n^{\operatorname{Re} z}$, the series converges absolutely for $\operatorname{Re} z > 1$.

The values of the Riemann series are known at even integers (Euler). They result, for example, from the evaluation of certain Fourier series (see example 20.1.3). Two useful values are

$$\zeta(2) = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}, \quad \zeta(4) = \sum_{k=1}^{\infty} \frac{1}{k^4} = \frac{\pi^4}{90}$$

¹⁰ see <http://www.madhavacompetition.com>, for texts and solutions. The contest is addressed to undergraduate students

¹¹ H. M. Edwards, *Riemann's Zeta Function*, Dover.

Exercise 4.3.13. Prove in the order:

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^z} = (1-2^{-z})\zeta(z), \quad \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)^z} = (1-2^{1-z})\zeta(z) \quad (4.9)$$

(since Riemann's series is absolutely convergent, the sum on even and odd n may be evaluated separately).

By collecting in the first series the terms $2n+1$ that are multiples of 3, obtain the sum on integers that are not divided by 2 and 3:

$$\sum_{n \neq 2k, 3k} \frac{1}{n^z} = \left(1 - \frac{1}{2^z}\right) \left(1 - \frac{1}{3^z}\right) \zeta(z)$$

Iteration gives the famous representation of Riemann's Zeta function as an infinite product on prime numbers:

$$\boxed{\frac{1}{\zeta(z)} = \prod_{p>1} \left(1 - \frac{1}{p^z}\right)} \quad (4.10)$$

Exercise 4.3.14. Show that¹²

$$\int_0^1 dx \int_0^1 dy \int_0^1 dz \frac{1}{1-xyz} = \zeta(3)$$

(Hint: expand the fraction in geometric series)

¹² This type of integral representation was used to prove irrationality of $\zeta(2)$ and $\zeta(3)$ in a way simpler than Apéry's proof of 1977 (see <https://doi.org/10.48550/arXiv.1308.2720>).

Chapter 5

Complex Functions

5.1 Differentiability and Cauchy-Riemann conditions

A complex function is a map from some set to \mathbb{C} . We focus on complex functions of a complex variable, $f : D \subseteq \mathbb{C} \rightarrow \mathbb{C}$ where the **domain** D , if not specified differently, is an *open connected* set in \mathbb{C} .

To stress that the function only depends on $z = x + iy$, and not also on \bar{z} (i.e. not freely on x and y), we sometimes denote it as $f(z)$.

Note that the real and imaginary parts of $f(z)$ are not themselves functions of the combination $x + iy$. For example: $z^2 = (x^2 - y^2) + i2xy$, $e^z = e^x \cos y + i e^x \sin y$. We then write:

$$f(z) = u(x, y) + i v(x, y)$$

Definition 5.1.1. A complex function $f(z)$ is continuous in z_0 if:

$$\forall \epsilon > 0 \quad \exists \delta > 0 \quad \text{such that} \quad |f(z) - f(z_0)| < \epsilon \quad \forall z \text{ in } |z - z_0| < \delta. \quad (5.1)$$

Proposition 5.1.2. $f(z)$ is continuous in $z_0 = x_0 + iy_0$ iff $u(x, y)$ and $v(x, y)$ are both continuous in (x_0, y_0) .

Proof. The inequality $|f(z) - f_0| \geq |u(x, y) - u_0|$ (and similar for v) implies continuity of u (and v) from continuity of f . The other way is proven by means of $|f(z) - f_0| \leq |u(x, y) - u_0| + |v(x, y) - v_0|$. (u_0 is short for $u(x_0, y_0)$ etc.) \square

Definition 5.1.3. $f(z)$ is *differentiable* in $z_0 \in D$ if the following limit exists

$$\boxed{f'(z_0) = \lim_{z \rightarrow z_0} \frac{f(z) - f(z_0)}{z - z_0}} \quad (5.2)$$

i.e. there is a number $f'(z_0)$ such that: $\forall \epsilon > 0$ there is a δ_ϵ such that

$$\left| \frac{f(z) - f(z_0)}{z - z_0} - f'(z_0) \right| < \epsilon \quad \forall z: |z - z_0| < \delta_\epsilon.$$

Then, in a neighbourhood of z_0 it is $f(z) = f(z_0) + f'(z_0)(z - z_0) + r(z, z_0)(z - z_0)$, where $r(z, z_0)$ vanishes as $z \rightarrow z_0$.

It is clear that differentiability of f at z_0 implies continuity at z_0 .

Example 5.1.4. $|z|^2$ is not differentiable in $z_0 \neq 0$. Let $h = |h|e^{i\theta}$ and evaluate

$$\frac{|z_0 + h|^2 - |z_0|^2}{h} = \frac{|h|^2 + \bar{z}_0 h + z_0 \bar{h}}{h} = |h|e^{-i\theta} + \bar{z}_0 + z_0 e^{-2i\theta}$$

The limit $h \rightarrow 0$ does not exist because it is non-unique: it depends on the angle θ . This does not occur for the function z^2 (it is everywhere differentiable):

$$\frac{(z_0 + h)^2 - z_0^2}{h} = \frac{h^2 + 2z_0 h}{h} = h + 2z_0$$

The existence of the limit (5.2) is more demanding than in real analysis of one variable, as z may approach z_0 from any direction. It implies a strong constraint on the real and imaginary parts of f .

Theorem 5.1.5 (Cauchy-Riemann conditions). *If $f(z) = u(x, y) + i v(x, y)$ is differentiable in z_0 , then the partial derivatives of u and v exist in (x_0, y_0) and the Cauchy-Riemann conditions hold in (x_0, y_0) :*

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \quad , \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}} \quad (5.3)$$

Proof. The incremental ratio is evaluated with $z = z_0 + h$ and $z = z_0 + ih$ respectively (h real). By hypothesis the limits $h \rightarrow 0$ exist and coincide:

$$\begin{aligned} \frac{u(x_0 + h, y_0) - u(x_0, y_0)}{h} + i \frac{v(x_0 + h, y_0) - v(x_0, y_0)}{h} &\rightarrow f'(z_0) \\ \frac{u(x_0, y_0 + h) - u(x_0, y_0)}{ih} + i \frac{v(x_0, y_0 + h) - v(x_0, y_0)}{ih} &\rightarrow f'(z_0) \end{aligned}$$

Therefore, the real and imaginary parts exist separately as partial derivatives, and yield identities useful for the evaluation of f' :

$$\operatorname{Re} f'(z_0) = \frac{\partial u}{\partial x} \Big|_{(x_0, y_0)} = \frac{\partial v}{\partial y} \Big|_{(x_0, y_0)} \quad \operatorname{Im} f'(z_0) = -\frac{\partial u}{\partial y} \Big|_{(x_0, y_0)} = \frac{\partial v}{\partial x} \Big|_{(x_0, y_0)}$$

□

Besides the Cauchy-Riemann conditions, we obtained the useful rules

$$f'(z) = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} = \frac{\partial u}{\partial x} - i \frac{\partial u}{\partial y} \quad (5.4)$$

The converse of the theorem requires further conditions on u and v :

Proposition 5.1.6. *If u and v have continuous partial derivatives in x and y in a disk centred in z_0 and if the Cauchy-Riemann conditions hold in z_0 , then $f(z)$ is differentiable in z_0 .*

Proof. By means of Taylor's expansion, and Cauchy-Riemann conditions at z_0 :

$$\begin{aligned} f(z_0 + h) - f(z_0) &= u(x_0 + h_x, y_0 + h_y) - u(x_0, y_0) + i v(x_0 + h_x, y_0 + h_y) - i v(x_0, y_0) \\ &= (\partial_x u + i \partial_x v)_0 h_x + o(h_x) + (\partial_y u + i \partial_y v)_0 h_y + o(h_y) \\ &= (\partial_x u + i \partial_x v)_0 (h_x + i h_y) + o(h_x) + o(h_y) \end{aligned}$$

Divide by h . The limit $h \rightarrow 0$ exists and is $f'(z_0) = (\partial_x u + i \partial_x v)(z_0)$. □

The standard rules of derivation for functions of a real variable continue to hold for differentiable functions of a complex variable (on suitable domains):

$$\begin{aligned} (\lambda f + g)' &= \lambda f' + g' && \text{(linearity)} \\ (fg)' &= f'g + fg' && \text{(Leibnitz property)} \\ (1/f)' &= -f' / f^2 && (f \neq 0) \\ f(g(z))' &= f'(g(z)) g'(z) && \text{(composite function)} \end{aligned}$$

Definition 5.1.7. A function $f(z)$ which is differentiable at all points of a domain D is **holomorphic** on D . A function holomorphic on \mathbb{C} is **entire**.

Example 5.1.8. *The function $z \rightarrow z^n$, $n \in \mathbb{Z}$, is differentiable:*

$$\frac{d}{dz} z^n = n z^{n-1}.$$

For $n \geq 0$ it is entire, while for $n < 0$ it is holomorphic on $\mathbb{C}/\{0\}$.

Example 5.1.9. The exponential function $e^z = e^x \cos y + ie^x \sin y$ has real and imaginary parts that are differentiable in x and y and solve the Cauchy-Riemann conditions. Then it is differentiable in z , with derivative (5.4)

$$\frac{d}{dz} e^z = \frac{\partial}{\partial x} e^{x+iy} = e^z$$

Since this holds at all points in \mathbb{C} , the exponential function is entire.

Also $\sin z$, $\cos z$, $\sinh z$ and $\cosh z$ are entire functions and $\frac{d}{dz} \sin z = \cos z$, $\frac{d}{dz} \cos z = -\sin z$, $\frac{d}{dz} \sinh z = \cosh z$ etc.

A direct check is $f(z) = \sin z = \sin x \cosh y + i \cos x \sinh y$. The functions $u(x, y) = \sin x \cosh y$ and $v(x, y) = \cos x \sinh y$ solve the C.R. equations, and $f'(z) = \partial_x u + i \partial_x v = \cos z$.

Example 5.1.10. $f(z) = \text{Log } z$ with domain $\mathbb{C}/(-\infty, 0]$. The real part is $u(x, y) = \frac{1}{2} \log(x^2 + y^2)$ and, with the single-valued $-\frac{\pi}{2} \leq \text{Arctan} \leq \frac{\pi}{2}$, the imaginary part is:

$$v(x, y) = 2 \text{Arctan} \frac{y}{\sqrt{x^2 + y^2} + x}$$

u and v are differentiable and solve the C.R. equations. Using (5.4):

$$\frac{d}{dz} \text{Log } z = \frac{\partial u}{\partial x} - i \frac{\partial u}{\partial y} = \frac{x}{x^2 + y^2} - i \frac{y}{x^2 + y^2} = \frac{\bar{z}}{|z|^2} = \frac{1}{z}.$$

Exercise 5.1.11. Prove that if f is holomorphic on D and $f'(z) = 0$ everywhere on D , then f is constant on D .

Remark 5.1.12. z and \bar{z} can be viewed as independent variables inasmuch as x and y . A function $f(x, y)$ can be written as a function of the independent variables $z = x + iy$ and $\bar{z} = x - iy$, with partial derivatives

$$\frac{\partial}{\partial z} = \frac{\partial x}{\partial z} \frac{\partial}{\partial x} + \frac{\partial y}{\partial z} \frac{\partial}{\partial y} = \frac{1}{2} \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \quad (5.5)$$

$$\frac{\partial}{\partial \bar{z}} = \frac{\partial x}{\partial \bar{z}} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \bar{z}} \frac{\partial}{\partial y} = \frac{1}{2} \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \quad (5.6)$$

$$4 \frac{\partial^2}{\partial z \partial \bar{z}} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \quad (5.7)$$



Figure 5.1 Augustin Luis Cauchy (Paris 1789, Sceaux 1857). Despite a complicated life during the political turmoil that followed the Revolution, he has been one of the most productive mathematicians of all ages, with works in analysis and at the foundation of continuum mechanics. He introduced mathematical rigour and discovered the fundamental integral representation of holomorphic functions (the Cauchy integral formula).

Karl Weierstrass (Ostenfelde 1815, Berlin 1897) was professor in Berlin. His fame as a lecturer attracted several students: Cantor, Frobenius, Fuchs, Grassmann, Killing, Mertens, Kovalevskaya, Runge, Schur, H. A. Schwarz. He studied analytic functions as power series. He did not bother much about priorities, and published many results late in his career (a detailed biography is <https://arxiv.org/pdf/1508.02928>)

Bernhard Riemann (Breselenz (Hannover) 1826, Verbania 1866). The young Riemann was oriented to become a pastor, and to study theology at Göttingen. Gauss encouraged him to study mathematics. In 1854 he completed his thesis *Über die Hypothesen welche der Geometrie zu Grunde liegen* (On the hypothesis which underlie geometry) which contains his ideas on Riemannian geometry, that generalize Gauss' results about surfaces. He succeeded to Dirichlet in the direction of the department, but died young of tuberculosis during a journey to lake Maggiore. He studied holomorphic functions as maps, and developed the theory of multi-sheet manifolds (Riemann surfaces) to investigate multi-valued functions.

The condition that a function only depends on z yields the C.R. conditions:

$$0 = \frac{\partial f}{\partial \bar{z}} = \frac{1}{2}(\partial_x + i\partial_y)(u + iv) = \frac{1}{2}(\partial_x u - \partial_y v) + \frac{i}{2}(\partial_y u + \partial_x v).$$

Exercise 5.1.13. Show that the Cauchy-Riemann conditions for $f = u + iv$ in polar coordinates are

$$\frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial v}{\partial \theta}, \quad \frac{\partial v}{\partial r} = -\frac{1}{r} \frac{\partial u}{\partial \theta}$$

5.2 Conformal maps

What makes holomorphic functions very special is that they depend upon a *single* variable z that spans a two-dimensional real space.

To visualize $f = u + iv$ one may plot the real functions $\operatorname{Re} f = u(x, y)$ and $\operatorname{Im} f = v(x, y)$ in \mathbb{R}^3 . However, it is far more interesting to view f as a *map* $w = f(z)$ from points (x, y) of a domain D to points (u, v) of the $w = u + iv$ plane (we already studied the linear map, the inversion and the Möbius map).

In this picture, the derivative f' of a function gains a simple geometric meaning.

The following theorem shows that a holomorphic map *locally* performs a *dilation* by a factor $|f'(z)|$ and an anticlockwise *rotation* of angle $\arg f'(z)$.

Theorem 5.2.1. *A holomorphic map with $f' \neq 0$ preserves angles (it is a conformal map)*

Proof. Consider a differentiable function $\gamma : t \in [a, b] \rightarrow \mathbb{C}$, where $[a, b]$ is an interval of the real line. The range $\{\gamma(t), t \in [a, b]\}$ is a curve in the complex plane. The cartesian components of the tangent vector are the real and imaginary parts of $\dot{\gamma}(t)$, we thus identify $\dot{\gamma}(t)$ as the tangent vector. We require $\dot{\gamma}(t) \neq 0$ for all t . Let $z_0 = \gamma(t_0)$, with tangent vector $\dot{\gamma}(t_0)$.

A holomorphic map $w = f(z)$ takes γ to the curve $f(\gamma)$, with tangent vector $f'(z_0)\dot{\gamma}(t_0)$ at $w_0 = f(z_0)$. The direction $\theta = \arg \dot{\gamma}(t_0)$ of the tangent vector at z_0 is rotated to the direction $\theta' = \theta + \arg f'(z_0)$ at w_0 , and the length of the tangent vector is scaled by the factor $|f'(z_0)|$.

Let two curves intersect in z_0 with tangents forming an angle α (see Fig.5.2). Since the images of the tangent vectors in w_0 are both rotated by the angle $\arg f'(z_0)$, the images of the curves continue to intersect in w_0 with the angle α . \square

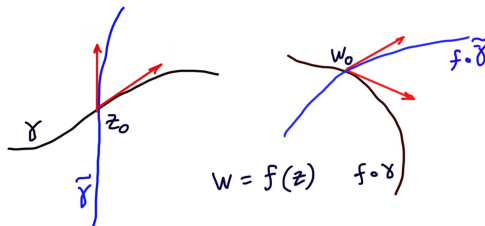


Figure 5.2 *The curves γ and $\tilde{\gamma}$ in z -plane are mapped to the w plane by a holomorphic function f . The tangents in z_0 form an angle that is equal to the angle formed by the tangents in $w_0 = f(z_0)$.*

In the study of holomorphic maps it is often useful to evaluate how a grid of orthogonal lines in some domain is mapped to, or back from, another grid of orthogonal lines. The straight lines $u = U$ and $v = V$ in w -plane are orthogonal and are the images of the curves $u(x, y) = U$ and $v(x, y) = V$ in the z plane. The vectors $\operatorname{grad} u = (\partial_x u, \partial_y u)$ and

$\text{grad } v = (\partial_x v, \partial_y v)$ are respectively orthogonal to the level lines $u(x, y) = U$ and $v(x, y) = V$ and point towards increasing values of u and v . At a point of intersection of the curves in z plane, the vectors are orthogonal by the Cauchy-Riemann conditions:

$$\text{grad } u \cdot \text{grad } v = \partial_x u \partial_x v + \partial_y u \partial_y v = 0 \quad (5.8)$$

The same is true for the tangent vectors: the two vectors tangent to the curves at a point are orthogonal¹.

The map $w = f(z)$ of a domain where f is holomorphic, univalent (one-to-one), with $f'(z) \neq 0$, represents a local change of variables from (x, y) to (u, v) . One evaluates:

$$\partial_u^2 + \partial_v^2 = \frac{1}{|f'(z)|^2} (\partial_x^2 + \partial_y^2) \quad (5.9)$$

$$du^2 + dv^2 = |f'(z)|^2 (dx^2 + dy^2) \quad (5.10)$$

$$du \wedge dv = |f'(z)|^2 dx dy \quad (5.11)$$

Let us analyse some examples of maps. By restricting the domain, a map can be made one-to-one.

Example 5.2.2. *The quadratic map $w = z^2$*

$$u(x, y) = x^2 - y^2 \quad v(x, y) = 2xy$$

Since $\arg w = 2 \arg z$, the set $-\frac{\pi}{2} < \text{Arg } z \leq \frac{\pi}{2}$ is mapped onto the whole w -plane. The whole z -plane covers the w -plane twice, a point w being the image of two points $\pm z$.

The derivative of the map is $2z$. An infinitesimal square of area $dx dy$ centred in z is mapped to an infinitesimal "square" centred in $w = z^2$ with area $dudv = 4|z|^2 dx dy$, rotated by the angle $\arg(2z)$.

The lines $u = U$ and $v = V$ in w -plane are the images of a grid of hyperbolas

$$x^2 - y^2 = U, \quad xy = \frac{V}{2}$$

¹ The tangent and the normal vectors at a point of a curve are orthogonal. The vector $\mathbf{t} = (t_x, t_y)$ tangent to a curve $f(x, y) = c$ points in a direction of null variation of $f(x, y)$. This means that the directional derivative vanishes: $0 = \mathbf{t} \cdot \nabla f$. If vectors are represented as complex numbers, orthogonality is expressed by a $\pm\pi/2$ rotation: $t_x + it_y \propto i(\partial_x f + i\partial_y f)$.

that intersect orthogonally. The lines $x = X$ or $y = Y$ are confocal parabolas in w -plane with focus in $w = 0$, which intersect orthogonally (see Fig.5.3):

$$u = -\frac{1}{4X^2}v^2 + X^2, \quad u = \frac{1}{4Y^2}v^2 - Y^2.$$

Note that in the origin the angles are not conserved (actually they are doubled by the map): this is possible since the derivative is zero in $z = 0$.

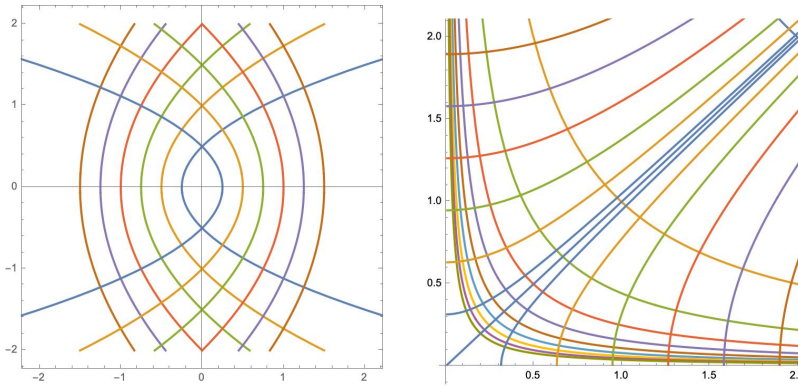


Figure 5.3 The quadratic map $w = z^2$. Left: the confocal parabolas in w -plane are the images of the coordinate square grid $x - y$ in z -plane. Right: the hyperbolas in w -plane are the pre-images of the coordinate square grid $u - v$ in w -plane (only a quadrant is shown).

Example 5.2.3. The exponential map $w = e^z$

$$u(x, y) = e^x \cos y \quad v(x, y) = e^x \sin y$$

A point w that is image of z is also image of $z + 2\pi i k$. A choice of domain for univalence is the strip $-\pi < \text{Im}z \leq \pi$. Now \exp is one-to-one from the strip to the w -plane \mathbb{C} with $w = 0$ removed. The circles $u^2 + v^2 = r^2$ are images of $x = \log r$ and the radial lines $\text{Arg } w = \theta$ emanating from $w = 0$ are images of horizontal lines $y = \theta$.

Example 5.2.4. The Joukowski map² $w = \frac{1}{2}(z + \frac{1}{z})$

$z = \pm 1$ are fixed points, and $z = \pm i$ are mapped to $w = 0$. The map is not one-to-one: z and $1/z$ have the same image. The pre-images of a point w solve the equation $z^2 - 2wz + 1 = 0$ and their product is one. Therefore the Joukowski map is invertible on a domain that does

² The Russian mathematician, airplane designer, professor of mechanics Nikolay Y. Joukowski (1847, 1921) used complex maps to study aerodynamics and flows. In 1918 he founded The Central Aero-Hydrodynamical Institute, which played a major role in the development of the aero-cosmic industry of the Soviet Union.

not contain both z and $1/z$.

$$\text{If } z = e^{\xi+i\theta} \text{ it is: } u = \cosh \xi \cos \theta \quad v = \sinh \xi \sin \theta$$

The circles $|z| = e^\xi$ and the radial lines $\text{Arg } z = \theta$ are mapped respectively to confocal ellipses and hyperbolas with foci in ± 1

$$\frac{u^2}{\cosh^2 \xi} + \frac{v^2}{\sinh^2 \xi} = 1, \quad \frac{u^2}{\cos^2 \theta} - \frac{v^2}{\sin^2 \theta} = 1 \quad (5.12)$$

that cross at right angles. The angular directions of the asymptotes of the hyperbola are $\pm\theta$.

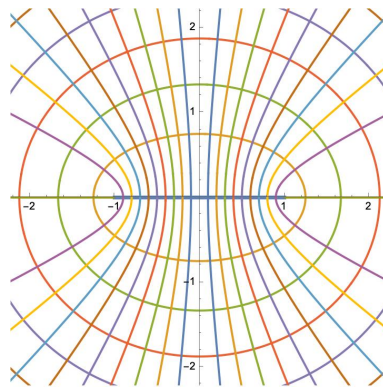


Figure 5.4 The Joukowski map $w = \frac{1}{2}(z + 1/z)$ maps the unit circle to $[-1, 1]$ (degenerate ellipse), $|z| > 1$ to $\mathbb{C} \setminus [-1, 1]$, circles to ellipses, radial lines to hyperbolas. The lines are confocal and intersect at right angles.

- $|z| > 1$ is mapped to $\mathbb{C} \setminus [-1, 1]$
- The wedge $\pi/2 - \theta < \text{Arg } z < \pi/2 + \theta$ is mapped to the region between the branches of the hyperbola with parameter θ .
- $\text{Im } z > 0$ is mapped to $\mathbb{C} \setminus (-\infty, -1] \cup [1, \infty)$. The boundary $\text{Im } z = 0$ is mapped to the cuts in w -plane as follows: $(0, 1]$ and $[1, \infty)$ are both mapped to the cut $[1, \infty)$, $(-\infty, -1]$ and $[-1, 0)$ are both mapped to $(-\infty, -1]$ (they contain x and $1/x$).

Conformal maps have important applications in physics and engineering (see chapter on electrostatics). They are a powerful tool to solve differential equations in two real variables in domains with complicated boundaries, by mapping them to domains with simpler boundaries. The cornerstone is the following theorem, of remarkable generality:

Theorem 5.2.5 (Riemann mapping theorem). Every simply connected domain in \mathbb{C} (but not \mathbb{C}) can be mapped bi-holomorphically onto the unit disk (or the half plane).

An important class of conformal transformations are the Schwarz-Christoffel maps, from polygons to the half-plane³. For the rectangle it is an elliptic function, prop.15.3.2.

5.2.1 Harmonic functions

We shall prove that, unlike real functions, the existence of the derivative f' on a domain D where f is holomorphic, implies that f is *differentiable infinitely many times* on D and admits convergent Taylor series expansion in any disk contained in D (*analyticity*). Because of this, the words "holomorphic" and "analytic" are equivalent.

Analyticity implies that the real and imaginary parts u and v of f are $\mathcal{C}^\infty(D)$. The Cauchy-Riemann property shows that **the real and imaginary parts of a holomorphic function are harmonic functions**:

$$\partial_x^2 u = \partial_x(\partial_y v) = \partial_y(\partial_x v) = -\partial_y^2 u, \quad \partial_x^2 v = -\partial_x(\partial_y u) = -\partial_y(\partial_x u) = -\partial_y^2 v$$

$$\boxed{\nabla^2 u = 0, \quad \nabla^2 v = 0} \tag{5.13}$$

As u and v originate from the same holomorphic function, they are "conjugate" harmonic functions.

Example 5.2.6. $f(z) = e^{z^2}$ is entire, then $u(x, y) = e^{x^2-y^2} \cos(2xy)$ and $v(x, y) = e^{x^2-y^2} \sin(2xy)$ are conjugate harmonic functions on the plane.

$f(z) = 1/z$ is holomorphic on $\mathbb{C} \setminus \{0\}$, then $x/(x^2 + y^2)$ and $-y/(x^2 + y^2)$ are conjugate harmonic on $\mathbb{C} \setminus \{0\}$.

Given a real harmonic function $u(x, y)$ on a domain D , the Cauchy-Riemann equations provide the *conjugate* harmonic function $v(x, y)$ on D up to a constant. The function $f = u + iv$ is holomorphic on D .

Example 5.2.7. Find the conjugate of the harmonic function $u(x, y) = x^3 y - xy^3$, and the associated analytic function.

1) use the C.R. equation $\partial_y v = \partial_x u = 3x^2 y - y^3$. The integral in y gives $v = \frac{3}{2}x^2 y^2 - \frac{1}{4}y^4 + \lambda(x)$. The second C.R. equation is: $\partial_x v = -\partial_y u$ i.e. $3xy^2 + \lambda'(x) = -x^3 + 3xy^2$. Then $\lambda(x) = -\frac{1}{4}x^4 + \lambda_0$ and $v(x, y) = \frac{3}{2}x^2 y^2 - \frac{1}{4}(y^4 + x^4)$ up to a constant λ_0 . The associated holomorphic function is $u + iv = x^3 y - xy^3 - \frac{i}{4}(x^4 - 6x^2 y^2 + y^4) = -\frac{i}{4}z^4$.

³ References: P. Henrici, *Applied and computational complex analysis*, vol. 3, Wiley (1976); T. Driscoll and L. Trefethen, *Schwarz-Christoffel mapping*, Cambridge Univ. Press. (2002); Z. Nehari, *Conformal Mapping*, reprinted by Dover.

2) use the formula $f'(z) = u_x - i u_y = 3x^2 y - y^3 - i x^3 + i 3x y^2 = 3x y(x + i y) - i(x^3 - i y^3) = 3x y z - i[(x + i y)^3 - 3i x^2 y + 3x y^2] = -i z^3$ (necessarily we end up with only z). An integral gives $f(z)$, and the imaginary part is $v(x, y)$.

Proposition 5.2.8. *If $\varphi(u, v)$ is harmonic on D_w (a domain in the plane $w = u + i v$) and if $w = f(z)$ is a holomorphic map on D to D_w , then $\varphi(u(x, y), v(x, y))$ is harmonic on D .*

Proof. Direct evaluation of partial derivatives checks the statement. In alternative, φ is the real part of a holomorphic function $g(w)$. Then $g(f(z))$ is holomorphic in the variable z , and $\operatorname{Re} g(f(z))$ is harmonic. \square

Exercise 5.2.9. *Show that if f is holomorphic, then⁴:*

$$\nabla^2 |f(z)|^2 = 4|f'(z)|^2 \quad (5.14)$$

$$\nabla^2 \log[1 + |f(z)|^2] = \frac{4|f'(z)|^2}{[1 + |f(z)|^2]^2} \quad (5.15)$$

5.3 Inverse functions

Let f be a holomorphic function on a domain D : we discuss conditions for the existence of a holomorphic inverse function f^{-1} .

Definition 5.3.1. A function g is a *branch* of f^{-1} with domain $U \subseteq f(D)$ if:

- 1) g is continuous on U ,
- 2) $f(g(w)) = w$ for all $w \in U$.

The branch function g of f^{-1} is univalent (injective) on U if:

$$g(w_1) = g(w_2) \Rightarrow f(g(w_1)) = f(g(w_2)) \text{ and } w_1 = w_2$$

The following result is a special case of the implicit function theorem in two real variables.

Theorem 5.3.2 (Inverse function theorem). *Suppose that $f(z)$ is holomorphic on a domain D , and $g(w)$ is a branch of $f^{-1}(w)$ with domain U . Let $f(z_0) = w_0 \in U$. If $f'(z_0) \neq 0$ then g is differentiable at w_0 and $g'(w_0) = 1/f'(z_0)$.*

Consequently, if $f'(z) \neq 0$ in $g(U)$, then g is holomorphic on U and

$$\boxed{g'(w) = \frac{1}{f'(g(w))}} \quad (5.16)$$

⁴ From: G. Pólya and G. Szegő, *Problems and Theorems in Analysis I*, Springer, 1978, page 115.

We now discuss the analytic structure of some relevant inverse functions. In these examples, the branch is chosen in order to reproduce the inverse function of real analysis, when restricted to real variable (*principal branch*).

5.3.1 The square root

The function $f(z) = z^2$ maps \mathbb{C} to a double cover of the w -plane. It is useful to view the image as a two-sheet Riemann surface, i.e. two copies of the w -plane.

In real analysis, the square root $u = \sqrt{x}$ is defined on the half-line $x \geq 0$, and maps the half-line monotonically to $u \geq 0$. Therefore, a convenient choice is to identify the first sheet as the *image* of the half-plane

$$-\frac{\pi}{2} < \text{Arg } z < \frac{\pi}{2}$$

which includes the positive real axis. The first sheet has a cut: the negative real axis $\text{Arg } w = \pi$, which is the image of the imaginary axis in z plane.

The second sheet is the image of the half-plane $\pi > |\text{Arg } z| > \frac{\pi}{2}$. The two sheets share an edge: the line $\text{Arg } w = \pi$.

By walking anticlockwise on a circle around the origin $z = 0$ starting at $\text{Arg } z = -\pi/2$, the image point walks in the first sheet starting at $\text{Arg } w = \pi$.

At $\text{Arg } z = \pi/2$ a full circle is run in the first sheet, and the walker enters the second sheet being at the other edge of the cut $\text{Arg } w = \pi$.

Another circle is completed as $\text{Arg } z = 3\pi/2$. At this point we are again at $\text{Arg } z = -\pi/2$, i.e. the image point is on the side of the cut where the walk in the first sheet started.

The principal branch of the square root has domain in the first sheet,

$$\sqrt{\cdot} : \rho e^{i\theta} \rightarrow \sqrt{\rho} e^{i\theta/2}, \quad |\theta| < \pi \quad (5.17)$$

The half line $(-\infty, 0] = \{w \text{ s.t. } \text{Arg } w = \pi\}$ is a *branch cut*, where the square root is discontinuous. Near the cut, for $\epsilon \rightarrow 0^+$:

$$\sqrt{-|x| + i\epsilon} \rightarrow i\sqrt{|x|}, \quad \sqrt{-|x| - i\epsilon} \rightarrow -i\sqrt{|x|}$$

On the domain $\mathbb{C}/(-\infty, 0]$ the principal branch is holomorphic and

$$\frac{d}{dw} \sqrt{w} = \frac{1}{2\sqrt{w}} \quad (5.18)$$

5.3.2 The logarithm

The function $f(z) = e^z$ is defined for all z but, being periodic, it is not invertible. On a strip $-\pi < \text{Im } z < +\pi$ the map is one-to-one with the w -plane with a cut given by the half-line

$\arg w = \pi$ removed. The whole z -plane is mapped to a *helix* (the Riemann surface of the log): a stack of an infinite number of sheets (copies of the w -plane with cut).

Each sheet is a domain of a *branch* of the log:

$$\log w = \log|w| + i \arg w \quad (2k-1)\pi < \arg w < (2k+1)\pi$$

It has discontinuity $2\pi i$ across the cut *if one remains on the same sheet*. However, the Riemann surface allows one to enter a new sheet by crossing the cut: a 2π ascent round the helix axis moves from one sheet to the next one, where the new branch of $\log w$ differs by $2\pi i$ from the previous one.

A walk parallel to the imaginary axis in z -plane in the positive direction corresponds to a helicoidal path in the Riemann surface.

Each sheet defines a branch of the log which is analytic with derivative

$$\frac{d}{dw} \log w = \frac{1}{e^{\log w}} = \frac{1}{w} \quad (5.19)$$

The principal log (Log) is the branch in the first sheet, $\mathbb{C}/(-\infty, 0]$, where $\text{Log } z = \log|z| + i \text{Arg}z$, $|\text{Arg}z| < \pi$.

Chapter 6

Electrostatics*

Several two-dimensional problems in electrostatics, magnetostatics, fluid-dynamics, elasticity, may be elegantly solved in the complex plane, with proper conformal maps that take care of the geometry. In this chapter we consider electrostatics¹.

6.1 The fundamental solution

The fundamental solution or Green function² of 2D electrostatics is the solution of the Poisson equation for a unit point charge localized at $z' = x' + iy'$:

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = -\frac{1}{\epsilon_0} \delta(x - x') \delta(y - y') \quad (6.1)$$

The solution is easily obtained if the point charge is viewed as the section of a wire orthogonal to the plane, with unit linear charge.

The 3D electric field is radial. Gauss theorem applied to a cylinder coaxial with the wire gives $\mathbf{E} = E\mathbf{n}$ with

$$E(x, y) = \frac{1}{2\pi\epsilon_0} \frac{1}{\sqrt{(x - x')^2 + (y - y')^2}}$$

¹ A specialized text in this topic is: E. Durand, *Électrostatique*, 3 voll, Masson, Paris 1964.

² George Green (Nottingham 1793, 1841) was a miller. For more than forty years he worked hard in his father's windmill, while self-teaching mathematics and physics. In 1828 he published at his own expense his most important and astonishing paper: *Essay on the application of mathematical analysis to the theories of electricity and magnetism*, that contains the first exposition of the theory of potential. After his father's death, he applied to Cambridge's university, and graduated in mathematics in 1838 (the same year as Sylvester). After his death his achievements were rescued from obscurity by Lord Kelvin, and are nowadays an important tool in every area of physics (including quantum field theory. See J. Schwinger, *The Greening of quantum Field Theory: George and I*. <https://doi.org/10.48550/arXiv.hep-ph/9310283>).

The electrostatic potential in 2D of a point unit charge is $\mathbf{E}(x, y) = -\nabla\varphi$ i.e.:

$$\boxed{\varphi(x, y) = -\frac{1}{2\pi\epsilon_0} \log \sqrt{(x-x')^2 + (y-y')^2}.} \quad (6.2)$$

By the superposition principle (linearity of Poisson's equation), the electrostatic potential generated by a charge distribution is:

$$\varphi(x, y) = -\frac{1}{2\pi\epsilon_0} \int dx' dy' \log \sqrt{(x-x')^2 + (y-y')^2} \rho(x', y')$$

It solves Poisson's equation and it is *harmonic in empty space*. For this reason, it is very useful to regard it as the real part of a *complex potential* which, in empty space, is *holomorphic* and depends on $z = x + iy$:

$$\boxed{\Phi(z) = \varphi(x, y) + i\psi(x, y)}$$

Necessarily, the conjugated field $\psi(x, y)$ is harmonic. It can be obtained from φ by solving the Cauchy-Riemann equations and is defined up to a constant; sometimes it is found by good guess. For the point charge it is

$$\Phi(z) = -\frac{1}{2\pi\epsilon_0} \log(z-z') = -\frac{1}{2\pi\epsilon_0} [\log|z-z'| + i \arg(z-z')]$$

The fields φ and ψ are harmonic in $\mathbb{C}/\{\text{cut}\}$. The cut joins the source point z' to infinity and can be chosen freely, to avoid the points of interest.

Being a function of z , the complex potential is more manageable than the potential. For a charge distribution, $\Phi(z)$ may be obtained by superposition.

The physical meaning of the field ψ is now given. The function Φ maps the z plane to the plane $w = \varphi + i\psi$; the orthogonal straight lines $\varphi(x, y) = U$ and $\psi(x, y) = V$ correspond in the z plane to orthogonal curves that describe respectively *equipotential lines* and *lines of force*.

For the point charge, the equipotential lines are circles centred in the point source z' , and the field lines are half-lines originating from z' .

The electric field $\mathbf{E} = -\nabla\varphi$ is best evaluated as a complex field: $\bar{E} \equiv E_x - iE_y = -\partial_x\varphi + i\partial_y\varphi = -\partial_x(\varphi + i\psi)$ by the C-R equation. Then:

$$\boxed{\bar{E}(z) = -\frac{d}{dz}\Phi(z)} \quad (6.3)$$

The complex electric field is holomorphic. The corresponding vector field \mathbf{E} is orthogonal (by definition) to equipotential lines, and tangent to the lines of force.

Example 6.1.1 (The uniformly charged segment). *The electrostatic complex potential of a segment $[a, b]$ of the real axis with uniform charge density σ (a thin slab across the plane) is*

$$\Phi(z) = -\frac{\sigma}{2\pi\epsilon_0} \int_a^b ds \log(z-s)$$

To evaluate the electric field (6.3) assume that $-\frac{d}{dz}$ can enter the integral and use $-\frac{d}{dz} \log(z-s) = \frac{d}{ds} \log(z-s)$:

$$E_x - iE_y = -\frac{\sigma}{2\pi\epsilon_0} \log \frac{z-b}{z-a} = -\frac{\sigma}{2\pi\epsilon_0} \left[\log \left| \frac{z-b}{z-a} \right| - i \arg \frac{z-b}{z-a} \right]$$

At $z = x \pm i\epsilon$, $a < x < b$, it is $\text{Log} \frac{z-b}{z-a} = \log \frac{b-x}{x-a} \pm i\pi$. Then $E_y = \pm \sigma/2\epsilon_0$; E_x is non-zero because the uniformly charged segment is not equipotential. At each point of $[a, b]$ (and only there) there are two determinations ($E_x \pm iE_y$)(x) that correspond to vectors pointing to opposite sides; it is singular at the end-points. Elsewhere, the vector field is unique.

Example 6.1.2. *Electrostatic potential of n charges q/n , equally spaced on a circle of radius R .*

Let $\zeta_1 \dots \zeta_n$ be the roots of unity, the complex potential is

$$\Phi(z) = -\frac{q}{n} \frac{1}{2\pi\epsilon_0} \sum_k \log(z - R\zeta_k) = -\frac{q}{n} \frac{1}{2\pi\epsilon_0} \log(z^n - R^n)$$

The potential is $\varphi(x, y) = -\frac{q}{n} \frac{1}{2\pi\epsilon_0} \log|z^n - R^n|$. In the continuum limit $n \rightarrow \infty$ (uniformly charged ring - or cylindrical surface in 3D):

$$\varphi(x, y) = -\frac{q}{2\pi\epsilon_0} \begin{cases} \log R & r < R \\ \log r & r > R \end{cases} \quad (6.4)$$

Example 6.1.3 (The dipole). *The complex potential of two point charges $\pm Q$ in $\pm i\delta/2$ is*

$$\Phi(z) = -Q \frac{1}{2\pi\epsilon_0} [\log(z - i\delta/2) - \log(z + i\delta/2)]$$

For $|z| \gg \delta$ one approximates $\log(z \pm i\delta/2) \approx \log z \pm i\delta/(2z)$. If $\delta \rightarrow 0$ and Q is rescaled such that $d = Q\delta$ is finite, we obtain the potential at a point z of a dipole placed in the origin and oriented as the imaginary axis:

$$\Phi(z) = i \frac{d}{2\pi\epsilon_0 z} = \frac{d}{2\pi\epsilon_0} \left[\frac{y}{x^2 + y^2} + i \frac{x}{x^2 + y^2} \right].$$

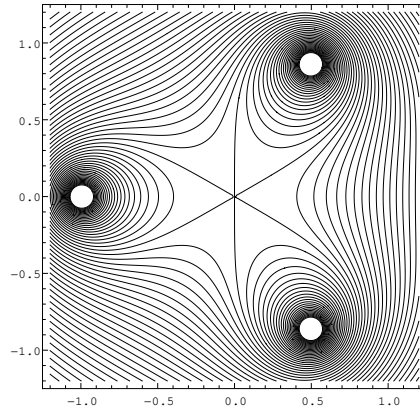


Figure 6.1 The equipotential lines of 3 unit charges (i.e. three wires with same linear charge crossing the plane).

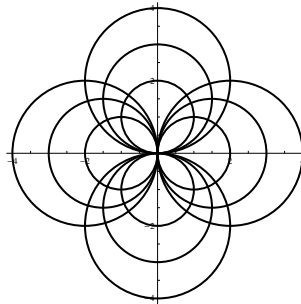


Figure 6.2 Equipotential lines and field lines for the dipole.

The equipotential lines are circles tangent to the real axis at the origin; the flux lines are circles through the origin and tangent to the imaginary axis (see Fig.6.2). The electric field of the dipole is

$$\bar{E}(z) = i \frac{d}{2\pi\epsilon_0 z^2} = \frac{d}{2\pi\epsilon_0} \left[\frac{2xy}{(x^2 + y^2)^2} + i \frac{x^2 - y^2}{(x^2 + y^2)^2} \right] = E_x - iE_y.$$

The intensity of the field is $|E(z)| = d/(2\pi\epsilon_0|z|^2)$.

The solution $\Phi_{\text{ref}}(w)$ of an electrostatic problem in a region Ω_w with prescribed point charges and boundary conditions can be used to solve a problem in Ω_z where the point charges and the conducting surfaces are displaced by the conformal map $f : \Omega_z \rightarrow \Omega_w$.

The function

$$\Phi(z) = \Phi_{\text{ref}}(f(z))$$

is holomorphic in Ω_z , and its real part is the harmonic potential in Ω_z .

In the following examples, a solution Φ_{ref} is found for simple geometries in the w -plane, and related more complex problems in z plane are solved by conformal mapping.

6.2 Thin metal plate

Consider in 3D a thin infinite metallic plate, with (uniform) charge density σ , at electrostatic potential φ_0 . The problem is studied in 2D, with the section of the plate chosen as the real axis of the $w = u + iv$ plane.

The potential solves the Laplace equation with $\varphi(u, 0) = \varphi_0$ and $-(\partial_v \varphi)(u, 0) = \sigma/\epsilon_0$. The solution is simple: $\varphi(u, v) = -\frac{1}{\epsilon_0} \sigma v + \varphi_0$ (equipotential lines parallel to the u -axis). It is the real part of the holomorphic potential

$$\Phi_{\text{ref}}(w) = \varphi_0 + \frac{i}{\epsilon_0} \sigma w + ic$$

where c is real and arbitrary. The electric field is $\vec{E} = -i\sigma/\epsilon_0$ (uniform and orthogonal to the plate).

The simple solution is useful for solving more difficult problems: if $f(z)$ is the conformal map of some empty domain to the half-plane $\text{Im } w > 0$, then

$$\Phi(z) = \varphi_0 + \frac{i}{\epsilon_0} \sigma f(z) + ic \tag{6.5}$$

is the complex potential in the new domain. Its real part is harmonic and takes the value φ_0 on the boundary of the domain, which f maps to the real axis $v = 0$. We consider two examples.

6.2.1 Right-angle dihedron, with conducting walls

$f(z) = z^2$ maps the quadrant $\{z: x > 0, y > 0\}$ to $\text{Im } w > 0$.

The complex potential $\Phi(z) = \varphi_0 + \frac{i}{\epsilon_0} \sigma z^2 + ic$ solves the electrostatic problem in the empty quadrant with potential φ_0 at the boundary.

The real part is $\varphi(x, y) = -(2\sigma/\epsilon_0)xy + \varphi_0$, with hyperbola as equipotential lines. Also the lines of force are hyperbolae: $\psi(x, y) = (\sigma/\epsilon_0)(x^2 - y^2)$.

The electric field is $\vec{E} = -i\frac{2\sigma}{\epsilon_0}z$, or $\mathbf{E}(x, y) = \frac{2\sigma}{\epsilon_0}(\mathbf{y}\mathbf{i} + x\mathbf{j})$.

The linear charge at the boundary of the quadrant is not uniform: $\sigma(x) = 2\sigma x$ ($x \geq 0$) and

$\sigma(y) = 2\sigma y$ ($y \geq 0$). Charge is depleted from the corner because of the electrostatic repulsion exerted by the other side. The total charge in $0 < x < L$ is σL^2 , and equals the total charge in the image segment $0 < u < L^2$.

6.2.2 Obtuse dihedron, with conducting walls

$f(z) = z^{2/3}$ maps the sector $0 < \arg z < \frac{3}{2}\pi$ to $\text{Im } w > 0$.

The complex potential in the sector is $\Phi(z) = \varphi_0 + i(\sigma/\epsilon_0) z^{2/3} + ic$. The electrostatic potential is $\varphi(x, y) = \varphi_0 - (\sigma/\epsilon_0) \rho^{2/3} \sin(\frac{2}{3}\theta)$. The linear charge on the boundary line $\theta = 0$ is:

$$\sigma(x) = \epsilon_0 E_y(x, 0) = \epsilon_0 \text{Im} \frac{d\Phi}{dz} \Big|_{y=0} = \frac{2}{3} \sigma x^{-1/3}.$$

The charge accumulates near the edge $x = 0$. The charge in the segment $0 < x < L$ is $\sigma L^{2/3}$ and equals the charge in the image segment $0 < u < L^{2/3}$.

6.3 Two adjacent thin metal plates

In 3D consider two adjacent thin metal plates at potentials 0 and V separated by an insulating line. The problem is 2D ($w = u + iv$ plane), with the two plates being the positive and negative parts of the real axis.

The Laplace equation for the electrostatic potential with b.c. $\varphi(u, 0) = 0$ if $u < 0$ and $\varphi(u, 0) = V$ if $u > 0$, is found in polar coordinates:

$$\nabla^2 \varphi(r, \theta) = 0, \quad \varphi(r, 0) = V, \quad \varphi(r, \pi) = 0 \quad r > 0$$

The solution is $\varphi(r, \theta) = \frac{1}{\pi} V(\pi - \theta)$ (independent of r) i.e. $\varphi(w) = \frac{1}{\pi} V(\pi - \text{Arg } w)$. It is the real part of the complex potential, holomorphic in $v \neq 0$:

$$\Phi_{\text{ref}}(w) = V + \frac{iV}{\pi} \text{Log } w + ic$$

This solution can be used to solve more difficult problems.

6.3.1 Semi-infinite plates at right angles, at potentials 0 and V

The complex potential is $\Phi(z) = V + \frac{iV}{\pi} \text{Log}(z^2)$. The real part is the electrostatic potential of the new geometry: $\varphi(x, y) = V - \frac{V}{\pi} \text{Arg}(z^2)$, with boundary values $\varphi(0, y) = 0$ and $\varphi(x, 0) = V$. The electric field is

$$\bar{E} = -\frac{2iV}{\pi z} \rightarrow E_x = -\frac{2V}{\pi} \frac{y}{x^2 + y^2}, \quad E_y = \frac{2V}{\pi} \frac{x}{x^2 + y^2}$$

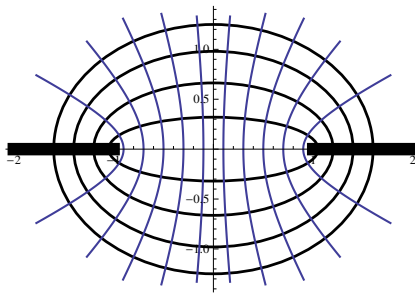


Figure 6.3 Equipotential lines and field lines for two coplanar thin metal plates at potentials 0 and V .

The charge on the metallic boundary $y = 0, x > 0$ is $\sigma(x) = \frac{1}{4\pi} E_y(x, 0) = \frac{V}{2\pi^2 x}$. On the boundary $x = 0, y > 0$ it is $\sigma(y) = \frac{1}{4\pi} E_x(0, y) = -\frac{V}{2\pi^2 y}$.

6.3.2 Coplanar thin metal plates, with gap

Two thin conducting plates have potentials 0 and V and are separated by a gap of width 2. In the plane $z = x + iy$, the plates are the semi-infinite lines $x \leq -1$ and $x \geq 1$ of the real axis (see Fig.6.3).

The electrostatic potential solves the Laplace equation with boundary conditions $\varphi(x, 0) = 0$ if $x \leq -1$ and $\varphi(x, 0) = V$ if $x \geq 1$. The b.c. are implemented by a conformal map.

The domain where φ is harmonic (z -plane with two cuts in the real axis) is the image of the half-plane $\mathbb{H} = \{w : \text{Im } w > 0\}$ for the Jukowski map

$$z = \frac{1}{2} \left(w + \frac{1}{w} \right)$$

In components the Jukowski map is ($w = r e^{i\theta}, 0 \leq \theta \leq \pi$):

$$x = \frac{1}{2} \left(r + \frac{1}{r} \right) \cos \theta, \quad y = \frac{1}{2} \left(r - \frac{1}{r} \right) \sin \theta$$

The half-line $\theta = 0$ is mapped to the cut $\{x \geq 1, y = 0\}$, while the half-line $\theta = \pi$ is mapped to the other cut $\{x \leq -1, y = 0\}$.

The complex potential of this problem is

$$\Phi(z) = V + \frac{iV}{\pi} \text{Log } w(z)$$

where $w(z)$ is the inverse of the Jukowski map.

The real part is $\varphi(x, y) = \frac{1}{\pi} V [\pi - \theta(x, y)]$. The equipotential lines have constant $\theta(x, y)$, they

are hyperbola with foci ± 1 :

$$\frac{x^2}{\cos^2 \theta} - \frac{y^2}{\sin^2 \theta} = 1$$

The lines of force are the images of circles (constant r), i.e. ellipses with foci ± 1 (orthogonal to hyperbola and to the two cuts. See Fig.6.3).

6.4 Point charge and semi-infinite conductor

Consider of a grounded semi-infinite conductor and a parallel wire at distance v_0 , with linear charge density Q . The charged wire induces a surface charge that contributes to the electrostatic potential.

In w -plane the problem is that of a point charge Q in $w_0 = u_0 + i v_0$ ($v_0 > 0$) in presence of the half plane $\text{Im } v \leq 0$ at potential zero. At the surface of the conductor ($v = 0$), the lines of force are perpendicular.

The evaluation of the field is done by replacing the semi-infinite conductor with an image charge $-Q$ in $\overline{w_0}$. By symmetry, the real axis has constant (zero) potential. Up to a constant, the complex field is:

$$\Phi_{\text{ref}}(w) = -\frac{Q}{2\pi\epsilon_0} \log(w - w_0) + \frac{Q}{2\pi\epsilon_0} \log(w - \overline{w_0}) \quad (6.6)$$

The real part is the electrostatic potential of the pair $\pm Q$, which is equivalent to the system “real charge and grounded conductor”:

$$\varphi(u, v) = -\frac{Q}{4\pi\epsilon_0} \log \frac{(u - u_0)^2 + (v - v_0)^2}{(u - u_0)^2 + (v + v_0)^2}$$

For $v = 0$ it is equal to zero. The complex electric field at the surface is

$$(E_u - i E_v)(u + i0) = \frac{Q}{2\pi\epsilon_0} \left[\frac{1}{u - w_0} - \frac{1}{u - \overline{w_0}} \right] = i \frac{Q}{\pi\epsilon_0} \frac{v_0}{(u - u_0)^2 + v_0^2}$$

The surface charge density $\sigma(u) = \epsilon_0 E_v(u, 0)$ is negative, and the total induced charge neutralizes the point charge:

$$Q_{\text{ind}} = \int_{-\infty}^{+\infty} du \sigma(u) = -Q \frac{v_0}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{(u - u_0)^2 + v_0^2} = -Q.$$

The solution (6.6) valid for a point charge in the half-plane \mathbb{H} is used to solve other problems, where a point charge sits in a vacuum region Ω_z , bounded by a line that is not

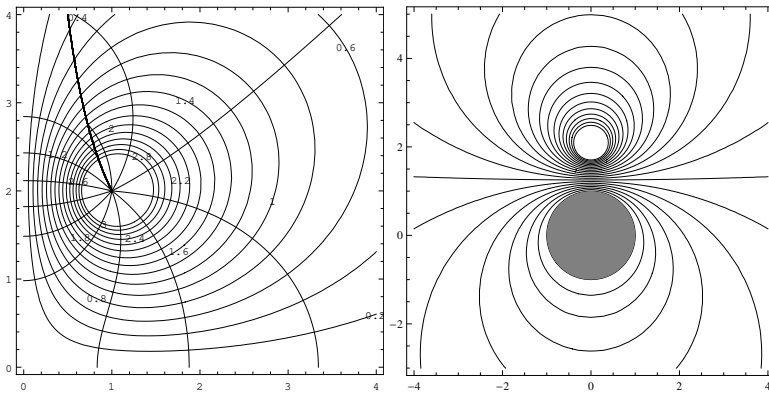


Figure 6.4 *Left: Equipotential lines for a point charge in a right angle with conducting walls (a dark line is spurious). Right: equipotential lines of a point charge in (0,2) in presence of a conducting disk (gray) of unit radius.*

the x -axis. If $f : \Omega_z \rightarrow \mathbb{H}$, the complex potential in Ω_z is $\Phi(z) = \Phi_{\text{ref}}(f(z))$. Being a composition of holomorphic functions, it is holomorphic, and its real and imaginary parts are harmonic in Ω_z . The real part is the electrostatic potential $\varphi(x, y)$ of the new problem.

6.4.1 Point charge in a right angle

Consider a point charge Q in $z_0 = x_0 + iy_0$ in the first quadrant of the z -plane. This quadrant is Ω_z , and is bounded by conducting half-lines at potential $\varphi = 0$. The quadrant is flattened to the half-plane \mathbb{H} by the map $w = z^2$. The charge has image w_0 . The complex potential for the quadrant is $\Phi(z) = \Phi_{\text{ref}}(z^2)$, where $\Phi_{\text{ref}}(w)$ is (6.6). The electrostatic potential is the harmonic function $\varphi(x, y) = \varphi_{\text{ref}}(x^2 - y^2, 2xy)$:

$$\varphi(x, y) = -\frac{Q}{4\pi\epsilon_0} \log \frac{(x^2 - y^2 - x_0^2 + y_0^2)^2 + 4(xy - x_0y_0)^2}{(x^2 - y^2 - x_0^2 + y_0^2)^2 + 4(xy + x_0y_0)^2} \tag{6.7}$$

It is $\varphi(x, 0) = 0$ and $\varphi(0, y) = 0$. The equipotential lines are shown in fig.6.4.

6.4.2 Point charge and conducting disk

A point charge Q is at distance d from the center of a grounded disk of radius R ($d > R$). The setting corresponds to a wire parallel to a conducting grounded cylinder. The problem of determining the complex field is solved by the conformal map that takes the solved reference problem in w -plane (point charge and half plane) to the present one in z -plane.

The solution is

$$\Phi(z) = \Phi_{\text{ref}}(f(z)) = -\frac{Q}{2\pi\epsilon_0} \log \frac{w(z) - w_0}{w(z) - \overline{w_0}}$$

Let id , be the position of the point charge. The map from the exterior of the disk $|z| > R$ (the Ω region) to the upper half-plane $\text{Im } w > 0$, that also maps id to $w_0 = i$, is the Möbius map:

$$f(z) = i \frac{d+R}{d-R} \frac{z-iR}{z+iR}$$

The complex potential generated by the disk and the point charge Q in id is:

$$\Phi(z) = -\frac{Q}{2\pi\epsilon_0} \left[\log(z-id) - \log\left(z - i\frac{R^2}{d}\right) + \log\frac{R}{d} \right] \quad (6.8)$$

It coincides with the potential of two point charges: the actual charge Q at id and an image charge $-Q$ at iR^2/d (inside the disk). The potential is

$$\varphi(x, y) = -\frac{Q}{4\pi\epsilon_0} \left[\log[x^2 + (y-d)^2] - \log\left[x^2 + \left(y - \frac{R^2}{d}\right)^2\right] + 2\log\frac{R}{d} \right]$$

(see Fig.6.4). At the surface of the disk, $|z| = R$, the electrostatic potential φ is zero. The electric field is:

$$\overline{E}(z) = -\Phi'(z) = \frac{Q}{2\pi\epsilon_0} \left[\frac{1}{z-id} - \frac{1}{z-iR^2/d} \right]$$

At the surface of the disk the electric field is radial, and the surface density is:

$$\sigma(\theta) = -\frac{Q}{2\pi R} \frac{d^2 - R^2}{d^2 + R^2 - 2dR\sin\theta}$$

with total induced charge $Q_{\text{ind}} = R \int_0^{2\pi} d\theta \sigma(\theta) = -Q$.

6.5 The planar capacitor

Consider in 3D an infinite planar capacitor; its section in the complex $w = u + iv$ plane is the infinite strip between two conducting lines $v = \pm d/2$ at potentials $\pm V/2$. In the strip the electrostatic potential is linear, $\varphi(u, v) = v(V/d)$, and it is the real part of the complex potential

$$\Phi(w) = -i \frac{V}{d} w \quad (6.9)$$

The complex electric field is uniform $\bar{E} = iV/d$, i.e. $E_v = -V/d$. The internal charge densities are $4\pi\sigma = -V/d$ on the lower plate and $4\pi\sigma = V/d$ on the upper one.

The solution of the infinite planar capacitor can be used to study more complex geometries. The following one is interesting for the study of the field near the aperture of a finite capacitor, and was obtained by J. K. Maxwell, by conformal map.

6.5.1 The semi-infinite planar capacitor

Consider the conformal map

$$z(w) = 2\pi(w/d) + e^{2\pi(w/d)}$$

It maps conjugate points w, \bar{w} to conjugate points z, \bar{z} , then the x axis is a symmetry axis and we study the upper half. In components the map is

$$x = 2\pi \frac{u}{d} + e^{2\pi(u/d)} \cos\left(2\pi \frac{v}{d}\right), \quad y = 2\pi \frac{v}{d} + e^{2\pi(u/d)} \sin\left(2\pi \frac{v}{d}\right).$$

The lines $(u, \pm d/2)$ are mapped to $x = \frac{2\pi}{d}u - e^{2\pi u/d}$, $y = \pm\pi$. Since $x'(u) = (2\pi/d)(1 - e^{2\pi u/d}) = 0$ in $u = 0$, the range of $x(u)$ is $(-\infty, -1]$. Therefore the map takes the lines $v = \pm d/2$ to the half-lines $x < -1$, $y = \pm\pi$.

The map takes the interior of an infinite capacitor (the strip $-d/2 < v < d/2$) to both the interior and the exterior of a semi-infinite capacitor. If the plates have potentials $\pm V/2$, the complex potential of the semi-infinite capacitor is:

$$\Phi(z) = -i \frac{V}{d} w(z)$$

Equipotential lines. The real axis $v = 0$ is mapped to $x = \frac{2\pi}{d}u + e^{2\pi u/d}$, $y = 0$, i.e. the real axis of the z plane. The equipotential lines $v = (d/2\pi)c$, $0 < c < \pi$, are mapped to lines that run inside the capacitor and, near the end of the capacitor, bend upward. If $c > \pi/2$ the lines fold back to the top of the condenser. The equation of such equipotential lines can be

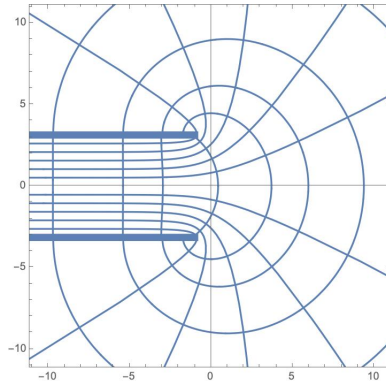


Figure 6.5 The semi-infinite planar capacitor.

obtained by elimination of u in $x = 2\pi \frac{u}{d} + e^{2\pi(u/d)} \cos c$, $y = c + e^{2\pi(u/d)} \sin c$:

$$x = \log \frac{y-c}{\sin c} + (y-c) \cot c \quad (6.10)$$

Electric field. Field lines are orthogonal to equipotential lines. They are the images of segments of constant u inside the infinite capacitor: $2\pi u/d = c$. They are given parametrically (in $s \in [-\pi, \pi]$) by eqs. $x - c = e^c \cos s$ and $y - c = e^c \sin s$ (see note³).

The electric field is

$$\bar{E}(z) = i \frac{V}{d} \left(\frac{dz}{dw} \right)^{-1} = i \frac{V}{2\pi} \frac{1}{1 + e^{2\pi w(z)/d}}$$

Deep in the condenser the field is uniform: $E_x \approx 0$ and $E_y \approx -V/2\pi$. It diverges at $w = \pm id/2$, i.e. at the ends of the conducting boundaries of the capacitor $z = -1 \pm i\pi$.

To avoid the occurrence of divergent fields near the tips of planar capacitors, one may deform the shape of the plates to trace equipotential lines $v = \pm(d/2\pi)c$, i.e. (6.10) (Rogowski's capacitor).

³ Deep in the capacitor ($c \ll -1$) it is $x = c$, $-\pi < y < \pi$. For $c \gg 1$ the lines are circular arcs that end on the exterior of the capacitor's plates, $(x-c)^2 + y^2 = e^{2c}$ (s finite); for small s the lines $x - c \approx e^c - (1/2)y^2 e^{-c}$ are approximately straight segments inside the capacitor, near the aperture.

Chapter 7

Complex Integral

7.1 Paths and curves

A *path* is a continuous map of a real interval to the complex plane,

$$\gamma : [a, b] \rightarrow \mathbb{C}, \quad (a < b).$$

The image is a *curve* γ , and the path $\gamma(t)$ is its parametrization. The increasing value of the parameter assigns an orientation to the curve. Different paths may yield the same curve. Since closed intervals are compact sets in \mathbb{R} and a path is a continuous function, the curve γ is a compact set¹ in \mathbb{C} .

We list some definitions that apply to paths. They imply geometric properties of curves that would otherwise be difficult to phrase:

- A path is *closed* if $\gamma(a) = \gamma(b)$ (we then say that the curve is closed).
- A path is *simple* if $\gamma(t_1) = \gamma(t_2) \Leftrightarrow t_1 = t_2$, $t_{1,2} \neq a, b$ (the curve does not self-intersect, except possibly at the endpoints).
- A *Jordan curve* is a simple closed curve γ .

A theorem of topology (Jordan, Veblen) states that \mathbb{C}/γ is the union of two disjoint sets: the bounded interior and the unbounded exterior of γ .

The complex integral on a curve in \mathbb{C} , will be defined for “smooth curves” i.e. curves that are parametrised by *smooth* functions $\gamma(t)$:

$\gamma(t)$ is differentiable on $[a, b]$,

$\dot{\gamma}(t)$ is continuous on $[a, b]$ and $\dot{\gamma}(t) \neq 0$ on $[a, b]$.

The complex number $\dot{\gamma}(t) = \dot{x}(t) + i\dot{y}(t)$ gives the components of the vector tangent to the curve at $\gamma(t)$ (we shall often identify a complex number with a vector). The tangent vector never vanishes.

The vector $i\dot{\gamma}(t)$ is normal to the curve.

¹ According to the Heine Borel theorem, a set in \mathbb{C} is compact iff it is closed and bounded.

If a curve is not simple, the point where the curve self-intersects has two or more tangent vectors.

A path is *piecewise smooth* if it is continuous (it is a path) and is smooth on each subinterval of some finite partition of $[a, b]$.

A curve can be given different parametrizations. For example the complex segment $[z_1, z_2]$ can be parameterized by $\gamma_1(t) = z_1 + t(z_2 - z_1)$ or by $\gamma_2(t) = z_1 + t^2(z_2 - z_1)$, $t \in [0, 1]$; both paths trace the same segment, but with different “time laws”.

In general, let $\gamma_1 : [a_1, b_1] \rightarrow \mathbb{C}$ be a smooth path, and let $\tau(s)$ be a real map of $[a_2, b_2]$ to $[a_1, b_1]$ with $d\tau/ds > 0$, $\tau(a_2) = a_1$ and $\tau(b_2) = b_1$. The smooth path $\gamma_2(s) = \gamma_1(\tau(s))$ with $s \in [a_2, b_2]$ is a reparametrization of the same curve γ .

Two parametrizations $\gamma_1(\tau)$ and $\gamma_2(s)$ of a curve, at a geometric point of the curve with interval coordinates τ or s , produce parallel tangent vectors $\dot{\gamma}_1(\tau)$ and $\dot{\gamma}_2(s)$ (with same direction if $d\tau/ds > 0$):

$$\dot{\gamma}_2(s) = \dot{\gamma}_1(\tau) \frac{d\tau}{ds}, \quad \tau(s) = \tau.$$

7.2 Complex integral

Given a **continuous complex function on a smooth oriented curve**, $f : \gamma \rightarrow \mathbb{C}$, the integral of f on γ is *defined* as:

$$\boxed{\int_{\gamma} f(z) dz = \int_a^b dt \dot{\gamma}(t) f(\gamma(t))} \quad (7.1)$$

where $\gamma(t)$ is a parametrization of the curve².

The value of the integral *does not depend on the parametrization of the curve*. If $\gamma_2(s) = \gamma_1(\tau(s))$ it is

$$\int_{a_2}^{b_2} ds \dot{\gamma}_2(s) f(\gamma_2(s)) = \int_{a_2}^{b_2} ds \frac{d\tau}{ds} \dot{\gamma}_1(\tau) f(\gamma_1(\tau(s))) = \int_{a_1}^{b_1} d\tau \dot{\gamma}_1(\tau) f(\gamma_1(\tau)).$$

Therefore, the integral of a function on an oriented curve is a geometric object. This is apparent in the equivalent construction of the integral sketched below.

² By expanding the product $\dot{\gamma}(t) f(\gamma(t)) = (\dot{x} + i\dot{y})[u(x, y) + i v(x, y)]$ one obtains four real Riemann integrals that are well defined, since all functions are continuous on closed intervals.

Given an oriented curve γ from point z' to point z'' , and a function f continuous on it, consider the sum

$$\sum_{k=0}^{n-1} (z_{k+1} - z_k) \frac{f(z_{k+1}) + f(z_k)}{2}$$

where z_k are $n + 1$ finitely spaced points of the curve, with $z_0 = z'$ and $z_n = z''$. Omitting technicalities, in the limits $n \rightarrow \infty$, $|z_{k+1} - z_k| \rightarrow 0$, the sum gives a parametrization-independent definition of an integral.

If a parametrization of the curve is used: $z_{k+1} - z_k = \gamma(t_{k+1}) - \gamma(t_k) \approx \dot{\gamma}(t_k)(t_{k+1} - t_k)$, and the sum yields the above defined integral.

If the curve γ is an interval $[a, b]$ of the real line, a parameterisation is $\gamma(x) = x$, and the complex integral coincides with the Riemann integral of a continuous function $f : [a, b] \rightarrow \mathbb{C}$.

Note that the complex integral differs from the line integral:

$$\int_{\gamma} |dz| f(z) = \int_a^b dt \sqrt{\dot{x}^2 + \dot{y}^2} f(x(t) + iy(t))$$

Example 7.2.1. Evaluate $\int_{\gamma} z^2 dz$ on the following curves:

i) The real segment $[a, b]$ ($a < b$).

A parametrization is $\gamma(x) = x$ with $a \leq x \leq b$. Then $\dot{\gamma}(x) = 1$ and

$$\int_{[a,b]} z^2 dz = \int_a^b dx x^2 = \frac{1}{3}(b^3 - a^3)$$

ii) The semicircle with diameter the real segment $[a, b]$ (from a to b counterclockwise, i.e. the semicircle is below the real axis).

A parametrization is $\gamma(\theta) = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)e^{i\theta}$, $\pi \leq \theta \leq 2\pi$. It is $\gamma(\pi) = a$, $\gamma(2\pi) = b$, and $\dot{\gamma} = \frac{i}{2}(b-a)e^{i\theta}$

$$\int_{\gamma} z^2 dz = \frac{i}{2}(b-a) \int_{\pi}^{2\pi} d\theta e^{i\theta} \left[\frac{1}{2}(a+b) + \frac{1}{2}(b-a)e^{i\theta} \right]^2 = \frac{1}{3}(b^3 - a^3)$$

$$I_k = \int_{\pi}^{2\pi} d\theta e^{ik\theta} = \int_{\pi}^{2\pi} d\theta [\cos(k\theta) + i \sin(k\theta)]. \quad I_0 = \pi, \quad I_1 = -2i, \quad I_2 = 0.$$

Note that the two integrals give the same result, which only depends on the extrema of the curve.

If a curve γ is parametrized by $\gamma(t)$, $t \in [a, b]$, the curve with opposite orientation $-\gamma$ is parametrized by the path $\gamma(a + b - t)$, $t \in [a, b]$. The integrals have opposite signs:

$$\begin{aligned} \int_{-\gamma} dz f(z) &= - \int_a^b dt \dot{\gamma}(a + b - t) f(\gamma(a + b - t)) \\ &= \int_b^a ds \dot{\gamma}(s) f(\gamma(s)) = - \int_{\gamma} dz f(z) \end{aligned} \quad (7.2)$$

7.2.1 Two useful inequalities

Proposition 7.2.2. *If the complex function f is integrable on a real interval $I = [a, b]$, then:*

$$\left| \int_a^b dt f(t) \right| \leq \int_a^b dt |f(t)| \quad (7.3)$$

Proof. Let $\int_I f = e^{i\theta} \int_I |f|$, then

$$\left| \int_I f(t) dt \right| = \int_I e^{-i\theta} f dt = \int_I \operatorname{Re}(e^{-i\theta} f) dt \leq \int_I |f| dt.$$

We used $\operatorname{Re} \int f dt = \operatorname{Re} \int (u + iv) dt = \int u dt = \int \operatorname{Re} f dt$. □

If a complex curve is parametrized as $\gamma(t)$, the real function $|f(\gamma(t))|$ is continuous on $[a, b]$ and has a maximum. The previous inequality gives:

Proposition 7.2.3 (Darboux's inequality). *If f is a complex continuous function on a smooth path γ , then:*

$$\left| \int_{\gamma} dz f(z) \right| \leq L(\gamma) \sup_{z \in \gamma} |f(z)| \quad (7.4)$$

where $L(\gamma) = \int_a^b dt |\dot{\gamma}(t)|$ is the length of the path (it is a finite number as γ is required to have continuous derivative on $[a, b]$). Then $\dot{\gamma}_1$ and $\dot{\gamma}_2$ are bounded).

Example 7.2.4. Consider the integral $I = \int_{\sigma} dz e^z$ on the interval $\sigma = [0, 2 + i\pi]$. Darboux's inequality gives $|I| < \sqrt{4 + \pi^2} \sup_{t \in [0, 1]} |e^{t(2+i\pi)}| = e^2 \sqrt{4 + \pi^2}$. The exact value of the integral is obtained through the primitive (as explained below): $I = e^{2+i\pi} - e^0 = -e^2 - 1$, then $|I| = e^2 + 1$.

7.3 Primitive

The evaluation of an integral is straightforward if the function has a primitive.

Definition 7.3.1. If $f(z)$ is continuous on a domain D , a primitive of f is a function $F(z)$ that is *holomorphic on D* such that

$$F'(z) = f(z), \quad \forall z \in D$$

If f is continuous on D and has a primitive on it, and γ is a path in D , the integral of f on γ only depends on the endpoints of the path:

$$\begin{aligned} \int_{\gamma} f(z) dz &= \int_a^b dt \dot{\gamma}(t) f(\gamma(t)) = \int_a^b dt \dot{\gamma}(t) F'(\gamma(t)) \\ &= \int_a^b dt \frac{d}{dt} F(\gamma(t)) = F(\gamma(b)) - F(\gamma(a)). \end{aligned} \quad (7.5)$$

If the path is closed, $\gamma(b) = \gamma(a)$, then the integral is zero.

Example 7.3.2. The function e^z is the primitive of e^z on \mathbb{C} ; therefore $\int_{\gamma} dz e^z = e^b - e^a$ on any curve joining the complex point a to b .

The existence of a primitive is implied by and implies strong properties of f on the domain:

Theorem 7.3.3 (Theorem of the primitive). *Let $f(z)$ be a continuous function on an open connected set D . The following statements are equivalent:*

1. *for any two points a and b in D the integral of f along a (piecewise) smooth path with endpoints a and b does not depend on the path;*
2. *the integral of f along any closed (piecewise) smooth path in D is zero;*
3. *there is a function $F(z)$ holomorphic at all points of D such that $F'(z) = f(z)$ at all points of D*

Proof. To prove that $1 \rightarrow 2$, $2 \rightarrow 1$ and $3 \rightarrow 1$ is trivial. The only non-trivial statement to prove is 1 implies 3. Define $F(z)$ as the integral of f from an arbitrary point $a \in D$ to z along a path; by hypothesis 1 the function depends on z (and a) but not on the path.

To prove that F is holomorphic consider a disk with center z contained in D (D is open), choose $z+h$ in the disk (we'll take the limit $h \rightarrow 0$) and consider the path from a to $z+h$ obtained by prolonging the path from a to z by the segment $\sigma = [z, z+h]$. Parametrize σ

as $\zeta(t) = z + ht$ ($d\zeta = hdt$). Then:

$$\frac{F(z+h) - F(z)}{h} = \frac{1}{h} \int_{\sigma} d\zeta f(\zeta) = \int_0^1 dt f(z+ht) = f(z) + \int_0^1 dt [f(z+ht) - f(z)].$$

Since f is continuous: $\forall \epsilon > 0 \exists \delta$ such that $|f(z+ht) - f(z)| < \epsilon$ if $t|h| < \delta$, then:

$$\left| \frac{F(z+h) - F(z)}{h} - f(z) \right| \leq \int_0^1 dt |f(z+ht) - f(z)| \leq \epsilon$$

if $|h| \leq \delta$, i.e. $F'(z) = f(z)$. □

7.4 The Cauchy transform

Let γ be a (piecewise) smooth path (no matter if open or closed) and f a continuous function on γ . For $z \notin \gamma$ the ratio $\varphi(\zeta) = f(\zeta)/(\zeta - z)$ is continuous on γ . The following integral exists, and is the *Cauchy transform* of f :

$$(\mathcal{C}f)(z) = \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z}, \quad z \notin \gamma, \quad (7.6)$$

It plays an important role in Cauchy's theory of holomorphic function, together with the integrals³

$$(\mathcal{C}_n f)(z) = \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z)^n}, \quad z \notin \gamma, \quad n = 2, 3, \dots \quad (7.7)$$

Theorem 7.4.1. *The functions $\mathcal{C}_n f$, $n = 1, 2, \dots$, are holomorphic in \mathbb{C}/γ and*

$$(\mathcal{C}_n f)'(z) = n(\mathcal{C}_{n+1} f)(z) \quad (7.8)$$

Proof. The proof is first given for $n = 1$.

Choose $z \in \mathbb{C}/\gamma$. Being \mathbb{C}/γ an open set, there is an open disk centred in z of radius δ that is not crossed by γ . Let $z+h$ belong to such disk and evaluate:

$$\begin{aligned} (\mathcal{C}f)(z+h) - (\mathcal{C}f)(z) &= \int_{\gamma} \frac{d\zeta}{2\pi i} f(\zeta) \left[\frac{1}{\zeta - z - h} - \frac{1}{\zeta - z} \right] \\ &= h \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z - h)(\zeta - z)} \end{aligned}$$

³ see Lars Ahlfors, Complex Analysis, 3rd ed. McGraw-Hill, p.121.

Let $M = \sup_{z \in \gamma} |f(z)|$; by the Darboux inequality:

$$\left| h \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z - h)(\zeta - z)} \right| \leq \frac{L(\gamma)M}{2\pi} \sup_{\zeta \in \gamma} \frac{|h|}{|\zeta - z - h||\zeta - z|}$$

For all $\zeta \in \gamma$ it is: $|\zeta - z| > \delta$ and $|\zeta - z - h| \geq ||\zeta - z| - |h|| = |\zeta - z| - |h| \geq \delta - |h|$. Then:

$$\frac{|h|}{|\zeta - z - h||\zeta - z|} \leq \frac{|h|}{(\delta - |h|)\delta} \rightarrow 0 \quad \text{for } h \rightarrow 0.$$

This result shows continuity of $\mathcal{C}f$. Now, divide by h and subtract $(\mathcal{C}_2 f)(z)$:

$$\begin{aligned} \frac{(\mathcal{C}f)(z+h) - (\mathcal{C}f)(z)}{h} - (\mathcal{C}_2 f)(z) &= \int_{\gamma} \frac{d\zeta}{2\pi i} \left[\frac{f(\zeta)}{(\zeta - z - h)(\zeta - z)} - \frac{f(\zeta)}{(\zeta - z)^2} \right] \\ &= h \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z - h)(\zeta - z)^2} \end{aligned}$$

The afore discussion shows that

$$\left| h \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z - h)(\zeta - z)^2} \right| \leq \frac{L(\gamma)M}{2\pi} \frac{|h|}{(\delta - |h|)\delta^2} \rightarrow 0 \quad \text{for } h \rightarrow 0.$$

Then $\mathcal{C}f$ is holomorphic and $(\mathcal{C}f)' = \mathcal{C}_2 f$.

For $n > 1$ the proof runs similarly. Consider:

$$\begin{aligned} (\mathcal{C}_n f)(z+h) - (\mathcal{C}_n f)(z) &= \int_{\gamma} \frac{d\zeta}{2\pi i} f(\zeta) \left[\frac{1}{(\zeta - z - h)^n} - \frac{1}{(\zeta - z)^n} \right] \\ &= \int_{\gamma} \frac{d\zeta}{2\pi i} f(\zeta) \frac{(\zeta - z)^n - (\zeta - z - h)^n}{(\zeta - z - h)^n (\zeta - z)^n} \\ &= nh \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - z - h)^n (\zeta - z)} + \mathcal{O}(h^2), \end{aligned}$$

Now divide by h and subtract $n\mathcal{C}_{n+1}f(z)$. It remains to show that

$$n \int_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} \left[\frac{1}{(\zeta - z - h)^n} - \frac{1}{(\zeta - z)^n} \right]$$

vanishes for $h \rightarrow 0$, as in the case $n = 1$. □

Example 7.4.2. Let $f(z) = z^k$ on a **closed** curve γ . The Cauchy transform at $z \notin \gamma$ is:

$$\oint \frac{dz'}{2\pi i} \frac{z'^k}{z' - z} = \oint \frac{dz'}{2\pi i} \frac{z'^k - z^k}{z' - z} + z^k \oint \frac{dz'}{2\pi i} \frac{1}{z' - z} = z^k (\mathcal{C}1)(z)$$

The first integral in the r.h.s. is zero because the ratio is a polynomial in z' and is holomorphic; the second one is the function itself, times the Cauchy transform of unity. The nice result holds for any polynomial:

$$\oint \frac{dz'}{2\pi i} \frac{p(z')}{z' - z} = p(z) \oint \frac{dz'}{2\pi i} \frac{1}{z' - z} \quad (7.9)$$

It predates an important property of holomorphic functions (the Cauchy integral formula).

7.5 Index of a closed curve

The Cauchy transform on a closed curve of the unit function is the Index of the closed curve. We discover that it has a topological meaning, captured by the following example.

7.5.1 An instructive integral

Let C be the (anticlockwise) circle with center 0 and radius r . The following integral is easily computed for any integer n , and is independent of the radius:

$$\oint_C \frac{dz}{z^n} = \frac{i}{r^{n-1}} \int_0^{2\pi} d\theta [\cos(n-1)\theta - i \sin(n-1)\theta] = 2\pi i \delta_{n,1} \quad (7.10)$$

What is special about $1/z$ to give a non-zero result?

The functions $1/z, 1/z^2, \dots, 1/z^n, \dots$ are holomorphic in the punctured plane $\mathbb{C}_0 = \mathbb{C}/\{0\}$, but with a difference: a primitive in \mathbb{C}_0 (where the circle runs) exists for them, but not for $n = 1$. $\log z$ is not a primitive of $1/z$ on \mathbb{C}_0 : it has branch cut that joins the origin to infinity. The curve C always crosses the cut.

However, if a ray from 0 (included) to ∞ is cut away from \mathbb{C} , then the log with branch cut along the ray is a primitive of $1/z$ in the new domain \mathbb{C}/ray .

Consider the open curve C_a obtained by removing the intersection (call it a) of the ray with C . The integral on C_a is the difference of primitives at the sides of the cut:

$$\int_{C_a} \frac{dz'}{z'} = \log a^+ - \log a^- = 2\pi i$$

$2\pi i$ is the discontinuity of $\log z$ across the cut.

The result *does not depend* on the curve joining the points a^\pm : the curve C_a may be deformed to γ_a (with fixed a). Since only a point has been removed, where $1/z$ is continuous,

the integrals on C , C_a and γ coincide. Therefore:

$$\oint_{\gamma} \frac{dz'}{z'} = 2\pi i$$

for any simple closed curve γ enclosing the origin. The contribution $2\pi i$ solely arises from the single crossing of the branch cut.

The result is invariant under a translation:

$$\oint_{\gamma} \frac{dz'}{z' - z_0} = \begin{cases} 0 & \text{if } \gamma \text{ does not encircle the point } z_0 \\ 2\pi i & \text{if } \gamma \text{ encircles (only once) the point } z_0 \end{cases}$$

This introduces the interesting topic of the index.

7.5.2 The index of a closed curve

Definition 7.5.1. Let γ be a (piecewise) smooth closed oriented curve and $z \notin \gamma$. The Index (or winding number) of γ with respect to z is

$$\text{Ind}(\gamma, z) = \oint_{\gamma} \frac{dz'}{2\pi i} \frac{1}{z' - z} \quad (7.11)$$

It is the Cauchy transform of $f(z) = 1$ on a closed curve. Therefore it is a holomorphic function on any open set not traversed by the curve. Indeed it is constant in each set:

$$\frac{d}{dz} \text{Ind}(\gamma, z) = \oint_{\gamma} \frac{dz'}{2\pi i} \frac{1}{(z' - z)^2} = 0, \quad z \notin \gamma$$

As $|z| \rightarrow \infty$, the index function vanishes. Being a constant, it is zero in $\text{Ext}(\gamma)$.

It can be easily understood that the constant is an integer that enumerates the number of windings of γ around the point z .

From the point z draw a half-line σ , with any direction that avoids self-intersections of the curve. The half-line crosses the curve in a number of points. Now, consider the domain \mathbb{C}/σ ; in this domain the primitive $\frac{1}{2\pi i} \log(z' - z)$ (as a function of z') is holomorphic. The integral for the index is now evaluated for the curve with points removed along the chosen cut: it is the difference of the primitive at points at the two ends of each piece of the curve. Each difference is ± 1 (because of the discontinuity $\pm 2\pi i$ of the log), with $+1$ when the crossing is anticlockwise, and -1 for a clockwise crossing:

$$\text{Ind}(\gamma, z) = \oint_{\gamma} \frac{dz'}{2\pi i} \frac{1}{z' - z} = N^+ - N^- \quad (7.12)$$

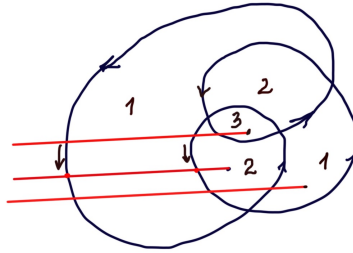


Figure 7.1 Indices of an oriented curve. To evaluate the index in a patch, fix a point in it, draw a half-line left from the point, and count the crossings from above (N_+) and from below (N_-). The index in the patch is $N_+ - N_-$.

where N^+ and N^- are the numbers of anticlockwise and clockwise turns of γ around z .

7.5.3 2D Gauss theorem and Index function*

Consider a 2D electrostatic field $\mathbf{E}(\mathbf{x}) = E_x \mathbf{i} + E_y \mathbf{j}$. The integral on a curve γ of $\bar{E}(z) = E_x - iE_y$ is⁴:

$$\begin{aligned} \int_{\gamma} \bar{E}(z) dz &= \int_a^b dt (\dot{x} + i\dot{y})(E_x - iE_y) \\ &= \int_a^b dt (E_x \dot{x} + E_y \dot{y}) + i(E_x \dot{y} - E_y \dot{x}) \\ &= \int_{\gamma} \mathbf{E}(\mathbf{x}) \cdot d\boldsymbol{\ell} + i \int_{\gamma} \mathbf{E}(\mathbf{x}) \cdot \mathbf{n} d\ell \end{aligned} \quad (7.13)$$

The real part is the work done by the electric field, the imaginary part is the flux of \mathbf{E} through the curve, \mathbf{n} is the vector normal to the curve.

Suppose that γ joins a to b in a domain where a complex potential Φ is holomorphic. Since $\bar{E} = -d\Phi/dz$, l.h.s. integral is $-\Phi(b) + \Phi(a)$: the work and the flux are independent of the curve joining fixed end-points a and b .

If the curve is closed, both work and flux are zero (no net charge is encircled).

Now a different situation: the closed curve encircles point-charges Q_i at z_i . The complex potential is

$$\Phi(z) = -\frac{1}{2\pi\epsilon_0} \sum_i Q_i \log(z - z_i).$$

⁴ the components of the tangent and normal vectors are the real and imaginary parts of $\dot{\gamma} = \dot{x} + i\dot{y}$ and $i\dot{\gamma} = -\dot{y} + i\dot{x}$. The normalization factor is $|\dot{\gamma}| = \sqrt{\dot{x}^2 + \dot{y}^2}$.

It is holomorphic except for cuts joining each z_i to ∞ . Such discontinuities affect the imaginary part of the integral, while the real part of the integral (7.13) remains zero, i.e. the work done by the field on a closed line is always zero. The evaluation of the integral gives an imaginary result (the flux):

$$\oint_{\gamma} dz \bar{E}(z) = - \oint_{\gamma} dz \frac{d\Phi}{dz} = \frac{1}{2\pi\epsilon_0} \sum_j Q_j \oint_{\gamma} \frac{dz}{z - z_j} = \frac{i}{\epsilon_0} \sum_j Q_j \text{Ind}(\gamma, z_j)$$

Therefore $\int_{\gamma} \mathbf{E}(\mathbf{x}) \cdot \mathbf{n} d\ell = \frac{1}{\epsilon_0} \sum_j Q_j \text{Ind}(\gamma, z_j)$. For a simple curve $\text{Ind}(\gamma, z_j) = 0, 1$. The result is the Gauss theorem: the flux of the electric field through a closed curve is proportional to the total charge encircled.

Chapter 8

Cauchy Theorems for Rectangles

The fundamental theorem that the integral on a closed curve of a holomorphic function is zero was proven by Cauchy with the requirement that f' is continuous (1825). In 1884 Edouard Goursat offered a proof *which seems to me a little simpler than the usual proofs. It relies only on the definition of the derivative and on the remark that the definite integrals $\int dz$ and $\int zdz$, taken along any closed contour, are equal to zero*¹. Years later, in 1900, he realized that continuity of f' is unnecessary. The proof given below is based on his ideas.

The theorem allows to construct a primitive of f and extend the validity to arbitrary closed paths in a rectangular domain where the function is holomorphic. The Cauchy integral formula follows.

For entire functions the results hold everywhere in \mathbb{C} .

8.1 The integral on a rectangle

Theorem 8.1.1. *If f is holomorphic on a domain, and R is a rectangular region in the domain, with boundary ∂R :*

$$\oint_{\partial R} dz f(z) = 0 \tag{8.1}$$

Proof. Let L be the length of the diagonal of R , and choose an orientation of the boundary. Halve the sides of R and obtain four rectangles R_{1k} (the index 1 stands for generation, $k = 1..4$); let $I(R_{1k})$ be the values of the integrals on the oriented boundaries of the rectangles. It is $I(R) = \sum_{k=1}^4 I(R_{1k})$ because integrals on shared sides (they have opposite orientations) cancel. Denote I_1 the integral with largest modulus among the four, and R_1 the corresponding rectangle. Then $|I(R)| \leq \sum_k |I(R_{1k})| \leq 4|I_1|$.

Now repeat with R_1 : a partition of R_1 into four rectangles R_{2k} gives $I_1 = \sum_{k=1}^4 I(R_{2k})$. Select

¹ Goursat, E. Démonstration du théorème de Cauchy. Acta Math. 4, 197–200 (1884), <https://link.springer.com/article/10.1007/BF02418419>

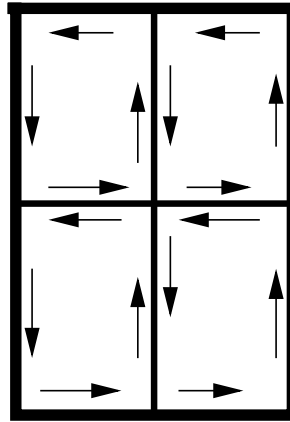


Figure 8.1 The integral on a rectangular path is the sum of four integrals on smaller rectangles; the contributions of oppositely oriented sides cancel.

the rectangle R_{2k} with largest value $|I(R_{2k})|$, and let I_2 be the value of such integral, and R_2 the rectangle. It is $|I(R)| \leq 4^2 |I_2|$.

By iterating the process, a sequence of rectangles $R_1 \supset R_2 \supset \dots \supset R_n \supset \dots$ is selected. At generation n :

$$|I(R)| \leq 4^n |I_n|$$

The middle points of the rectangles form a sequence whose limit point a belongs to the intersection of all the rectangles in the sequence.

Since $f(z)$ is holomorphic, it is true that given $\epsilon > 0$, there exists δ such that

$$\frac{f(z) - f(a)}{z - a} = f'(a) + r(z, a)$$

with remainder $|r(z, a)| < \epsilon$ for all z such that $|z - a| < \delta$.

In R_n two points have separation at most $L/2^n$, therefore a rephrasing is: $\forall \epsilon \exists n$ (generation) such that $f(z) = f(a) + f'(a)(z - a) + r(z, a)(z - a)$ where $|r(z, a)| < \epsilon$ for all $z \in R_n$. This gives the estimate:

$$\begin{aligned} |I_n| &= \left| \oint_{\partial R_n} dz [f(a) + f'(a)(z - a) + r(z, a)(z - a)] \right| \\ &= \left| \oint_{\partial R_n} dz r(z, a)(z - a) \right| \leq \epsilon \times \text{perimeter of } R_n \times \sup_{z \in \partial R_n} |z - a| \\ &< \epsilon \frac{4L}{2^n} \frac{L}{2^n} \end{aligned}$$

Note that $\int_{\partial R} dz[f(a) + f'(a)(z-a)] = 0$ as a primitive exists. Since $|I(R)| \leq 4\epsilon L^2$ for arbitrary ϵ , it is $I(R) = 0$. \square

The hypothesis of the theorem can be weakened to allow for a function that is holomorphic up to a point (or a finite collection of points) in the domain, where the function remains continuous. This will be useful to prove the Cauchy integral formula.

Proposition 8.1.2. *Let $f(z)$ be a function that is continuous on a domain D and holomorphic on $D \setminus \{a\}$. Then $\oint_{\partial R} dz f(z) = 0$ for any rectangle R in D .*

Proof. If $a \notin R$ Theorem 8.1.1 holds. If $a \in R$ decompose R as $R_a \cup R_1 \cup \dots \cup R_k$ where R_a is a square with side ϵ that contains a (an interior or a boundary point of R), and $R_1 \dots R_k$ are rectangles that complete the partition. The contour integral is $I(R) = I(R_a) + \sum_i I(R_i)$. The integrals $I(R_i)$ are zero by Theorem 8.1.1. Since $|f(z)| < M$ on R (because f is continuous on the compact set R), Darboux's inequality gives $|I(R)| = |I(R_a)| \leq (4\epsilon)M$. \square

Example 8.1.3 (Fourier transform of the Gaussian).

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2 - ikx} = \frac{1}{\sqrt{2}} e^{-\frac{1}{4}k^2}, \quad k \in \mathbb{R} \quad (8.2)$$

Proof: consider the integral $\oint_{\partial R} dz e^{-z^2}$ on the rectangle with corners $-a, b, b + i(k/2)$ and $-a + i(k/2)$ ($a, b > 0$). The integral is zero because the function is entire. The same integral is the sum of four integrals evaluated on the sides:

$$0 = \int_{-a}^b dx e^{-x^2} + i \int_0^{\frac{k}{2}} dy e^{-(b+iy)^2} - \int_{-a}^b dx e^{-(x+\frac{1}{2}ik)^2} - i \int_0^{\frac{k}{2}} dy e^{-(-a+iy)^2}$$

For $a, b \rightarrow \infty$, the integrals in y vanish, and the value of the first integral is $\sqrt{\pi}$.

Exercise 8.1.4. *Prove the useful integral:*

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-x^2 - xz} = e^{\frac{1}{4}z^2}, \quad z \in \mathbb{C}. \quad (8.3)$$

Exercise 8.1.5. *Evaluate the moments of the Gaussian distribution:*

$$\langle x^{2n} \rangle = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} dx x^{2n} e^{-\frac{x^2}{2\sigma^2}} = \frac{(2n)!}{2^n n!} \sigma^{2n} \quad (8.4)$$

Hint: expand in powers of k both sides of eq.(8.2). The coefficient $(2n)!/(2^n n!)$ is often written $(2n-1)!! = (2n-1)(2n-3)\dots 1$.

8.2 Cauchy theorem in rectangular domains

A consequence of the theorem for rectangles is that a primitive F can be explicitly constructed inside a rectangular domain R where f is holomorphic (up to a finite number of points where it remains continuous). It is built as the integral of f along a curve joining a fixed reference point in R to z .

Without loss of generality, we may assume that the rectangle has sides parallel to the axes and contains the origin. If $z = x + iy$ the curve is $[0, x] \cup [x, x + iy]$ and

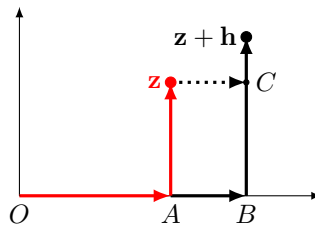
$$F(z) = \int_0^x dx' f(x') + i \int_0^y dy' f(x + iy')$$

Proposition 8.2.1. $F(z)$ is holomorphic and $F'(z) = f(z)$ for all $z \in R$.

Proof. Fix z and let $h = h_x + ih_y$; because of theorem 8.1.1, it is

$$\begin{aligned} F(z+h) &= \int_0^{x+h_x} dx' f(x') + i \int_0^{y+h_y} dy' f(x+h_x + iy') \\ &= F(z) + \int_x^{x+h_x} dx' f(x' + iy) + i \int_y^{y+h_y} dy' f(x+h_x + iy') \\ &= F(z) + \int_\gamma d\zeta f(\zeta) \end{aligned}$$

where the path γ is made of two segments at right angles: $[z, z+h_x] \cup [z+h_x, z+h]$. Divide by h and subtract $f(z)$ from both sides. Note that $\int_\gamma d\zeta = h$.



The integral on $A - B - C$ equals the integral $A - z - C$.

Then:

$$\frac{F(z+h) - F(z)}{h} - f(z) = \frac{1}{h} \int_\gamma d\zeta [f(\zeta) - f(z)]$$

By Darboux's inequality:

$$\left| \frac{F(z+h) - F(z)}{h} - f(z) \right| \leq \sup_{z \in \gamma} |f(z) - f(\zeta)| \frac{|h_x| + |h_y|}{|h|} \leq 2 \sup_{z \in \gamma} |f(z) - f(\zeta)|$$

Since f is continuous in z , the limit $h \rightarrow 0$ of the r.h.s. is zero. Then F' exists (i.e. F is holomorphic) in R and $F' = f$. \square

With a primitive available in R , by Theorem 7.3.3, we conclude that the integral of f on any closed (piecewise) smooth path in the rectangle R is zero²:

$$\oint_{\gamma} dz f(z) = 0 \quad (8.5)$$

If f is entire, this is true for any closed curve in \mathbb{C} .

Exercise 8.2.2 (Fresnel integrals). *Obtain the useful integrals:*

$$\int_0^{\infty} dx \cos(x^2) = \int_0^{\infty} dx \sin(x^2) = \frac{\sqrt{2\pi}}{4}$$

Hint: consider the integral $0 = \oint_{\mathcal{C}} dz e^{iz^2}$ on the closed path with sides $[0, R]$, $[0, Re^{i\pi/4}]$ and the circular arc $\{Re^{i\theta}, 0 \leq \theta \leq \pi/4\}$. For $R \rightarrow \infty$ the integral on the arc is zero (use the inequality $\sin \theta \geq 2\theta/\pi$ valid for $0 \leq \theta \leq \pi/2$. See Fig.14.2).

8.3 Cauchy integral formula

Theorem 8.3.1 (Cauchy's integral formula). *If f is a holomorphic function on a rectangle R , γ is a (piecewise) smooth closed curve in R and $a \in R \setminus \gamma$, then*

$$\oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - a} = f(a) \text{Ind}(\gamma, a), \quad a \notin \gamma \quad (8.6)$$

Proof. Consider the function

$$g(\zeta) = \begin{cases} \frac{f(\zeta) - f(a)}{\zeta - a} & \zeta \neq a, \\ f'(a) & \zeta = a. \end{cases}$$

² This property was known to Gauss, who announced it in a letter to Bessel in 1811 [Boyer]. Gauss refrained from publishing several results he obtained, if not fully developed. His motto was *pauca sed matura*.

g is continuous on R and holomorphic in $R/\{a\}$. Cauchy's theorem on rectangles holds (a may belong to the boundary), and enables the introduction of a primitive in $R/\{a\}$. Therefore the integral of g on a closed path is zero:

$$0 = \oint_{\gamma} d\zeta g(\zeta) = \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - a} - f(a) \text{Ind}(\gamma, a)$$

□

The Cauchy integral formula is remarkable: it shows that the values of a function holomorphic on a bounded region are determined by the values *at the boundary* of the region! It also shows that the Cauchy *transform* on a closed path of a holomorphic function coincides with the function itself, times the Index function. Since we proved that the Cauchy transform of a continuous function is holomorphic on \mathbb{C}/γ , the following important theorem follows:

Theorem 8.3.2. *The derivative f' of a function f holomorphic on a rectangle R , is holomorphic on R , as well as all derivatives $f^{(n)}$, and*

$$\frac{1}{n!} \text{Ind}(\gamma, z) f^{(n)}(z) = \oint_{\gamma} \frac{dz'}{2\pi i} \frac{f(z')}{(z' - z)^{n+1}}, \quad z \in R/\gamma \quad (8.7)$$

Theorem 8.3.3 (Morera³). *If the Cauchy integral of a continuous function f vanishes for all rectangular paths in R , then f is holomorphic on R .*

Proof. The property of vanishing integral on all rectangular paths implies that a primitive exists (recall that in proving Prop.8.2.1 the ingredients were continuity for the existence of integrals, and zero integral around rectangles), i.e. a function F holomorphic on R such that $F'(z) = f(z)$ for all $z \in R$. Being F holomorphic, also F' is holomorphic, i.e. f is holomorphic. □

Proposition 8.3.4 (Mean value theorem). *$f(z)$ is the mean value of f on any circle in the rectangle, centred in z :*

$$f(z) = \int_0^{2\pi} \frac{d\theta}{2\pi} f(z + re^{i\theta}) \quad (8.8)$$

Proof. Apply Cauchy's formula to a circle with center z and radius r . □

³ Giacinto Morera (1856, 1907).

Example 8.3.5. Let γ be the ellipse $|z - 1| + |z + 1| = 4$, consider the integral

$$\oint_{\gamma} dz \frac{e^{\pi z}}{2z - 3i}$$

The point $\frac{3}{2}i$ is in the ellipse, therefore the integral is $\frac{2\pi i}{2} e^{\pi(3i/2)} = \pi$.

Exercise 8.3.6. Let γ be the circle $|z| = 3$. Show that

$$\oint_{\gamma} dz \frac{\sin z}{z^2 - 3z + 2} = 2\pi i (\sin 2 - \sin 1)$$

Chapter 9

Entire Functions

Entire functions are holomorphic on the whole complex plane. Polynomials and the exponential are entire functions. An entire function admits primitives which are entire functions, and can be differentiated indefinitely.

9.1 Liouville theorem

The mean value theorem eq. (8.8) implies the inequality

$$|f(z)| \leq \sup_{\theta \in [0, 2\pi]} |f(z + re^{i\theta})|$$

for any radius r of circles centred on z . This means that $|f(z)|$ has no peaks. Indeed, the following remarkable theorem holds:

Theorem 9.1.1 (Liouville theorem). *If $f(z)$ is an entire function and $|f(z)| \leq M$ for all $z \in \mathbb{C}$, then $f(z)$ is constant.*

Proof. Given a point z and a circle C with center 0 and radius $R > |z|$, the Cauchy integral formula gives:

$$f(z) - f(0) = \oint_C \frac{d\zeta}{2\pi i} f(\zeta) \left[\frac{1}{\zeta - z} - \frac{1}{\zeta} \right] = \oint_C \frac{d\zeta}{2\pi i} \frac{zf(\zeta)}{(\zeta - z)\zeta} = z \int_0^{2\pi} \frac{d\theta}{2\pi} \frac{f(Re^{i\theta})}{Re^{i\theta} - z}$$

In the inequality

$$|f(z) - f(0)| \leq |z| \int_0^{2\pi} \frac{d\theta}{2\pi} \left| \frac{f(Re^{i\theta})}{Re^{i\theta} - z} \right| \leq |z| M \max_{\theta} \frac{1}{|Re^{i\theta} - z|} = M \frac{|z|}{R - |z|}.$$

R can be arbitrarily large, then $f(z) - f(0) = 0$ for all z , i.e. $f(z)$ is constant. □

In the proof, the boundedness of f is needed only on the circle C . This leads to several generalizations, like this one:

Corollary 9.1.2. *If $f(z)$ is entire and $\lim_{z \rightarrow \infty} |f(z)| = 0$, then $f(z) = 0$.*

Proof. By hypothesis: $\forall \epsilon > 0 \exists R_\epsilon$ such that $|f(z)| < \epsilon$ if $|z| > R_\epsilon$. Then for $R > R_\epsilon$ the Darboux inequality in the Cauchy formula gives $|f(z)| \leq \epsilon R / (R - |z|)$. \square

If f is entire and $f(z) - (az + b) \rightarrow 0$ for $|z| \rightarrow \infty$, then $f(z) = az + b$. More generally, if $f(z) - z^n \rightarrow 0$ at infinity, then $f(z)$ is a polynomial of degree n .

Exercise 9.1.3. *If f is entire and $\text{Im} f \geq 0$ for all z , then f is constant.*

Hint: consider $\exp(if)$.

9.2 Polynomials

Theorem 9.2.1 (The fundamental theorem of algebra). *A polynomial of order greater than zero has a zero.*

Proof. Suppose that a polynomial $p(z)$ of order greater than zero has no zeros. Then $1/p(z)$ is entire and vanishes for $z \rightarrow \infty$. By Cor.9.1.2 one gets the absurd result $1/p(z) = 0$ everywhere. \square

The theorem implies that a polynomial of degree n with complex coefficients has exactly n zeros z_1, \dots, z_n in \mathbb{C} .

Let the coefficient of the leading power be $a_0 = 1$ (monic polynomial):

$$\begin{aligned} p(z) &= z^n + a_1 z^{n-1} + \dots + a_n \\ &= (z - z_1)(z - z_2) \cdots (z - z_n). \end{aligned}$$

The two representations give useful relations among roots and coefficients:

$$\begin{aligned} \sigma_1 &= z_1 + z_2 + \dots + z_n = -a_1 \\ \sigma_2 &= z_1 z_2 + z_1 z_3 + \dots + z_{n-1} z_n = a_2 \\ &\dots \\ \sigma_n &= z_1 z_2 \cdots z_n = (-1)^n a_n. \end{aligned}$$

The quantities σ_k are the elementary symmetric polynomials of z_1, \dots, z_n . They are related to the sums $s_p = z_1^p + \dots + z_n^p$ by *Newton's identities* ($s_1 = \sigma_1$, $s_2 = \sigma_1^2 - 2\sigma_2$, etc.)

Exercise 9.2.2. Prove the useful identity for polynomials with simple roots

$$\boxed{\frac{1}{p(z)} = \sum_{k=1}^n \frac{1}{p'(z_k)} \frac{1}{z - z_k}} \quad (9.1)$$

Exercise 9.2.3. By expanding (9.1) in powers of $1/z$ and equating coefficients, obtain the identities for the roots:

$$0 = \sum_{k=1}^n \frac{z_k^\ell}{p'(z_k)} \quad (\ell = 0, \dots, n-2), \quad 1 = \sum_{k=1}^n \frac{z_k^{n-1}}{p'(z_k)}, \quad -a_1 = \sum_{k=0}^n \frac{z_k^n}{p'(z_k)}, \quad \dots \quad (9.2)$$

Exercise 9.2.4. Prove the useful formula, $n \geq m \geq 0$:

$$\oint_C \frac{dz}{2\pi i} \frac{(1+z)^n}{z^{m+1}} = \binom{n}{m} \quad (9.3)$$

where C is a Jordan curve around the origin. Next, prove

$$\sum_{n=m}^N \binom{N}{n} \binom{n}{m} = 2^{N-m} \binom{N}{m}$$

Exercise 9.2.5. If $f(z)$ is an entire function and γ is a simple closed path enclosing the points $z = 0, 1, \dots, n$ show that:

$$\oint_{\gamma} \frac{dz}{2\pi i} \frac{f(z)}{z(z-1)\cdots(z-n)} = \frac{(-1)^n}{n!} \sum_{k=0}^n (-1)^k \binom{n}{k} f(k)$$

Exercise 9.2.6. Let the simple closed path γ contain the unit disk and let $f(z)$ be an entire function; show that:

$$\oint_{\gamma} \frac{dz}{2\pi i} \frac{f(z)}{z^n - 1} = \frac{1}{n} \sum_{k=1}^n \omega^k f(\omega^k), \quad \omega = \exp\left(i \frac{2\pi}{n}\right)$$

9.2.1 Miscellanea*

Given a monic polynomial of order n with distinct zeros, the set $\{z : |p_n(z)| = C\}$ is a *lemniscate*. For $C = 0$ it consists of n points (the roots). By increasing C the lemniscate evolves from n distinct ovals encircling the roots, to ovals that merge into fewer closed lines.

• Borwein (1995): the length of the lemniscate $|p_n(z)| = 1$ is not greater than Kn , where $K \leq 8\pi e$. The result was improved to $K \leq 9.173$ (Eremenko and Hayman, 1999).

• Cartan: for a monic polynomial p_n the inequality $|p_n(z)| > (R/e)^n$ holds outside at most n circular disks, the sum of the radii being at most $2R$.

• Polya: For a monic polynomial, let $S = \{z : |p_n(z)| \leq 2\}$. Consider the projection of S on any line L in the complex plane (one or more segments). The total length of the segments never exceeds 4 (this and other statements are found in the delightful book by M. Aigner and G. Ziegler, *Proofs from THE BOOK*, Springer).

Theorems for the location of the zeros will be given in Sect.(14.4).

Exercise 9.2.7. *If the roots are simple, show that:*

$$\frac{p''(z_k)}{p'(z_k)} = \sum_{j \neq k} \frac{2}{z_k - z_j}, \quad \prod_k p'(z_k) = (-1)^{\frac{1}{2}n(n-1)} \prod_{i>j} (z_i - z_j)^2. \quad (9.4)$$

Exercise 9.2.8. *Prove the relations, valid for general polynomials:*

$$\frac{p'(z)}{p(z)} = \sum_{k=1}^n \frac{1}{z - z_k}, \quad \frac{p'(z)^2 - p''(z)p(z)}{p(z)^2} = \sum_{k=1}^n \frac{1}{(z - z_k)^2}$$

Exercise 9.2.9. *Let $p_k(z)$ be monic polynomials of degree $k = 1, \dots, n-1$. Show that:*

$$\det \begin{bmatrix} 1 & p_1(z_1) & \cdots & p_{n-1}(z_1) \\ 1 & p_1(z_2) & \cdots & p_{n-1}(z_2) \\ \vdots & \vdots & & \vdots \\ 1 & p_1(z_n) & \cdots & p_{n-1}(z_n) \end{bmatrix} = \det \begin{bmatrix} 1 & z_1 & \cdots & z_1^{n-1} \\ 1 & z_2 & \cdots & z_2^{n-1} \\ \vdots & \vdots & & \vdots \\ 1 & z_n & \cdots & z_n^{n-1} \end{bmatrix} = \prod_{i>j} (z_i - z_j)$$

The second matrix is the Vandermonde matrix, which is an important tool in linear algebra, matrix theory, and polynomial interpolation.

9.3 Picard's Little Theorem*

The function $f(z) = z$ is entire and takes all complex values; the exponential function is entire and takes all complex values but one, the value zero. Is there a non-constant entire function that avoids two values? The answer is no:

Theorem 9.3.1 (Picard's little theorem¹). *Let f be an entire function and a and b two distinct complex values such that, for all z , $f(z) \neq a$ and $f(z) \neq b$. Then $f(z)$ is constant.*

A sharpened version (Picard's great theorem) states that every transcendental entire function f assumes every complex number *infinitely many times* with at most one exception².

¹ Charles E. Picard (1856, 1941).

² See R. Remmert, *Classical topics in complex analysis*, GTM 172, Springer 1998. A function is transcendental if it's not algebraic. A function $\omega(z)$ is algebraic if it solves an equation $P(z, \omega) = 0$ where P is a polynomial both in z and ω .

Chapter 10

Cauchy Theorem and Integral Formula

The extension of Cauchy's theory from rectangular domains to general ones requires care. If f is holomorphic on D and has singularities in \mathbb{C}/D , a closed curve in D may encircle them. In 1971 Dixon gave a proof of Cauchy's theorem and integral formula that solves the topological problem with the index function¹.

Theorem 10.0.2 (Dixon). *Let γ be a piecewise smooth closed path in a domain D such that $\text{Ind}(\gamma, z) = 0 \forall z \notin D$. If f is holomorphic on D and $z \in D \setminus \gamma$:*

$$\text{Ind}(\gamma, z) f(z) = \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} \quad (\text{Cauchy integral formula}) \quad (10.1)$$

$$0 = \oint_{\gamma} d\zeta f(\zeta) \quad (\text{Cauchy theorem}) \quad (10.2)$$

Proof. We first prove Cauchy's integral formula (10.1). Consider the function $g : D \times D \rightarrow \mathbb{C}$

$$g(\zeta, z) = \begin{cases} \frac{f(\zeta) - f(z)}{\zeta - z} & \zeta \neq z \\ f'(\zeta) & \zeta = z \end{cases}$$

g is continuous and holomorphic in each variable.

¹ John D. Dixon, *A brief proof of Cauchy's integral theorem*, Proc. Am. Math. Soc. 29 n.3 (1971) 625-26 (<https://www-users.cse.umn.edu/~brubaker/docs/8701-F13/dixon.pdf>). See the textbook S. Lang, *Complex Analysis*, Springer.

Define the set $E = \{z \in \mathbb{C}, \text{Ind}(\gamma, z)\} = 0$. It is $D \cup E = \mathbb{C}$.

The following function exists $\forall z \in \mathbb{C}$:

$$h(z) = \begin{cases} \oint_{\gamma} \frac{d\zeta}{2\pi i} g(\zeta, z) & \text{if } z \in D \\ \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} & \text{if } z \in E \end{cases} \quad (10.3)$$

For $z \in E$ the function $h(z)$ is a Cauchy transform, hence it is holomorphic on E and vanishes as $|z| \rightarrow \infty$.

For $z \in D$ the function $h(z)$ is holomorphic (proof omitted). In particular for $z \in D/\gamma$ it is

$$h(z) = \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} - f(z)\text{Ind}(\gamma, z).$$

Then on the intersection of D and E the two definitions coincide, and h is entire.

By Liouville's theorem (Cor. 9.1.2), it is $h(z) = 0$ on \mathbb{C} , and (10.1) is proven.

To obtain (10.2), choose $a \in D/\gamma$ and apply (10.1) to the function $(z - a)f(z)$:

$$\text{Ind}(\gamma, z) (z - a)f(z) = \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{\zeta - a}{\zeta - z} f(\zeta).$$

Now let $z = a$ and Cauchy's theorem follows. □

Corollary 10.0.3. *A holomorphic function can be differentiated indefinitely on its domain.*

Exercise 10.0.4. *Use Cauchy's formula to evaluate the integral (Hint: $z = e^{i\theta}$):*

$$\int_0^{2\pi} d\theta \frac{1}{1 - 2x \cos \theta + x^2} = \frac{2\pi}{1 - x^2}, \quad 0 \leq x < 1. \quad (10.4)$$

Chapter 11

Power Series

11.1 Uniform convergence

We consider sequences of functions $f_n : E \rightarrow \mathbb{C}$, where E is some abstract set. At each point $P \in E$ there is a complex sequence $f_n(P)$, whose convergence is assessed by Cauchy's criterion.

• **Pointwise convergence on E .** Suppose that $\forall P \in E$ the sequence $f_n(P)$ converges to a finite complex number. The set of limit values defines a function $f : E \rightarrow \mathbb{C}$, and we say that $f_n \rightarrow f$ pointwise on E .

Since \mathbb{C} is complete, we only need Cauchy's criterion for convergence:

$$\forall P \in E \quad \forall \epsilon > 0 \quad \exists N_{\epsilon, P} \text{ such that } |f_n(P) - f_m(P)| < \epsilon \quad \forall m, n > N_{\epsilon, P}$$

• **Uniform convergence on E .** Suppose that the stronger condition holds: $\forall P \in E$ the sequence $f_n(P)$ is Cauchy with N_ϵ independent of P . Then f_n converges on E , and the distance $|f_n(P) - f_m(P)|$ is bounded on E by the same ϵ for all $P \in E$, $n, m > N_\epsilon$. We say that $f_n \rightarrow f$ uniformly on E :

$$\forall \epsilon > 0 \quad \exists N_\epsilon \text{ such that } |f_n(P) - f_m(P)| < \epsilon \quad \forall m, n > N_\epsilon, \quad \forall P \in E.$$

Definition 11.1.1. A series of functions $\sum_k f_k$ is uniformly convergent on E if the sequence of partial sums is uniformly convergent on E :

$$\forall \epsilon > 0 \quad \exists N_\epsilon : \left| \sum_{k=m+1}^{m+n} f_k(P) \right| < \epsilon \quad \forall m > N_\epsilon, \quad \forall n > 0, \quad \forall P \in E. \quad (11.1)$$

Theorem 11.1.2 (Weierstrass M-criterion). *If there are positive constants M_k such that $|f_k(P)| < M_k$ for all $P \in E$ and $\sum_k M_k$ is finite, then the series $\sum_k f_k$ is uniformly convergent on E .*

Proof. Let $S_m(P)$ be the sequence of partial sums. For all $P \in E$:

$$|S_{m+n}(P) - S_m(P)| \leq \sum_{k=m+1}^{m+n} |f_k(P)| \leq \sum_{k=m+1}^{m+n} M_k < \epsilon$$

for m large enough and all n , because the M -series converges. □

From now on, E is a set in \mathbb{C} .

Proposition 11.1.3. *The geometric series $\sum_k z^k$ is uniformly convergent on the closed disk $|z| \leq 1 - \eta$, $\eta > 0$.*

Proof. Use the M -criterion with $M_k = (1 - \eta)^k$. □

Uniform convergence of a series guarantees that integration can be made term by term:

Theorem 11.1.4 (Integral of series). *Given a piecewise smooth curve γ and a sequence f_k of functions continuous on γ , if $\sum_k f_k$ is uniformly convergent on γ then:*

$$\int_{\gamma} dz \sum_{k=0}^{\infty} f_k(z) = \sum_{k=0}^{\infty} \int_{\gamma} dz f_k(z) \quad (11.2)$$

Proof. The partial sums $S_m(z)$ are continuous functions on γ which is a compact set, then uniform convergence implies that the limit series $S(z) = \sum_{k=0}^{\infty} f_k(z)$ is continuous on γ , and the integral exists. Uniform convergence on γ means that $|S_m(z) - S(z)| < \epsilon$ for all $m > N$ and for all $z \in \gamma$. Darboux's inequality shows that summation and integration commute:

$$\left| \sum_{k=0}^m \int_{\gamma} dz f_k(z) - \int_{\gamma} dz \sum_{k=0}^{\infty} f_k(z) \right| \leq \int_{\gamma} |dz| |S_m(z) - S(z)| < \epsilon L(\gamma). \quad \square$$

Since derivatives of holomorphic functions can be evaluated as Cauchy integrals, the theorem adds another important property:

Theorem 11.1.5 (Derivative of a series). *Let f_n be a sequence of holomorphic functions on a domain D . If $S = \sum_n f_n$ is uniformly convergent on D then S is holomorphic on D and $S' = \sum_k f_k'$.*

Proof. The function S , being a uniform limit of continuous partial sums S_n , is continuous on D . Then the integral of S on a curve in D exists. Since for any closed curve in D the integral of S_n vanishes for all n , by the previous theorem also the integral of S is zero. Therefore S is holomorphic by Morera's theorem.

The derivative of S in z is given by Cauchy's formula on a circle encircling z of radius δ :

$$S'(z) - \sum_{k=1}^N f'_k(z) = \oint_{\gamma} \frac{dz'}{2\pi i} \frac{S(z') - \sum_{k=1}^N f_k(z')}{(z' - z)^2}$$

Now take the modulus and use the Darboux inequality

$$\left| S'(z) - \sum_{k=1}^N f'_k(z) \right| \leq C \sup_{z \in \gamma} \left| S(z) - \sum_{k=1}^N f_k(z) \right| \rightarrow 0$$

for $N \rightarrow \infty$. The same holds for higher order derivatives. \square

In some cases the requirement of uniform convergence on a domain is too restrictive. Theorems 11.1.4 and 11.1.5 can be proven under the weaker hypothesis of local uniform convergence (normal convergence).

Definition 11.1.6. A sequence of functions f_n converges *normally* to f on a domain D if it converges pointwise to f on D and, for any $z \in D$, there is a *closed* disk centred in z where convergence is uniform.

Theorem 11.1.7 (Integral of series). *Given a piecewise smooth curve γ and a sequence of continuous functions f_k on γ , if the series $\sum_k f_k(z)$ is normally convergent on γ then*

$$\int_{\gamma} dz \sum_{k=0}^{\infty} f_k(z) = \sum_{k=0}^{\infty} \int_{\gamma} dz f_k(z) \quad (11.3)$$

Theorem 11.1.8. *If a sequence f_k is normally convergent to f on a domain D and all functions f_k are holomorphic, then f is holomorphic and the sequence of n -th derivatives $f_k^{(n)}$ converges to $f^{(n)}$ normally.*

Theorem 11.1.9 (Derivative of series). *If the series $\sum_k f_k$ is normally convergent on a domain D , and every term f_k is holomorphic on D , then the series is holomorphic on D . Moreover, the series can be differentiated term by term any number of times:*

$$\frac{d^n}{dz^n} \sum_{k=0}^{\infty} f_k(z) = \sum_{k=0}^{\infty} \frac{d^n f_k}{dz^n}(z), \quad n = 1, 2, \dots \quad (11.4)$$

for all $z \in D$, and each differentiated series is normally convergent.

11.2 Power series

A fundamental class of series of complex functions are power series:

$$f(z) = \sum_{n=0}^{\infty} c_n(z-a)^n \quad (11.5)$$

$a \in \mathbb{C}$ is the *center* of the power series, the coefficients c_n are complex numbers. Two notable examples are the geometric and exponential series. They converge absolutely, the first one in the open disk $|z| < 1$, the second one everywhere.

This is a fundamental theorem:

Theorem 11.2.1 (Abel, Weierstrass). *If the power series $\sum_k c_k(z-a)^k$ is convergent at a point z_0 , then the series converges:*

- 1) *absolutely for all z in the open disk $|z-a| < |z_0-a|$,*
- 2) *uniformly in the closed disk $|z-a| \leq (1-\eta)|z_0-a|$, $\eta > 0$.*

Proof. 1) Convergence of the series in z_0 implies that $|c_k(z_0-a)^k| \rightarrow 0$ for $k \rightarrow \infty$. Then there is N such that $|c_k(z_0-a)^k| < 1$ for all $k > N$. This means that $|c_k(z-a)^k|$ is majored by $|(z-a)/(z_0-a)|^k$ for all $k > N$. The sum of the latter terms converges (absolutely) for all z in the open disk $|z-a| < |z_0-a|$.

2) If $|z-a| \leq |z_0-a|(1-\eta)$ it follows that, for $k > N$, it is $|c_k(z-a)^k| \leq (1-\eta)^k$. Then convergence is uniform by the Weierstrass M-criterion. \square

The theorem shows that one out of three possibilities occurs:

- $z = a$ is the only point where the series converges.
- There are points $z \neq a$ where the series converges, but the series diverges at other points.
- The series converges everywhere in \mathbb{C} .

The Abel - Weierstrass theorem shows that convergence in z implies convergence in any open disk centred in a of radius $r < |z-a|$. Case two implies the existence of a radius R such that for $|z-a| < R$ the series converges absolutely (and uniformly in any closed disk strictly contained in it) and diverges in $|z-a| > R$. The value R is the **radius of convergence** of the series. If $R = \infty$ the series converges absolutely everywhere, and uniformly on any closed bounded set.

In general nothing can be said about the series on the boundary $|z-a| = R$ ¹.

We give an important formula for the radius R , which results from the sufficient criteria for absolute convergence of series.

¹ If the series converges at a point z_0 with $|z_0-a| = R$, a theorem by Abel proves that on the radius $\zeta(t) = a + (z_0-a)t$ ($t \in [0,1]$) the series $f(t) = \sum c_k(z_0-a)^k t^k$ converges uniformly with respect to t and $\lim_{t \rightarrow 1} f(t) = f(1)$.

Theorem 11.2.2 (Cauchy - Hadamard).

$$\boxed{\frac{1}{R} = \limsup_k \sqrt[k]{|c_k|}} \quad (11.6)$$

If $\lim_{k \rightarrow \infty} \sqrt[k]{|c_k|}$ exists, it is equal to $1/R$.

Example 11.2.3. In $\sum_{k=1}^{\infty} (2z)^{2k}$ odd powers are missing and the sequence $\sqrt[k]{c_n} = 2, 0, 2, 0, \dots$ is not convergent, but its lim sup is 2. Then the series converges in the disk $|z| < \frac{1}{2}$ (as a geometric series, it converges for $|4z^2| < 1$).

Exercise 11.2.4. Evaluate the radius of convergence of the series:

$$\sum_{k=1}^{\infty} \frac{z^k}{k}, \quad \sum_{k=0}^{\infty} \frac{z^{2k}}{(2k)!}, \quad \sum_{k=1}^{\infty} (-1)^k z^{3k}, \quad \sum_{k=0}^{\infty} z^{k^2}, \quad \sum_{k=0}^{\infty} k^2 z^k$$

Theorem 11.2.5. The power series

$$S(z) = \sum_{k=0}^{\infty} c_k (z-a)^k \quad \text{and} \quad S'(z) = \sum_{k=1}^{\infty} k c_k (z-a)^{k-1}$$

have the same radius of convergence.

Proof. In the proof we put $a = 0$. Suppose that S and S' have radii R and R' respectively. Since $|c_k z^k| < |z| |k c_k z^{k-1}|$ for all z , by the comparison test, the series S converges absolutely if S' does, i.e. $|z| < R'$ is a sufficient condition for S to absolutely converge. Then $R \geq R'$.

For z such that $|z| < R$ it is $k|z|^{k-1} < \frac{R^k}{R-|z|}$. Then it is $|k c_k z^{k-1}| < \frac{1}{R-|z|} |c_k R^k|$ and the series S' converges absolutely if S does, i.e. $R \leq R'$.

We used the inequality $\frac{1}{1-r} > 1 + r + \dots + r^{n-1} > nr^{n-1}$, $0 \leq r < 1$. □

Corollary 11.2.6. A power series $\sum_n c_n (z-a)^n$ is a holomorphic function on the open disk of convergence (where it is also infinitely many times differentiable).

Exercise 11.2.7. Evaluate $\sum_{n=1}^{\infty} n^2 z^n$ (Note that $z \frac{d}{dz} z^n = n z^n$).

Theorem 11.2.8 (Power series for holomorphic functions). Let f be holomorphic in a domain, and let D be an open disk centred in a of radius r in the domain, with (positively

oriented) boundary C . Then, for any z in the disk, f has the power series expansion

$$f(z) = \sum_{k=0}^{\infty} c_k (z-a)^k, \quad c_k = \oint_C \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta-a)^{k+1}} = \frac{1}{k!} f^{(k)}(a) \quad (11.7)$$

Proof. For any z in the disk $D(a, r)$, $f(z)$ is given by the Cauchy integral

$$f(z) = \oint_C \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta-z}.$$

Since $r = |\zeta - a| > |z - a|$, the kernel admits an expansion in geometric series

$$\frac{1}{\zeta-z} = \frac{1}{\zeta-a-(z-a)} = \sum_{k=0}^{\infty} \frac{(z-a)^k}{(\zeta-a)^{k+1}} \quad (11.8)$$

The sum can be taken out of the integral because the series converges uniformly in the interior of the disk. \square

Corollary 11.2.9. *A holomorphic function can be differentiated indefinitely and*

$$f^{(k)}(a) = k! \oint_{C(a,r)} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta-a)^{k+1}} \quad (11.9)$$

Darboux's inequality gives *Cauchy's Inequality*

$$|f^{(k)}(a)| \leq \frac{k!}{r^k} \sup_{\theta \in [0, 2\pi]} |f(a + re^{i\theta})| \quad (11.10)$$

Remark 11.2.10. *The radius of convergence of the power series centred in a of an analytic function is the largest admissible radius of a disk centred in a in the domain of analyticity: $R = |\xi - a|$ where ξ is the singular point nearest to a .*

Example 11.2.11. *The function $f(z) = [(z-2i)(z-3)]^{-1}$ is singular at $z = 2i$ and $z = 3$. A power expansion in the origin has radius 2. An expansion with center $a = 1$ has radius 2 because the singular point 3 has distance $|3-1| = 2$ smaller than the distance $|2i-1| = \sqrt{5}$ of the singular point $2i$.*

Exercise 11.2.12. *Integrate term by term the geometric series to obtain:*

$$\text{Log}(1-z) = - \sum_{k=1}^{\infty} \frac{z^k}{k} \quad |z| < 1 \quad (11.11)$$

Convergence is absolute. However, the series is also convergent on $|z| = 1$, $z \neq 1$. A theorem by Abel ensures that the value on the unit circle $\text{Log}(1 - e^{i\theta})$ coincides with the limit of the series as $|z| \rightarrow 1$ on the radius ending in $e^{i\theta}$.

Exercise 11.2.13. From the expansion (11.11) obtain:

$$\sum_{k=1}^{\infty} \frac{\rho^k}{k} \cos(k\theta) = -\frac{1}{2} \log(1 - 2\rho \cos\theta + \rho^2), \quad \rho < 1.$$

Note: If $\rho = 1$, $\theta \neq 0$ the series still converges: $\sum_{k=1}^{\infty} \frac{\cos(k\theta)}{k} = -\log\left(2\left|\sin\frac{\theta}{2}\right|\right)$.

Example 11.2.14. Evaluate the coefficients of the power series

$$\frac{e^{tz}}{1-z} = \sum_{n=0}^{\infty} c_n(t) z^n$$

It is convenient to compare the series $e^{tz} = (1-z) \sum_n c_n z^n = \sum_n z^n (c_n - c_{n-1})$, with $c_0 = 1$, $c_{-1} = 0$. This gives the recursive rule $c_n - c_{n-1} = t^n / n!$ i.e.

$$c_n(t) = 1 + t + \frac{t^2}{2!} + \dots + \frac{t^n}{n!}.$$

Example 11.2.15. Evaluate the coefficients of the power series

$$\frac{1}{z^2 + z - 1} = \sum_{n=0}^{\infty} c_n z^n$$

The radius of convergence of the series is dictated by the size of the smallest root of the binomial: $R = \frac{1}{2}(\sqrt{5} - 1)$. The quick way to obtain the coefficients is to write the l.h.s. as a combination of two geometric series. However, the following procedure is interesting.

Multiply the series by the denominator to get $1 = \sum_n z^n (c_{n-2} + c_{n-1} - c_n)$ i.e. $c_n = c_{n-1} + c_{n-2}$ and $c_0 = 1$ ($c_{-1} = 0$). The recursion generates the Fibonacci numbers 1, 1, 2, 3, 5, 8, 13, ... The general solution can be found: $c_n = ax_1^n + bx_2^n$, where $x_{1,2}$ solve the quadratic equation $x^2 - x - 1 = 0$ and a, b are specified by the initial conditions.

If x_1 is the root with largest modulus, Hadamard's criterion for the radius of the power series gives $1/R = |x_1|$, i.e. $R = |x_2|$ (note that $x_1 x_2 = 1$).

The recursion can be written $(c_n / c_{n-1}) = 1 + (c_{n-2} / c_{n-1})$. In the large n limit $c_n / c_{n-1} \rightarrow \phi$ and $\phi = 1 + 1/\phi$ (then, by the ratio criterion, $R = 1/\phi$). The number $\phi = \frac{1}{2}(\sqrt{5} + 1)$ is the golden mean, and is the limit of ratios of Fibonacci numbers. Its continued fraction expansion is peculiar, $\phi = 1 + 1/(1 + 1/(1 + 1/(1 + \dots)))$, and makes this number the "most irrational" one.

Example 11.2.16 (Euler numbers). They are the coefficients E_{2n} in the power series

$$\frac{1}{\cos z} = \sum_{n=0}^{\infty} (-1)^n E_{2n} \frac{z^{2n}}{(2n)!}$$

The radius of convergence of the series is $\pi/2$ (the pole closest to the origin). This gives us the estimate $|E_{2n}| \approx (2n)!(2/\pi)^{2n}$ (up to factors that grow less than powers of n)². Multiplication by $\cos z$ gives a Cauchy product of series:

$$1 = \sum_{k=0}^{\infty} z^{2k} \frac{(-1)^k}{(2k)!} \sum_{\ell=0}^k \binom{2k}{2\ell} E_{2\ell}$$

Comparison of powers in z gives, for the power $k = 0$: $E_0 = 1$. Higher powers are absent in the l.h.s. therefore:

$$\sum_{\ell=0}^k \binom{2k}{2\ell} E_{2\ell} = 0, \quad k \geq 1.$$

Example 11.2.17 (Bernoulli numbers). They are defined by the power series

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} B_n \frac{z^n}{n!}$$

The radius of convergence of the series is 2π . If we subtract the series evaluated at $-z$, we get $-z = 2 \sum_{\text{odd}} B_n z^n / n!$. Therefore $B_1 = -\frac{1}{2}$ and $B_{\text{odd} > 1} = 0$. Then the series can be rewritten as:

$$\frac{z}{2} \coth \frac{z}{2} = \sum_{n=0}^{\infty} B_{2n} \frac{z^{2n}}{(2n)!} \quad (11.12)$$

Multiplication by $\cosh(z/2)$ gives a Cauchy product of series, and recursive relations for the Bernoulli numbers³.

Exercise 11.2.18. Obtain the coefficients in

$$\sum_{n=1}^{\infty} H_n z^n = -\frac{\log(1-z)}{1-z}. \quad (11.13)$$

A: the coefficients $H_n = 1 + 1/2 + \dots + 1/n$ are named Harmonic numbers.

² the actual behaviour is: $|E_{2n}| \approx 2^{2n+2} (2n)! \pi^{-2n-1}$ (NIST Handbook of Mathematical Functions, Cambridge 2010).

³ The Bernoulli numbers were discovered almost at the same time in Japan by Seki Kowa (1640, 1708), the most eminent Wasan (Japanese calculator).

11.2.1 The binomial series

The function $(1 - z)^a$ is singular in $z = 1$ if a is a negative integer. If $a \notin \mathbb{Z}$ the function has a branch cut from infinity to $z = 1$. In any case the function is analytic in the unit disk, where it admits the power expansion:

$$(1 - z)^a = 1 - az + \frac{1}{2!}a(a-1)z^2 - \frac{1}{3!}a(a-1)(a-2)z^3 + \dots$$

The useful *Pochhammer's symbols* a_k are: $a_0 = 1$, $a_1 = a$,

$$a_k = a(a+1)\dots(a+k-1)$$

We then obtain:

$$(1 - z)^a = \sum_{k=0}^{\infty} (-a)_k \frac{z^k}{k!} \quad |z| < 1 \quad (11.14)$$

The sum truncates if a is a positive integer. The binomial symbol may be introduced, to recover the familiar Newton's expression:

$$\binom{a}{k} = \frac{(-1)^k}{k!} (-a)_k = \frac{a(a-1)\dots(a-k+1)}{k!}$$

Exercise 11.2.19. Show that

$$\frac{1}{(1 - z)^n} = \sum_{k=0}^{\infty} \binom{n+k-1}{k} z^k, \quad |z| < 1, \quad n = 1, 2, \dots \quad (11.15)$$

11.2.2 Polylogarithms*

Polylogarithms generalize the power series of the logarithm.

$$\text{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s} \quad |z| < 1 \quad (11.16)$$

For $\text{Re } s > 1$ it is $\text{Li}_s(1) = \zeta(s)$. Being uniformly convergent in the disk, derivation and integration of the series term by term give

$$z \frac{d}{dz} \text{Li}_s(z) = \text{Li}_{s-1}(z), \quad \text{Li}_{s+1}(z) = \int_0^z \frac{dz'}{z'} \text{Li}_s(z')$$

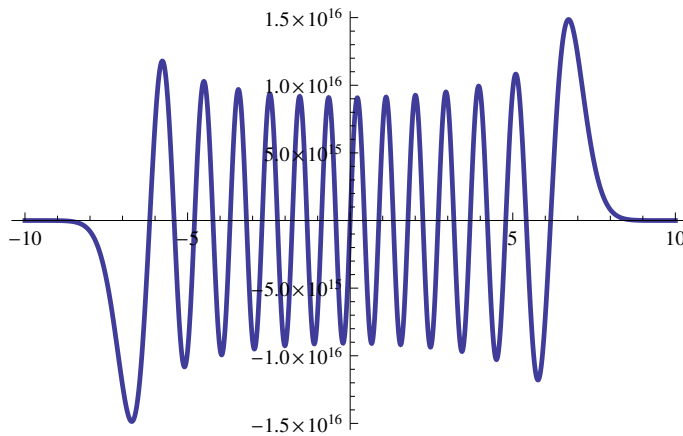


Figure 11.1 The Hermite polynomial $H_{25}(x)$ multiplied by $\exp(-x^2/2)$. Note the 25 real zeros and the wild oscillations in value.

With $\text{Li}_1(z) = -\log(1 - z)$, the dilogarithm is⁴

$$\text{Li}_2(z) = -\int_0^z \frac{dz'}{z'} \log(1 - z') = -\int_0^1 \frac{dt}{t} \log(1 - zt)$$

The integral is well defined for $\mathbb{C}/[1, \infty)$, and is an analytic continuation of the power series.

Exercise 11.2.20. Prove (using the series) the reflection rule:

$$\text{Li}_s(-z) = -\text{Li}_s(z) + 2^{1-s} \text{Li}_s(z^2).$$

With the integral expression, for real x , prove:

$$\text{Li}_2(x) = \frac{\pi^2}{6} - \log x \log(1 - x) - \text{Li}_2(1 - x), \quad (\text{Euler}).$$

11.3 Generating functions and polynomials

11.3.1 Hermite polynomials

The function $H(z, x) = e^{-z^2+2xz}$ is entire for any value $x \in \mathbb{R}$, and can be expanded in power series of z with center $z = 0$:

$$e^{-z^2+2xz} = \sum_{k=0}^{\infty} H_k(x) \frac{z^k}{k!} \tag{11.17}$$

⁴ <http://maths.dur.ac.uk/~dma0hg/dilog.pdf>

The coefficients are functions of x . It is instructive to evaluate them by the methods introduced so far, as contour integrals around the origin:

$$H_k(x) = k! \oint \frac{d\zeta}{2\pi i} \frac{H(\zeta, x)}{\zeta^{k+1}} = k! \sum_{\ell=0}^{\infty} \frac{(2x)^\ell}{\ell!} \oint \frac{d\zeta}{2\pi i} e^{-\zeta^2} \zeta^{\ell-k-1}$$

Since terms with $\ell \geq k+1$ vanish because of Cauchy's theorem for entire functions, $H_k(x)$ turns out to be a polynomial of degree k (Hermite polynomial). The evaluation can proceed further.

$$\begin{aligned} &= k! \sum_{\ell=0}^k \frac{(2x)^\ell}{\ell!} \oint \frac{d\zeta}{2\pi i} e^{-\zeta^2} \zeta^{\ell-k-1} = k! \sum_{\ell=0}^k \frac{(2x)^{k-\ell}}{(k-\ell)!} \oint \frac{d\zeta}{2\pi i} e^{-\zeta^2} \zeta^{-\ell-1} \\ &= k! \sum_{\ell=0}^{\lfloor k/2 \rfloor} \frac{(2x)^{k-2\ell}}{(k-2\ell)!} \oint \frac{d\zeta}{2\pi i} e^{-\zeta^2} \zeta^{-2\ell-1} \end{aligned}$$

where $\lfloor k/2 \rfloor$ is the integer part of $k/2$. The Cauchy integral is the coefficient of the term $z^{2\ell}$ of the power expansion of e^{-z^2} . The explicit expression of Hermite polynomials is obtained:

$$H_k(x) = k! \sum_{\ell=0}^{\lfloor k/2 \rfloor} \frac{(-1)^\ell}{\ell!(k-2\ell)!} (2x)^{k-2\ell} \quad (11.18)$$

$H(z, x)$ is the *generating function* of Hermite polynomials and encodes their analytic properties. We learn a lot from it with little effort:

1) the change z to $-z$ in (11.17) is compensated by x to $-x$, then Hermite polynomials have definite parity: $H_k(-x) = (-1)^k H_k(x)$.

2) the identities $\partial_x H(z, x) = 2zH(z, x)$ and $\partial_z H(z, x) = 2(-z+x)H(z, x)$, when translated to the power series expansion⁵, give the recurrence relations

$$H'_k(x) = 2k H_{k-1}(x), \quad H_{k+1}(x) = 2xH_k(x) - 2k H_{k-1}(x) \quad (11.19)$$

with initial conditions $H_0(x) = 1$ and $H_1(x) = 2x$ that can be obtained by direct expansion of $H(z, x)$.

3) the identity $(2z\partial_z - 2x\partial_x + \partial_x^2) H(z, x) = 0$ corresponds to the second order equation (which has another non-polynomial independent solution)

$$H''_k - 2xH'_k + 2kH_k = 0 \quad (11.20)$$

⁵ Derivation of the series term by term is possible because it is uniformly convergent both in z and x , in any compact set.

4) Hermite polynomials can be evaluated by Rodrigues' formula⁶:

$$\begin{aligned} H_k(x) &= \left[\frac{\partial^k}{\partial t^k} H(t, x) \right]_{t=0} = \left[e^{x^2} \frac{\partial^k}{\partial t^k} e^{-(t-x)^2} \right]_{t=0} \\ &= (-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2} \end{aligned} \quad (11.21)$$

5) The integral $\int_{-\infty}^{\infty} dx e^{-x^2} H_k(x) H_j(x)$ is symmetric in k and j . We evaluate it for $k \geq j$ by using Rodriguez's formula for $H_k(x)$, and doing k integration by parts:

$$\begin{aligned} \int_{-\infty}^{\infty} dx e^{-x^2} H_k(x) H_j(x) &= (-1)^k \int_{-\infty}^{\infty} dx H_j(x) \frac{d^k}{dx^k} e^{-x^2} \\ &= \int_{-\infty}^{\infty} dx e^{-x^2} \frac{d^k}{dx^k} H_j(x) = 2^k k! \sqrt{\pi} \delta_{jk} \end{aligned} \quad (11.22)$$

because $H_k(x) = 2^k x^k + \dots$ (use eq.11.19). This is the *orthogonality* property of Hermite polynomials.

The Cauchy product $H(z, x) H(z, y) = H(z\sqrt{2}, \frac{x+y}{\sqrt{2}})$ gives the summation formula (by equating the coefficients of equal powers of z):

$$\sum_{\ell=0}^k \binom{k}{\ell} H_{\ell}(x) H_{k-\ell}(y) = 2^{k/2} H_k\left(\frac{x+y}{\sqrt{2}}\right).$$

Exercise 11.3.1. Evaluate the Cauchy product of the exponential series for e^{-z^2} and e^{2tz} and obtain the absolutely convergent power series of the generating function (11.17).

There are several other generating functions whose power series expansion yield special functions that are important in mathematical physics⁷. Some examples are briefly presented below, some will be considered in the study of orthogonal polynomials (see Section 19.3).

⁶ Olinde Rodrigues (1795, 1851)

⁷ A beautiful little book on special functions is: N. N. Lebedev, *Special functions and their applications*, Dover Ed. A modern reference book is the *NIST Handbook of Mathematical Functions*, Cambridge Univ. Press, online at <https://dlmf.nist.gov>

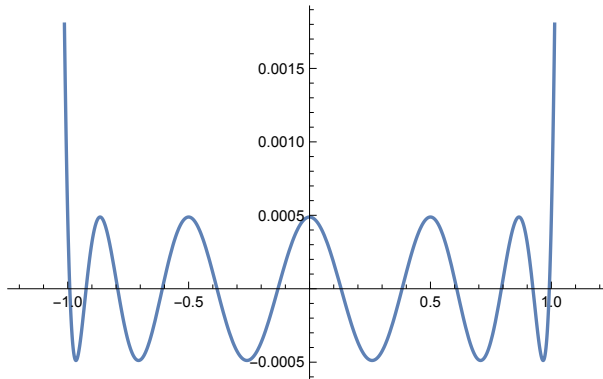


Figure 11.2 The monic polynomial $T_{12}(x)2^{-11}$. The 12 zeros are in $[-1, 1]$, where the polynomial is bounded by $1/2048$, and blows outside.

11.3.2 Chebyshev polynomials (of the first kind)

The power series expansion in $z = 0$ of $[(1 - ze^{i\theta})(1 - ze^{-i\theta})]^{-1}$ is easily done by means of the geometric series. It gives:

$$\frac{1 - z \cos \theta}{1 - 2z \cos \theta + z^2} = \sum_{k=0}^{\infty} z^k \cos(k\theta), \quad |z| < 1 \quad (11.23)$$

With $\cos \theta = x$, the identity becomes:

$$\frac{1 - xz}{1 - 2xz + z^2} = \sum_{k=0}^{\infty} z^k T_k(x), \quad |z| < 1 \quad (11.24)$$

where $T_k(x)$ are the Chebyshev polynomials 2.5.2. The identity $(1 - xz) = (1 - 2xz + z^2) \sum_{k=0}^{\infty} T_k(x)z^k$ gives $T_0(z) = 1$, $T_1(x) = x$ and the recurrence relation

$$0 = T_k(x) - 2xT_{k-1}(x) + T_{k-2}(x).$$

The k roots of $T_k(x)$ are real and in the interval $[-1, 1]$. On this interval $|T_k(x)| \leq 1$.

Chebyshev polynomials share the unique and important property: among all *monic* polynomials of degree k , the one that deviates the least from zero on $[-1, 1]$ is the polynomial $2^{1-k}T_k(x)$.

Exercise 11.3.2. Study the Chebyshev polynomials of the second kind:

$$\frac{1}{1 - 2xz + z^2} = \sum_{k=0}^{\infty} U_k(x)z^k, \quad |z| < 1$$

11.3.3 Legendre polynomials

In his *Recherches sur l'attraction des spheroides homogènes* (1783), Adrien Marie Legendre introduced the important expansion in multipoles:

$$\boxed{\frac{1}{|\mathbf{r} - \mathbf{R}|} = \frac{1}{\sqrt{R^2 - 2Rr \cos\theta + r^2}} = \frac{1}{R} \sum_{\ell=0}^{\infty} P_{\ell}(\cos\theta) \left(\frac{r}{R}\right)^{\ell}} \quad (11.25)$$

θ is the angle between the vectors, $R > r$, $P_k(\cos\theta)$ is a Legendre polynomial of order k in $\cos\theta$. The generating function

$$P(z, \cos\theta) = \frac{1}{\sqrt{1 - 2z \cos\theta + z^2}} = (1 - ze^{i\theta})^{-1/2} (1 - ze^{-i\theta})^{-1/2}$$

is analytic in the disk $|z| < 1$, where the two factors can be expanded in binomial series. The coefficients of the Cauchy product are the Legendre functions:

$$\begin{aligned} \frac{1}{\sqrt{1 - 2z \cos\theta + z^2}} &= \sum_{n,m} z^{n+m} \frac{(-1/2)_m}{m!} \frac{(-1/2)_n}{n!} e^{i(m-n)\theta} \\ &= \sum_{k=0}^{\infty} z^k P_k(\cos\theta) \\ P_k(\cos\theta) &= \sum_{m=0}^k \frac{(-1/2)_m}{m!} \frac{(-1/2)_{k-m}}{(k-m)!} \cos(2m-k)\theta \end{aligned}$$

As P_k is an expression of $\cos(n\theta)$ with $n = 0, \dots, k$, it may be rewritten as a polynomial of order k in the variable $x = \cos\theta$. In the variable x , $|x| \leq 1$, it is:

$$\frac{1}{\sqrt{1 - 2xz + z^2}} = \sum_{k=0}^{\infty} z^k P_k(x) \quad (11.26)$$

From the identity $(1 - 2xz + z^2) \frac{\partial P(z, x)}{\partial z} = (x - z)P(z, x)$ one obtains the recurrence relation $(k+1)P_{k+1}(x) = x(2k+1)P_k(x) - kP_{k-1}(x)$.

11.3.4 Laguerre polynomials*

The polynomials arise in the study of the radial Schrödinger equation for the Hydrogen atom. The generating function is:

$$L(z, x) = \frac{1}{1-z} \exp\left(-\frac{xz}{1-z}\right) = \sum_{k=0}^{\infty} L_k(x) z^k. \quad (11.27)$$

It is holomorphic in $|z| < 1$. If C is a circle $|z| = r < 1$:

$$L_k(x) = \oint_C \frac{dz}{2\pi i} \frac{L(z, x)}{z^{k+1}} = \sum_{n=0}^{\infty} \frac{(-x)^n}{n!} \oint_C \frac{dz}{2\pi i} \frac{z^{n-k-1}}{(1-z)^{n+1}}$$

The integral is zero if $n - k - 1 \geq 0$ i.e. L_k is a polynomial of degree k . Use (11.15) to evaluate the integral:

$$L_k(x) = \sum_{n=0}^k \frac{(-x)^n}{n!} \oint_C \frac{dz}{2\pi i} \sum_{m=0}^{\infty} \binom{n+m}{m} z^{m+n-k-1}$$

The series is uniformly convergent on C and the sum is extracted from the integral. The integral is non-zero only for $m + n - k - 1 = -1$, i.e. $m = k - n$:

$$L_k(x) = \sum_{n=0}^k \binom{k}{n} \frac{(-x)^n}{n!} \quad (11.28)$$

11.3.5 The Hypergeometric series*

Several functions of mathematical physics correspond to special choices of the real parameters a, b and $c \neq 0, -1, -2, \dots$ of the hypergeometric function, which is defined by the power series:

$${}_2F_1(a, b; c; z) = \sum_{n=0}^{\infty} \frac{a_n b_n}{c_n} \frac{z^n}{n!} = 1 + \frac{ab}{c} z + \frac{1}{2!} \frac{a(a+1)b(b+1)}{c(c+1)} z^2 + \dots \quad (11.29)$$

The series is absolutely convergent for $|z| < 1$, and is symmetric in a, c . For $a = -k$ the series terminates, and is a polynomial of degree k in z .

The hypergeometric function solves the differential equation

$$z(z-1) {}_2F_1''(z) + [c - (a+b-1)z] {}_2F_1'(z) - ab {}_2F_1(z) = 0$$

It has the integral representation ($\text{Re } c > \text{Re } b > 0$):

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(c-b)\Gamma(b)} \int_0^1 dt t^{b-1} (1-t)^{c-b-1} (1-zt)^{-a}$$

(the Gamma function is presented in the next chapter).

11.4 The Airy equation*

Power series are an effective representation of solutions of linear differential equations. The subject is vast⁸. As an example, the solution of the Airy equation is discussed. First, a useful theorem:

Theorem 11.4.1. *In the linear second order differential equation*

$$f''(z) + p(z)f'(z) + q(z)f(z) = 0 \quad (11.30)$$

if $p(z)$ and $q(z)$ are analytic on a disk $|z| < R$, then any solution of the equation is analytic on the same disk.

Airy's equation occurs in physics, for example in the study of a quantum particle in a uniform electric field⁹, WKB theory, radio waves. In general it is useful to study the equation in the complex plane:

$$f''(z) - zf(z) = 0 \quad (11.31)$$

The previous theorem assures that the two solutions are entire functions with absolutely convergent power series representation $f(z) = \sum_k c_k z^k$. Then

$$\sum_{k=2}^{\infty} k(k-1)c_k z^{k-2} - \sum_{k=0}^{\infty} c_k z^{k+1} = 0$$

i.e. $2c_2 + (6c_3 - c_0)z + (12c_4 - c_1)z^2 + (20c_5 - c_2)z^3 + \dots = 0$. The coefficients of the polynomial must vanish: c_0 and c_1 are undetermined, and $c_2 = 0$. Next:

$$k(k-1)c_k = c_{k-3}, \quad k = 3, 4, \dots$$

⁸ see Einar Hille, Ordinary differential equations in the complex domain, Dover reprint.

⁹ The Hamiltonian for an electron in a uniform electric field E along the x axis is $H = p^2/2m + eEx$. The eigenvalue equation is separable and for the x component is:

$$-\frac{\hbar^2}{2m}u''(x) + eExu(x) = \lambda u(x)$$

The linear potential eEx equals the energy λ at $x_0 = \lambda/eE$, therefore the classical motion is confined in $x \leq x_0$. The problem has a natural length $\ell = \hbar^2/3(meE)^{-1/3}$ and the rescaling $x - x_0 = \ell s$ brings the eigenvalue equation to Airy's form. For a field $E = 1$ keV/cm it is $\ell \approx 9$ nm.

Starting with $c_0 \neq 0$, $c_1 = 0$ one obtains $c_3 = c_0/(2 \cdot 3)$, $c_6 = c_3/(5 \cdot 6)$, $c_9 = c_6/(8 \cdot 9) \dots$ A good guess helps in getting the general coefficient:

$$\begin{aligned} \frac{c_{3k}}{c_0} &= \frac{1}{3k(3k-1)} \cdots \frac{1}{6 \cdot 5} \cdot \frac{1}{3 \cdot 2} = \frac{(3k-2) \cdots 10 \cdot 7 \cdot 4 \cdot 1}{(3k)!} \\ &= \frac{3^k}{(3k)!} \left(k - 1 + \frac{1}{3}\right) \cdots \left(2 + \frac{1}{3}\right) \left(1 + \frac{1}{3}\right) \frac{1}{3} = \frac{3^k}{\Gamma(3k+1)} \frac{\Gamma\left(k + \frac{1}{3}\right)}{\Gamma\left(\frac{1}{3}\right)} \end{aligned}$$

With the aid of the triplication formula¹⁰ for $\Gamma(3k+1)$:

$$\frac{c_{3k}}{c_0} = \frac{2\pi}{\Gamma\left(\frac{1}{3}\right)} \frac{1}{3^{2k+1/2} k! \Gamma\left(k + \frac{2}{3}\right)}$$

An appropriate choice of c_0 gives the solution:

$$f_0(z) = \sum_{k=0}^{\infty} \frac{z^{3k}}{9^k k! \Gamma\left(k + \frac{2}{3}\right)} = \frac{1}{\Gamma\left(\frac{2}{3}\right)} \left[1 + \frac{z^3}{6} + \frac{z^6}{180} + \dots\right]$$

An independent solution is obtained with $c_0 = 0$ and $c_1 \neq 0$:

$$f_1(z) = \sum_{k=0}^{\infty} \frac{z^{3k+1}}{9^k k! \Gamma\left(k + \frac{4}{3}\right)} = \frac{1}{\Gamma\left(\frac{4}{3}\right)} \left[z + \frac{z^4}{12} + \frac{z^7}{504} + \dots\right]$$

The two series have infinite radius and are entire functions.

The standard solutions are the *Airy functions* of the first and second kind:

$$\text{Ai}(z) = 3^{-2/3} f_0(z) - 3^{-4/3} f_1(z), \quad \text{Bi}(z) = 3^{-1/6} f_0(z) + 3^{-5/6} f_1(z).$$

For real variable $z = x$ both functions are oscillatory for $x \ll 0$. For $x \gg 0$ the function $\text{Ai}(x)$ decays to zero exponentially while $\text{Bi}(x)$ grows exponentially¹¹

¹⁰ $\Gamma(3z) = \frac{3^{3z-1/2}}{2\pi} \Gamma(z) \Gamma\left(z + \frac{1}{3}\right) \Gamma\left(z + \frac{2}{3}\right)$

¹¹ O. Vallée and M. Soares, *Airy functions and applications to physics*, World Scientific 2004; Carl M. Bender and Steven A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, Springer.

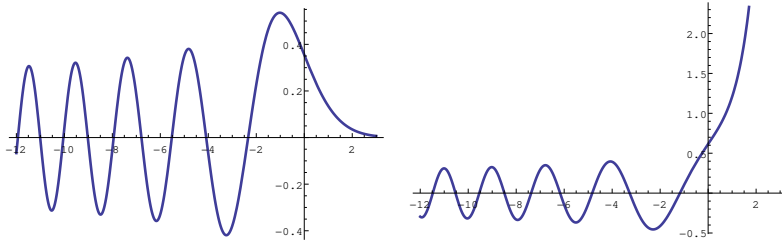


Figure 11.3 *The Airy functions $Ai(x)$ and $Bi(x)$.*

Chapter 12

Analytic Continuation

The power series representation of an analytic function implies that its zeros are *isolated*. An analytic function cannot vanish on a curve or a region in the domain, unless it is zero on the whole domain. This has far reaching and unexpected consequences, as the powerful concept of analytic continuation.

Some theorems about analytic maps are presented in the end.

12.1 Zeros of analytic functions

Theorem 12.1.1. *Let f be analytic on a domain D , and not identically zero on D . If $f(z_0) = 0$ at a point in D , then there is a punctured disk centred in z_0 where $f(z) \neq 0$.*

Proof. If f is not everywhere zero in a disk centred in z_0 , the function has a power series centred in z_0 , with some finite radius of convergence. If the zero is of order k , the coefficient c_k is nonzero and

$$f(z) = c_k(z - z_0)^k \left[1 + \frac{c_{k+1}}{c_k}(z - z_0) + \dots \right] = c_k(z - z_0)^k \varphi(z)$$

where $\varphi(z)$ is analytic in the disk, and $\varphi(z_0) = 1$. Since φ is continuous in z_0 , $\forall \epsilon \exists \delta$ such that $|\varphi(z) - 1| < \epsilon \forall z \in D(z_0, \delta)$ i.e. there is no zero of φ in $D(z_0, \delta)$, and there is no zero of f in the same disk with point z_0 removed. \square

It follows that a zero of an analytic function cannot be an accumulation point. An analytic function that vanishes on a disk or a line, or a set of points with an accumulation point in the domain, is zero on the whole domain.

Two functions analytic on the same domain that take the same values on a line, or a sequence of points with an accumulation point, necessarily coincide (if not, their difference would violate the theorem).

Example 12.1.2. The function $\sin(2z) - 2 \sin z \cos z$ is entire and vanishes on the real axis, therefore $\sin(2z) = 2 \sin z \cos z$ holds everywhere in \mathbb{C} .

12.2 Analytic continuation

Suppose that f is analytic on a set D that contains at least a convergent sequence of points and its limit point. If \tilde{f} is a function analytic on \tilde{D} such that $D \subset \tilde{D}$ and $\tilde{f} = f$ on D , then \tilde{f} is the **analytic continuation** of f to \tilde{D} .

Theorem 12.2.1. The analytic continuation of f to \tilde{D} is unique.

Proof. Suppose that f_1 and f_2 are two extensions. Then $f_1 - f_2$ is zero on D . This implies that $f_1 - f_2 = 0$ on the whole set \tilde{D} . \square

Suppose that f_1 and f_2 are analytic on D_1 and D_2 , and $f_1 = f_2$ on $D_1 \cap D_2$. If the intersection contains at least a convergent sequence of points, then the function $f = f_1$ on D_1 and $f = f_2$ on D_2 is analytic on $D_1 \cup D_2$.

Consider a series $f(z) = \sum_n a_n (z - a)^n$ that converges in the disk $|z - a| < R$. If in the disk we fix a point b and expand f with center b , we may obtain a new disk that leaks out of the prior. The two expansions coincide on the intersection, and together describe a single analytic function f on the union of the two disks. In this larger domain, one may choose another center and build a new expansion, and proceed. Then, disk by disk, an analytic continuation of f by power series is obtained.

Sometimes this is not possible. Consider the power series

$$g(z) = \sum_{n=0}^{\infty} z^{2^n} = z + z^2 + z^4 + z^8 + z^{16} + \dots$$

By the Cauchy-Hadamard criterion it converges in $|z| < 1$, and clearly diverges at $z = \pm 1$. Note that $g(z^2) = g(z) - z$, therefore the series is divergent also at $z = \pm i$. But $g(z^4) = g(z) - z - z^2$, then the series $g(z)$ also diverges at the roots of $z^4 = 1$. In this way one proves divergence at all points $z^{2^n} = 1$ $n = 1, 2, \dots$; such points are dense in the unit circle, which constitutes a barrier (*singular line*) for $g(z)$. Since the series diverges at all points $|z| = 1$, then it cannot be analytically continued.

12.3 Gamma function

The Gamma function stands out as the “Queen” of special functions. It was devised by Euler (1729) and extends the factorial $n!$ to complex numbers:

$$\Gamma(z) = \int_0^{\infty} ds e^{-s} s^{z-1} \quad \text{Re } z > 0 \quad (12.1)$$

With s^z is $e^{z \log s}$ note that:

$$|\Gamma(z)| \leq \int_0^\infty ds e^{-s} |s^{z-1}| = \Gamma(\operatorname{Re} z)$$

The Gamma function is holomorphic: let γ be an arbitrary closed path in $\operatorname{Re} z > 0$, and integrate. The integrals can be exchanged:

$$\oint_\gamma dz \Gamma(z) = \int_0^\infty ds e^{-s} \oint_\gamma dz e^{(z-1) \log s}$$

The last one is zero by Cauchy's formula. Then Morera's theorem assures that $\Gamma(z)$ is holomorphic. \square

The derivative $\Gamma'(z)$ is holomorphic on the same domain, and is related to the useful Digamma function (see sect.12.3.2).

For $z = x > 0$, integration by parts of (12.1) gives the property of the factorial: $\Gamma(x+1) = x\Gamma(x)$. Since $\Gamma(1) = 1$, it is

$$\Gamma(n+1) = n!$$

The property remains valid in the complex domain: since $\Gamma(z+1) - z\Gamma(z)$ is analytic and vanishes on the real positive axis, then it must vanish everywhere in its domain:

$$\boxed{\Gamma(z+1) = z\Gamma(z)} \quad (12.2)$$

Exercise 12.3.1. Show that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $\Gamma(n + \frac{1}{2}) = \sqrt{\pi} \frac{(2n)!}{4^n n!}$ (Hint: make the change $s = t^2$ in Euler's integral).

Exercise 12.3.2. Evaluate the volume V and the area A of the sphere of radius R in \mathbb{R}^n . (Hint: compare the integrals $\int d^n x \exp(-\sum x_k^2)$ in Cartesian and spherical coordinates).

$$V = \frac{\pi^{n/2}}{\Gamma(1 + \frac{n}{2})} R^n, \quad A = n \frac{V}{R}. \quad (12.3)$$

Exercise 12.3.3. Euler's Beta function. Evaluate the double integral $\Gamma(x)\Gamma(y)$, $x > 0$ and $y > 0$, by changing to squared variables and then to polar coordinates, and prove the useful

formula¹

$$B(x, y) \equiv \int_0^1 dt t^{x-1} (1-t)^{y-1} = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \quad (12.4)$$

Euler's integral (12.1) is well defined for $\operatorname{Re} z > 0$. However, by splitting the range of integration into $[0, 1] \cup [1, \infty)$, and integrating on $[0, 1]$ by series expansion, one obtains

$$\Gamma(z) = \int_1^\infty ds e^{-s} s^{z-1} + \sum_{k=0}^\infty \frac{(-1)^k}{k!} \frac{1}{z+k} \quad (12.5)$$

This expression provides the analytic continuation of Γ to $\operatorname{Re} z \leq 0$. It shows that $\Gamma(z)$ is the sum of an entire and a meromorphic function with simple poles at $-k$ with residue $(-1)^k/k!$, $k \in \mathbb{N}$.

An alternative definition on the punctured complex plane was obtained by Gauss (1811):

$$\Gamma(z) = \lim_{n \rightarrow \infty} \frac{n^z n!}{z(z+1)(z+2) \cdots (z+n)} \quad z \neq 0, -1, -2, \dots \quad (12.6)$$

From Gauss' formula one easily obtains the useful duplication formula (as well as the triplication, or multiplication by n)

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}} \Gamma(z) \Gamma\left(z + \frac{1}{2}\right) \quad (12.7)$$

Exercise 12.3.4. Evaluate the following integral that, for large n , links Euler's and Gauss' expressions of the Gamma function (integrate by parts):

$$\int_0^n ds s^{z-1} \left(1 - \frac{s}{n}\right)^n = \frac{n^z n!}{z(z+1) \cdots (z+n)} \quad (12.8)$$

In 1854 Weierstrass gave a representation for the reciprocal of the Gamma function, which is an entire function:

$$\frac{1}{\Gamma(z)} = z e^{Cz} \prod_{m=1}^\infty \left[\left(1 + \frac{z}{m}\right) e^{-z/m} \right] \quad (12.9)$$

¹ Atle Selberg, winner of a Fields medal (with Laurent Schwartz, 1950) for his studies on prime numbers, obtained an important multi-dimensional extension of the Beta function (Selberg's integral).

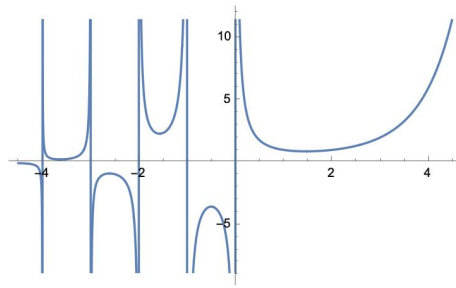


Figure 12.1 The Gamma function for real x . Note the poles at $0, -1, -2, \dots$. For large $x > 0$ it diverges factorially (according to the Stirling formula).

with Euler's constant

$$C = \lim_{n \rightarrow \infty} \left[1 + \frac{1}{2} + \dots + \frac{1}{n} - \log n \right] = 0.5772156\dots \quad (12.10)$$

Another useful representation is by Hankel's contour integral eq.(28.16).

Exercise 12.3.5. Prove the useful formulae:

$$\int_0^{\infty} dt \frac{t^{z-1}}{e^t - 1} = \Gamma(z)\zeta(z), \quad \operatorname{Re} z > 1, \quad (12.11)$$

$$\int_0^{\infty} dt \frac{t^{z-1}}{e^t + 1} = (1 - 2^{1-z})\Gamma(z)\zeta(z), \quad \operatorname{Re} z > 0. \quad (12.12)$$

(Hint: multiply and divide by e^{-t} and expand the denom. in geometric series).

The integrals appear in the theory of free bosons and free fermions. The second one is an analytic extension of Riemann's $\zeta(z)$ from $\operatorname{Re} z > 1$ to $\operatorname{Re} z > 0$.

Exercise 12.3.6. Show that $\lim_{z \rightarrow 0} [z\zeta(1-z)] = -1$.

12.3.1 Stirling's formula

The well known formula for the growth of the factorial arises from the Stirling's expansion of $\Gamma(x+1)$, when x is real and large:

$$\Gamma(x+1) = \sqrt{2\pi x} e^{-x(\log x - 1)} \left[1 + \frac{1}{12x} + \frac{1}{288x^2} + \mathcal{O}\left(\frac{1}{x^3}\right) \right] \quad (12.13)$$

Proof. Put $s = xt$ in the integral:

$$\Gamma(x+1) = \int_0^\infty ds e^{-s+x \log s} = x e^{x \log x} \int_0^\infty dt e^{-x(t-\log t)}$$

For $x \gg 1$, the neighborhood of the minimum of the exponent contributes most. The minimum is at $t = 1$, with expansion $t - \log t = 1 + \frac{1}{2}(t-1)^2 - \frac{1}{3}(t-1)^3 + \dots$

$$\begin{aligned} \Gamma(x+1) &= x e^{x \log x - x} \int_{-1}^\infty dt \exp \left[-x \left(\frac{1}{2} t^2 - \frac{1}{3} t^3 + \frac{1}{4} t^4 - \dots \right) \right] \\ &= \sqrt{x} e^{x \log x - x} \int_{-\sqrt{x}}^\infty dt \exp \left(-\frac{1}{2} t^2 + \frac{1}{3\sqrt{x}} t^3 - \frac{1}{4x} t^4 + \dots \right) \\ &= \sqrt{x} e^{x \log x - x} \int_{-\sqrt{x}}^\infty dt e^{-\frac{1}{2} t^2} \left[1 + \frac{t^3}{3\sqrt{x}} + \frac{1}{x} \left(\frac{t^6}{18} - \frac{t^4}{4} \right) + \dots \right] \end{aligned}$$

The integrals of odd powers are neglected since they are the sum $\int_{-\sqrt{x}}^{\sqrt{x}} dt \dots + \int_{\sqrt{x}}^\infty dt$ where the first integral is zero and the second one is exponentially small in x . For even powers the segment $(-\sqrt{x}, \sqrt{x})$ is where the function contributes for large x . The lower limit can be taken to $-\infty$ with an exponentially small error. Then:

$$\Gamma(x+1) = \sqrt{x} e^{x \log x - x} \int_{-\infty}^\infty dt e^{-\frac{1}{2} t^2} \left[1 + \frac{1}{x} \left(\frac{t^6}{18} - \frac{t^4}{4} \right) + \dots \right]$$

The result follows with the aid of $\int_{-\infty}^{+\infty} e^{-t^2} t^{2n} dt = \Gamma(n + \frac{1}{2})$. □

12.3.2 Digamma function*

The logarithmic derivative of the Gamma function is the Digamma function:

$$\boxed{\psi(z) = \frac{1}{\Gamma(z)} \frac{d\Gamma(z)}{dz} = \frac{1}{\Gamma(z)} \int_0^\infty ds e^{-s} s^{z-1} \log s} \quad (12.14)$$

with the main property:

$$\psi(z+1) = \frac{1}{z} + \psi(z).$$

For integer values it gives $\psi(n+1) = \frac{1}{n} + \dots + \frac{1}{2} + 1 + \psi(1)$. The behaviour of the harmonic series (12.10) implies that, for large n : $\psi(n) - \psi(1) \approx \log n + C$. Stirling's formula gives the

behaviour for large real x :

$$\psi(x+1) \approx \log x + \frac{1}{2x} - \frac{1}{12x^2} + \dots$$

then, $\psi(1) = -C$. Euler's constant (12.10) is deeply related to the properties of Riemann's zeta function².

12.4 Analytic maps*

Theorem 12.4.1 (Open mapping theorem). *If f is non-constant and analytic on a domain D , the image of an open subset in D is open (the converse is obviously true because f is continuous.)*

Proof. Consider an open subset O in D and a point $a \in O$. The function $g(z) = f(z) - f(a)$ vanishes in a ; then there is a disk centred on a of radius δ and contained in O where $g(z) \neq 0$ i.e. $|f(z) - f(a)| > 0$. This means that the point $f(a)$ has an open neighborhood in $f(O)$. \square

Theorem 12.4.2 (Maximum principle theorem). *If f is non-constant and analytic on a domain D , the maximum of $|f(z)|$ is attained at the boundary ∂D .*

Proof. Suppose that $|f|$ attains its maximum at an interior point $z_0 \in D$, with image $w_0 = f(z_0)$. Then there is an open disk $D(z_0, r)$ centred in z_0 and contained in D . Since the image of the disk is open (Open mapping theorem 12.4.1) and contains w_0 , there is a disk $|w - w_0| < r'$ contained in $f(D)$. Therefore there is a point w with $|w| > |w_0|$, and this contradicts the hypothesis. \square

If $f(z) \neq 0$ on D , the same theorem applies to the holomorphic function $1/f$ to give the *minimum principle*: the minimum of $|f(z)|$ is attained at the boundary of D .

Exercise 12.4.3. *Find the maxima of $|\cosh z|$ in the square of vertices $0, \pi, \pi + i\pi, i\pi$.*

Proposition 12.4.4 (Schwarz's Lemma). *Suppose that f is holomorphic and maps the open unit disk \mathbb{D} into itself, $f(\mathbb{D}) \subseteq \mathbb{D}$, with $f(0) = 0$. Then*

$$|f(z)| \leq |z|, \quad \forall z \in \mathbb{D}.$$

Proof. The function $f(z)/z$ has a removable singularity in $z = 0$, and is holomorphic in the disk. Since it gains the maximum modulus at the boundary, it is: $|f(z)/z| \leq 1$. In particular $|f'(0)| \leq 1$. \square

² a nice book is: J. Havil, *Gamma, exploring Euler's constant*, Princeton Univ Press, 2003. See also the paper by Z. Silagadze: *Basel problem, a physicist's solution*, arXiv:1908.0751.

If the map is a bijection of the unit disk and $f'(z) \neq 0$ (f is a conformal map), Schwarz's lemma applies to the inverse map f^{-1} as well. Then $|f'(0)| = 1$, and $|f(z)| = 1$ if $|z| = 1$. For such functions, the power expansion is: $f(z) = z + a_2 z^2 + a_3 z^3 + \dots$. Bieberbach's conjecture (1916) states that $|a_n| < n$ for all n . He only proved $|a_2| < 2$. Loewner proved $|a_3| < 3$ by means of Loewner's differential equation. The conjecture was proven by de Branges in 1984.

A limit case with real coefficients is the power expansion of Koebe's function:

$$z + 2z^2 + 3z^3 + 4z^4 + \dots = z \frac{d}{dz} (1 + z + z^2 + \dots) = \frac{z}{(1-z)^2}$$

It maps univalently the unit disk to the w -plane with cut $\{u < -1/4, v = 0\}$. The cut is the image of the unit circle³.

Here are some pearls from the theory of analytic functions:

Theorem 12.4.5 (Bohr, 1914). *If $f(z) = \sum_{k=0}^{\infty} c_k z^k$ is analytic and $|f(z)| < 1$ on the unit disk, then $\sum_{k=0}^{\infty} |c_k z^k| < 1$ on the disk $|z| < 1/3$. This radius is the best possible.*

Theorem 12.4.6 (Bloch, 1924). *If f is analytic on the unit disk \mathbb{D} with $f(0) = 0$ and $f'(0) = 1$ then there is a number B (Bohr's constant) independent of f such that there is a subset $\Omega \subset \mathbb{D}$ where f is one-to-one, and such that $f(\Omega)$ contains a disk of radius B . ($B = 0.4469$, <https://arxiv.org/abs/1702.01080>)*

Theorem 12.4.7 (MacDonald 1898, Whittaker 1935). *The number of zeros of a non-constant function f analytic in a region bounded by a contour $|f(z)| = c$ exceeds by unity the number of zeros of f' in the same region.*
<https://arxiv.org/abs/1702.03458>

Theorem 12.4.8 (Earle-Hamilton fixed point theorem, 1968). *Let f be a holomorphic function on a bounded domain D , such that the distance between $f(D)$ and \mathbb{C}/D is greater than a positive constant. Then f has a unique fixed point.*

³ A magnificent reference is: R. Roy, *Sources in the development of mathematics*, Cambridge, 2011.

Chapter 13

Laurent Series

13.1 Laurent series of holomorphic functions

A Laurent series with center a is the bilateral sum

$$\sum_{n=-\infty}^{\infty} c_n(z-a)^n = \sum_{n=0}^{\infty} c_n(z-a)^n + \sum_{n=1}^{\infty} c_{-n} \frac{1}{(z-a)^n} \quad (13.1)$$

It exists if both one-sided series converge. The two series are respectively called the *analytic* and the *principal* parts of the series.

The analytic part converges absolutely on a disk centred in a with radius R ,

$$\limsup \sqrt[n]{|c_n(z-a)^n|} < 1, \quad \rightarrow \quad |z-a| < R, \quad \frac{1}{R} = \limsup \sqrt[n]{|c_n|}$$

The principal part (negative powers) converges absolutely for

$$\limsup \sqrt[n]{|c_{-n}(z-a)^{-n}|} < 1, \quad \rightarrow \quad |z-a| > r = \limsup \sqrt[n]{|c_{-n}|}$$

Therefore, the Laurent series is well defined in the *annulus*

$$A(a, r, R) = \{z : r < |z-a| < R\}.$$

If the inner radius is zero and the point a is avoided, the annulus is the *punctured disk* $D'(a, R) = D(a, R) \setminus \{a\}$.

Exercise 13.1.1. Discuss the convergence of the Laurent series:

$$\sum_{k=-\infty}^{\infty} 3^{-|k|} z^k, \quad \sum_{k=-\infty}^{\infty} \frac{z^k}{\cosh(3k)}.$$

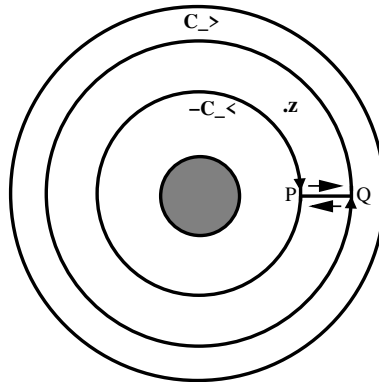


Figure 13.1 The integral on the closed path denoted by arrows equals the integral on the two circles, because the integrals on PQ and QP cancel.

Remark 13.1.2. Because the analytic and the principal parts are power series (in $z - a$ and its reciprocal), convergence in the annulus is absolute, and it is uniform in any compact subset. Thus a Laurent series can be integrated term by term on a path in the annulus. In particular, for a closed path encircling the center a with index 1, the integral of the analytic part is zero, and the integral of the principal part is $2\pi i c_{-1}$:

$$\oint_{\gamma} dz \sum_{n=-\infty}^{\infty} c_n (z - a)^n = 2\pi i c_{-1} \quad (13.2)$$

The following fundamental theorem was proven by Pierre Laurent¹:

Theorem 13.1.3 (Laurent). If $f(z)$ is analytic in the (open) annulus $A(a, r, R)$, then it has a unique Laurent expansion in it, with center a :

$$f(z) = \sum_{k=-\infty}^{\infty} c_k (z - a)^k, \quad c_k = \oint_{\gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta - a)^{k+1}} \quad (13.3)$$

γ is any closed positive path in the annulus that encircles the center once.

Proof. Let z be a point in the annulus and draw in the annulus two circles with center a and positive orientation: $C_{>}$ with radius $r_{>}$ and $C_{<}$ with radius $r_{<}$, and $r_{<} < |z - a| < r_{>}$.

¹ He was an engineer in the army, and communicated the theorem to Cauchy in 1843, in a private letter. The proof was published after his death. Weierstrass arrived to the same theorem independently and, as he often did, he published the proof years later. These two books by Reinhold Remmert: *Theory of complex functions*, and *Classical topics in complex function theory*, published by Springer, contain many interesting historical notes.

Choose a point $P \in C_<$ and a point $Q \in C_>$. Consider the closed positively oriented path

$$\Gamma = [PQ] \cup C_> \cup [QP] \cup (-C_<)$$

where $-C_<$ is the inner circle with reversed orientation. Since the segment joining P and Q is covered twice in opposite directions, it is:

$$\oint_{\Gamma} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} = \oint_{C_>} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} - \oint_{C_<} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z}$$

The path Γ encircles the point z ; by Cauchy's integral formula, the first integral is $f(z)$. Therefore:

$$f(z) = \oint_{C_>} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z} - \oint_{C_<} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{\zeta - z}$$

Write $\zeta - z = (\zeta - a) - (z - a)$ in the Cauchy kernels of the two integrals and expand in Geometric series (where respectively it is $|\zeta - a| > |z - a|$ and $|z - a| < |\zeta - a|$). Uniform convergence allows to take the sums out of the integrals

$$\begin{aligned} &= \oint_{C_>} \frac{d\zeta}{2\pi i} f(\zeta) \sum_{k=0}^{\infty} \frac{(z-a)^k}{(\zeta-a)^{k+1}} + \oint_{C_<} \frac{d\zeta}{2\pi i} f(\zeta) \sum_{k=0}^{\infty} \frac{(\zeta-a)^k}{(z-a)^{k+1}} \\ &= \sum_{k=0}^{\infty} (z-a)^k \oint_{C_>} \frac{d\zeta}{2\pi i} \frac{f(\zeta)}{(\zeta-a)^{k+1}} + \sum_{k=0}^{\infty} \frac{1}{(z-a)^{k+1}} \oint_{C_<} \frac{d\zeta}{2\pi i} f(\zeta) (\zeta-a)^k. \end{aligned}$$

The two circles can be deformed into an arbitrary simple closed path γ in the annulus, without changing the values of the integrals (the coefficients c_k and c_{-k}).

Suppose that f admits another (uniformly convergent) Laurent expansion in the annulus: $f(z) = \sum_{k \in \mathbb{Z}} \tilde{c}_k (z-a)^k$. The coefficient c_n in (13.3) is evaluated:

$$c_n = \oint_{\gamma} \frac{dz}{2\pi i} \sum_{k \in \mathbb{Z}} \tilde{c}_k (z-a)^{k-n-1} = \sum_{n \in \mathbb{Z}} \tilde{c}_k \oint_{\gamma} \frac{dz}{2\pi i} (z-a)^{k-n-1} = \tilde{c}_n$$

because the integrals vanish if $k - n - 1 \neq -1$. □

The Laurent expansion of a function that is analytic on the whole disk with center a has no principal part, and the analytic part coincides with the power expansion in the disk.

Example 13.1.4. *The function $1/\sin z$ has simple poles at $z = n\pi$, $n \in \mathbb{Z}$. With center in $z = 0$ it admits a Laurent expansion in each concentric annulus.*

In the punctured disk $0 < |z| < \pi$ the expansion is

$$\frac{1}{\sin z} = \frac{1}{z - z^3/3! + z^5/5! - \dots} = \frac{1}{z} + \frac{1}{6}z + \frac{7}{360}z^3 + \frac{31}{15120}z^5 + \mathcal{O}(z^7) = \frac{1}{z} + A(z)$$

where $A(z)$ is the analytic part, absolutely convergent in the disk $|z| < \pi$.

To find the expansion in $\pi < |z| < 2\pi$ one subtracts the principal parts of the expansions of $1/\sin z$ centred in $z = 0, z = \pm\pi$. The function

$$\varphi(z) = \frac{1}{\sin z} - \frac{1}{z} + \frac{1}{z - \pi} + \frac{1}{z + \pi}$$

is holomorphic in the disk $|z| < 2\pi$. In the disk $|z| < \pi$ it is $A(z) = \varphi(z) - \frac{1}{z - \pi} - \frac{1}{z + \pi}$. In the annulus $\pi < |z| < 2\pi$ we have the expansion:

$$\frac{1}{\sin z} = \frac{1}{z} - \frac{2z}{z^2 - \pi^2} + \varphi(z) = -2 \sum_{k=1}^{\infty} \frac{\pi^{2k}}{z^{2k+1}} - \frac{1}{z} + \varphi(z)$$

The analytic part is odd with the expansion:

$$\begin{aligned} \varphi(z) &= \left[\frac{1}{\sin z} - \frac{1}{z} \right] - \frac{2z}{\pi^2} \frac{1}{1 - (z/\pi)^2} \\ &= \left[\frac{1}{6} - \frac{2}{\pi^2} \right] z + \left[\frac{7}{360} - \frac{2}{\pi^4} \right] z^3 + \left[\frac{31}{15120} - \frac{2}{\pi^6} \right] z^5 + \dots \end{aligned}$$

The coefficients coincide with $c_{2k+1} = \oint_C \frac{dz}{2\pi i} \frac{1}{\sin z} z^{-2k+2}$ on a circle of radius $\pi < r < 2\pi$.

Exercise 13.1.5. Obtain the following Laurent expansion in $z = -1$, and the radius of the punctured disk

$$\frac{1}{z^3 + z + 2} = \frac{1}{4(z+1)} + \frac{1}{2\sqrt{7}} \sum_{k=0}^{\infty} \frac{(z+1)^k}{2^k} \sin[(k+2)\theta]$$

($\cos \theta = 3/4$ and $\sin \theta = \sqrt{7}/4$; the radius is $R = 2$)

13.2 Bessel functions (integer order)

The function $J(z, x) = \exp[\frac{1}{2}x(z - 1/z)]$ is analytic in the punctured complex plane $\mathbb{C}/\{0\}$, where it has the Laurent expansion

$$\exp \left[\frac{x}{2} \left(z - \frac{1}{z} \right) \right] = \sum_{k=-\infty}^{\infty} z^k J_k(x) \quad (13.4)$$

It is the generating function of Bessel's functions of integer order, which arise in the study of the Laplace operator in cylindrical coordinates².

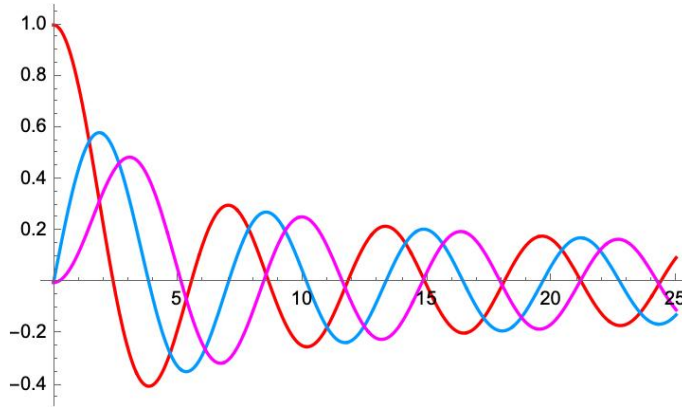


Figure 13.2 Bessel functions of the first kind J_0 (red), J_1 (blue), J_2 (fuchsia).

A change of sign of z is compensated by a change of sign of x : $J(-z, x) = J(z, -x)$ then $J_k(-x) = (-1)^k J_k(x)$. The exchange of z with $1/z$ amounts again to a change of sign of x , then

$$J_{-k}(x) = J_k(-x) = (-1)^k J_k(x)$$

With $z = e^{i\theta}$ the expansion is $e^{ix\sin\theta} = \sum_{k=-\infty}^{\infty} e^{ik\theta} J_k(x)$. An integral expression for Bessel functions is readily obtained:

$$J_k(x) = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i(x\sin\theta - k\theta)} \tag{13.5}$$

The generating function allows for a simple derivation of several properties. From $\partial_x J(z, x) = \frac{1}{2}(z - 1/z)J(z, x)$ and $z\partial_z J(z, x) = \frac{x}{2}(z + 1/z)J(z, x)$ one obtains

$$2J'_k(x) = J_{k-1}(x) - J_{k+1}(x), \tag{13.6}$$

$$\frac{2k}{x} J_k(x) = J_{k-1}(x) + J_{k+1}(x) \tag{13.7}$$

² Friedrich Wilhelm Bessel (1784, 1846) was the director of Königsberg's astronomical observatory (Prussia) and measured the first stellar distance by parallax, after correctly interpreting the apparent motion of *61 Cygni* (discovered by Piazzi in Palermo) as due to Earth's annual motion. The same instrument (built by Fraunhofer) enabled him to discover the oscillations of Sirius, due to an invisible companion star (a white dwarf) to be observed a century later. He developed an accurate theory for solar eclipses, and introduced Bessel's function to solve Kepler's equation for planetary motion (see sect.20.6.4).

The two equations for $J(z, x)$ also yield an equation where z and ∂_z only appear in the combination $z\partial_z$: $(z\partial_z)^2 J(z, x) = (x^2\partial_x^2 + x\partial_x + 1)J(z, x)$. This gives Bessel's equation for integer order:

$$\left[\frac{d^2}{dx^2} + \frac{1}{x} \frac{d}{dx} + 1 - \frac{k^2}{x^2} \right] J_k(x) = 0 \quad (13.8)$$

The other independent solution is Bessel's function of the second kind $Y_k(x)$.

Bessel functions are so important in physics, that it is worth studying their large x behaviour.

The change $J_k(x) = f_k(x)/\sqrt{x}$ in eq.(13.8) cancels the first derivative term: $f_k'' + f_k + f_k(\frac{1}{4} - k^2)/x^2 = 0$. For large x it is $f_k'' + f_k = 0$. Up to a phase and a constant we obtain the oscillating behaviour with decay in amplitude: $J_k(x) \approx \frac{C_k}{\sqrt{x}} \cos(x - \phi_k)$. The properties (13.7) imply $C_k = C_0$ and $\phi_k = \phi_0 + k\pi/2$. A detailed study³ of J_0 reveals that $C_0 = \sqrt{2/\pi}$ and $\phi_0 = \pi/4$:

$$J_k(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - k\frac{\pi}{2} - \frac{\pi}{4}\right) \quad (13.9)$$

Write eq.(13.8) for another index, say m . Multiply the first by $xJ_m(x)$ and the other by $xJ_k(x)$, and subtract:

$$\left(1 + x \frac{d}{dx}\right)(J_k' J_m - J_m' J_k) - \frac{k^2 - m^2}{x} J_k J_m = 0$$

Now integrate on the positive reals. The first two terms cancel by integration by parts. The orthogonality property is obtained:

$$\int_0^\infty \frac{dx}{x} J_k(x) J_m(x) = 0 \quad k \neq m \quad (13.10)$$

Exercise 13.2.1.

1) With the Cauchy product $J(z, x)J(z, y)$ obtain the summation formula

$$J_n(x+y) = \sum_{k=-\infty}^{\infty} J_k(x) J_{n-k}(y) \quad (13.11)$$

2) With the integral representation (13.5) show that $J_n(x)$ behaves as x^n for small x ($n \geq 0$).

3) Write the Helmholtz equation $(\nabla^2 + \lambda^2)u = 0$ in polar coordinates and solve it for $u(r, \theta) = R(r\sqrt{\lambda})e^{im\theta}$ (the radial equation becomes Bessel's equation).

³ See the nice booklet by Frank Bowman, Introduction to Bessel functions, Dover Ed.

4) $J(z, x)$ is the product of two exp series. Obtain the expansion

$$J_n(x) = \sum_{k=0}^{\infty} (-1)^k \frac{(x/2)^{n+2k}}{k!(n+k)!} \quad (13.12)$$

13.3 Fourier series

Consider a function f that is analytic in an annulus centred in the origin that contains the unit circle. In the annulus f has a Laurent expansion with coefficients f_k evaluated as integrals on the unit circle. In particular, on the unit circle $z = e^{i\theta}$:

$$f(e^{i\theta}) = \sum_{k=-\infty}^{\infty} c_k e^{ik\theta}, \quad c_k = \int_0^{2\pi} \frac{d\theta}{2\pi} f(e^{i\theta}) e^{-ik\theta}$$

This Laurent expansion on the unit circle, with $\hat{f}_k = \sqrt{2\pi} c_k$, defines the *Fourier* expansion of the 2π -periodic function $f(\theta) \equiv f(e^{i\theta})$:

$$f(\theta) = \sum_{k=-\infty}^{\infty} \hat{f}_k u_k(\theta), \quad \hat{f}_k = \int_0^{2\pi} d\theta \overline{u_k(\theta)} f(\theta) \quad (13.13)$$

where $\{u_k\}_{k \in \mathbb{Z}}$ is the *Fourier basis* of orthonormal 2π -periodic functions

$$\boxed{u_k(\theta) = \frac{e^{ik\theta}}{\sqrt{2\pi}}, \quad \int_0^{2\pi} d\theta \overline{u_m(\theta)} u_n(\theta) = \delta_{mn}} \quad (13.14)$$

The numbers \hat{f}_k are the *Fourier coefficients* of the periodic function $f(\theta)$.

In this discussion f is the restriction of a holomorphic function to the unit circle, where it is continuous and differentiable. The Fourier expansion of more general periodic functions will be studied in section 20.1.

13.4 Z-transform*

In signal and image processing the Z-transform of a bilateral $\{x_n\}_{-\infty}^{\infty}$ or a unilateral sequence $\{x_n\}_0^{\infty}$ is the Laurent series $Z[x_n] = \sum_{n=-\infty}^{\infty} x_n z^{-n}$, $z \in \mathbb{C}$ (note the sign of the exponent). The input sequence determines a domain of convergence of Z as a function of z . Operations on sequences correspond to operations on Laurent series.

Chapter 14

The Residue Theorem

14.1 Singularities.

If f is an analytic function, a zero a is isolated. For the reciprocal function $1/f$, a zero becomes an isolated singularity.

Definition 14.1.1. When a function $f(z)$ fails to be analytic at a point a , but is analytic in a punctured disk $D'(a, r)$ (a is removed from the disk $D(a, r)$), the point a is an **isolated singularity** of f .

The Laurent expansion of the function in the punctured disk $D'(a, r)$,

$$f(z) = \dots + \frac{c_{-k}}{(z-a)^k} + \dots + \frac{c_{-1}}{z-a} + c_0 + c_1(z-a) + \dots,$$

defines the principal and the analytic parts of f at its isolated singularity a . Since a punctured disk has inner radius equal to zero, the principal series exists at all points different from a , and converges uniformly on any compact set (for example, on any bounded curve) that does not contain the singular point.

According to the principal part being null, terminating, or containing an infinite number of terms, the singularity a is described by one of three types:

- The point a is a **removable singularity** if $c_{-k} = 0$ for all $k > 0$.
Example: $f(z) = \sin(z-a)/(z-a)$.
- The point a is a **pole of order k** if there is $k > 0$ such that $c_{-k} \neq 0$ and $c_{-k-n} = 0$ for all $n > 0$. It follows that $\lim_{z \rightarrow a} (z-a)^k f(z) = c_{-k}$.
Example: $f(z) = 1/(z-a)^3$ has a pole of order 3.
- The point a is an **essential singularity** if the principal part of the Laurent series has an infinite number of terms.
Example: $f(z) = \exp[(z-a)^{-1}]$

Remark 14.1.2. *There is a substantial difference between a pole and an essential singularity. If a is a pole for f , then $\lim_{z \rightarrow a} f(z) = \infty$. However, if a is an essential singularity, then $\lim_{z \rightarrow a} f(z)$ is undefined. Indeed, a theorem by Picard states that if a is an essential singularity of f , the image $f(D')$ of the punctured disk contains all complex points with at most one exception.*

Exercise 14.1.3. *Study the behaviour of $|1/z|$ and $|e^{1/z}|$ for $z \rightarrow 0$.*

Definition 14.1.4. A function is **meromorphic** on a domain D if it is analytic in D up to a set of isolated *poles* in D .

Theorem 14.1.5 (Picard's little theorem for meromorphic function). *Every function meromorphic on \mathbb{C} that omits three distinct complex values a, b and c is constant¹.*

14.2 Residues and their evaluation

Definition 14.2.1. The **residue** of a function f at the *isolated singularity* a is the coefficient c_{-1} of the Laurent expansion in the punctured disk,

$$\text{Res}[f, a] = c_{-1} = \oint_{\gamma} \frac{dz}{2\pi i} f(z) \quad (14.1)$$

where γ is any (piecewise) smooth simple path encircling the singularity a anticlockwise inside the punctured disk of analyticity.

In view of their importance, we give rules to calculate residues that avoid the evaluation of the contour integral.

- If $f(z)$ has a simple pole in a (a pole of order 1), its Laurent expansion is $f(z) = c_{-1}(z-a)^{-1} + \text{analytic part}$. Therefore the residue is

$$c_{-1} = \lim_{z \rightarrow a} (z-a)f(z) \quad (14.2)$$

- If $f(z)$ has a pole of order k in a , it is $(z-a)^k f(z) = c_{-k} + c_{-k+1}(z-a) + \dots + c_{-1}(z-a)^{k-1} + \dots$. Then $(k-1)$ derivatives give $(k-1)!c_{-1} +$ terms that vanish in $z = a$. The residue of f in a is

$$c_{-1} = \lim_{z \rightarrow a} \frac{1}{(k-1)!} \frac{d^{k-1}}{dz^{k-1}} \left[(z-a)^k f(z) \right] \quad (14.3)$$

¹ see: R. Remmert, *Classical topics in complex function theory*, GTM 172, Springer 1998.

- If a is an essential singularity, the residue is computed with (14.1).

Example 14.2.2. *In some cases the residue is more easily obtained by evaluating the first terms of the principal part.*

The function $1/\sin^3 z$ has poles of third order in $z = n\pi$. The formula for the residue in $z = 0$ is $c_{-1} = \lim_{z \rightarrow 0} \frac{1}{2} (d/dz)^2 [z^3/\sin^3 z]$. A simple alternative is to evaluate the P.P.

$$\frac{1}{\sin^3 z} = \frac{1}{z^3} \frac{1}{(1 - z^2/3! + \dots)^3} = \frac{1}{z^3} (1 + \frac{z^2}{2} + \mathcal{O}(z^4)) = \frac{1}{z^3} + \frac{1}{2z} + \text{anal. part}$$

The residue is $1/2$.

Example 14.2.3. *Standard expansions are centred in $z = 0$. To evaluate the residue of $f(z) = \text{Log } z/(1 - z^2)^3$ in $z = 1$, set $z = 1 + \epsilon$ and expand in small complex ϵ :*

$$\frac{\text{Log}(1 + \epsilon)}{(-2\epsilon - \epsilon^2)^3} = \frac{\epsilon - \frac{1}{2}\epsilon^2 + \mathcal{O}(\epsilon^3)}{-8\epsilon^3(1 + \frac{1}{2}\epsilon)^3} = -\frac{1 - \frac{1}{2}\epsilon + \mathcal{O}(\epsilon^2)}{8\epsilon^2} (1 - \frac{3\epsilon}{2} + \mathcal{O}(\epsilon^2)) = \frac{-1}{8\epsilon^2} + \frac{1}{4\epsilon} + \dots$$

The residue is $1/4$. We used: $\log(1 - z) = -z - \frac{z^2}{2} - \frac{z^3}{3} - \dots$

Example 14.2.4. *With the expansion $e^{1/z} = 1 + \frac{1}{z} + \dots + \frac{1}{4!z^4} + \dots$, one evaluates $\text{Res}[z^3 e^{1/z}, 0] = 1/24$.*

$\text{Res}[\tan z/z^5, 0] = 0$ because the function is even and the Laurent expansion in $z = 0$ only contains even powers.

Exercise 14.2.5. *Classify all points where the function is not holomorphic, and evaluate the residues at poles.*

$$f(z) = \frac{1}{\exp(1/z) - 1}$$

(Note that $z = 0$ is not an isolated singularity)

Theorem 14.2.6 (The Residue Theorem). *Let f be an analytic function on D/S , where $S = \{z_1, \dots, z_n\}$ is the set of its isolated singularities in the domain D . If γ is a closed piecewise smooth path in D/S such that $\text{Ind}(\gamma, z) = 0$ for all $z \notin D$, then:*

$$\oint_{\gamma} dz f(z) = 2\pi i \sum_{k=1}^n \text{Ind}(\gamma, z_k) \text{Res}[f, z_k]. \quad (14.4)$$

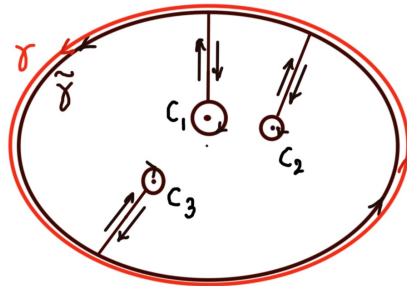


Figure 14.1 The integral on the simple curve γ (red, encircling singularities) is equal to sum of the integral on the black curve $\tilde{\gamma}$ with detours to avoid the singularities (its value is zero), to which one must subtract the added integrals on the segments (but they cancel) and on the circles in each punctured disk of the singularities (proportional to the residues).

Proof. Each singularity z_k is the center of a punctured disk in D where f is analytic and can be expanded in Laurent's series: $f(z) = P_k(z) + A_k(z)$. While the analytic part A_k converges in the full disk, the principal part P_k converges in \mathbb{C}/z_k .

The function $g(z) = f(z) - \sum_k P_k(z)$ is analytic on D . By Cauchy's theorem:

$$0 = \oint_{\gamma} dz g(z) = \oint_{\gamma} dz f(z) - \sum_k \oint_{\gamma} dz P_k(z)$$

The principal series can be integrated term by term because it converges uniformly on γ . The integrals $\oint_{\gamma} dz (z - z_k)^{-\ell}$ are zero for $\ell \neq 1$; the integral $\ell = 1$ is by definition $2\pi i \text{Ind}(\gamma, z_k)$. Then $\oint_{\gamma} dz P_k(z) = 2\pi i \text{Res}[f, z_k] \text{Ind}(\gamma, z_k)$. \square

Remark 14.2.7. It is remarkable that an integral that, in principle, requires the knowledge of the function on the whole curve, only requires the local knowledge of the function at the singular points enclosed by the curve.

14.3 Evaluation of integrals

The Residue Theorem is a fundamental tool for evaluating integrals. In all applications, one has to arrange the integral as an integral on a closed path in the complex plane, either by a change of variable, or by closing the set of integration with extra curves. The method is successful if the integral on such additional curves is known (e.g. zero), or is proportional to the initial integral. The choice of the correct closed path is a matter of wisdom. However, some cases are typical and are here illustrated by examples.

14.3.1 Trigonometric integrals

Integrals in $x \in [0, 2\pi]$ that only involve trigonometric functions may be attempted by writing the functions in terms of $e^{\pm ix}$ or powers, and putting $z = e^{ix}$. The new variable runs the unit circle C , and the Residue Theorem may apply.

Example 14.3.1.

$$\int_0^{2\pi} dx \frac{1}{2 + \cos x} = \oint_C \frac{dz}{iz} \frac{2}{4 + z + 1/z} = \oint_C dz \frac{-2i}{z^2 + 4z + 1}$$

The roots $z_{\pm} = -2 \pm \sqrt{3}$ are simple poles, and $|z_+| < 1$. Then:

$$= 2\pi i \lim_{z \rightarrow z_+} (z - z_+) \frac{-2i}{(z - z_+)(z - z_-)} = \frac{2\pi}{\sqrt{3}}$$

Example 14.3.2.

$$\begin{aligned} \int_0^{2\pi} dx \frac{\cos(4x)}{3 + \sin^2 x} &= \operatorname{Re} \int_0^{2\pi} dx \frac{e^{i4x}}{3 + \sin^2 x} = \operatorname{Re} \oint_C \frac{dz}{iz} \frac{4z^4}{12 - (z - 1/z)^2} \\ &= -4 \operatorname{Re} \oint_C \frac{dz}{i} \frac{z^5}{(z^2 - a)(z^2 - 1/a)} \quad (a = 7 - 4\sqrt{3}, 0 < a < 1) \\ &= -4 \operatorname{Re} 2\pi i [\operatorname{Res}(\sqrt{a}) + \operatorname{Res}(-\sqrt{a})] = \frac{\pi}{\sqrt{3}} (7 - 4\sqrt{3})^2 \end{aligned}$$

By taking the real part, one avoids the evaluation of two integrals. The poles are all simple, and only $\pm\sqrt{a}$ are in the unit disk.

Exercise 14.3.3.

$$\int_0^{2\pi} \frac{d\theta}{2\pi} \frac{\cos(k\theta)}{\cosh \xi - \cos \theta} = \frac{e^{-k\xi}}{\sinh \xi}, \quad \xi > 0, k = 0, 1, \dots \quad (14.5)$$

$$\int_0^{2\pi} dx \frac{\cos(2x)}{1 + \sin^2 x} = \pi(3\sqrt{2} - 4) \quad (14.6)$$

$$\int_{-1}^1 \frac{dx}{\sqrt{1-x^2}} \frac{1}{y-x} = \pi \frac{\operatorname{sign}(y)}{\sqrt{y^2-1}}, \quad |y| > 1 \quad (14.7)$$

14.3.2 Integrals on the real line

Several integrals on the whole real line are evaluated by *closing the interval* $[-R, R]$ with a semicircle in the upper or lower half-plane and promoting the real variable x to a complex

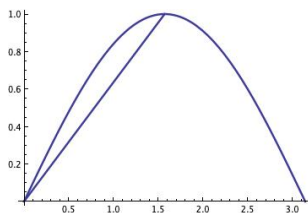


Figure 14.2 The inequality $\sin \theta \geq 2\theta/\pi$ on $0 \leq \theta \leq \frac{\pi}{2}$.

variable $z = x + iy$ (then $dz = dx$ on the real axis). If the Residue Theorem applies, it provides the value of the original integral if *if the contribution of the semicircle vanishes* in the limit $R \rightarrow \infty$.

Example 14.3.4.

$$\int_{\mathbb{R}} dx \frac{x^2}{x^4 + 1} = \lim_{R \rightarrow \infty} \int_{-R}^R dx \frac{x^2}{x^4 + 1} = \lim_{R \rightarrow \infty} \oint_{\gamma} dz \frac{z^2}{z^4 + 1}$$

γ is the closed path $[-R, R] \cup \sigma$, where σ is the semicircle $\{Re^{i\theta}, 0 \leq \theta \leq \pi\}$. Since the function decays as R^{-2} in every direction, for $R \rightarrow \infty$ the contribution of the semicircle vanishes (Darboux's inequality) (a semicircle in the lower half plane would be equally admissible). The path γ encircles the simple poles $z_1 = e^{i\pi/4}$ and $z_2 = e^{3i\pi/4}$. Then the integral is

$$= 2\pi i \lim_{z \rightarrow z_1} \frac{(z - z_1)z^2}{(z^4 + 1)} + 2\pi i \lim_{z \rightarrow z_2} \frac{(z - z_2)z^2}{(z^4 + 1)} = \frac{\pi}{\sqrt{2}}$$

Remark 14.3.5. The asymptotic behaviour $|f(Re^{i\theta})|R \rightarrow 0$ as $R \rightarrow \infty$ is a sufficient condition for the integral $\int_{\sigma} dz f(z)$ on the semicircle σ to vanish.

Exercise 14.3.6.

$$\int_{-\infty}^{+\infty} \frac{dx}{(1 + x^2)^2} = \frac{\pi}{2} \tag{14.8}$$

There is an important class of integrals where the choice of half-plane is not free, and the following result is useful:

Lemma 14.3.7 (Jordan). Let f be a complex function, continuous on the semicircle $\sigma = \{Re^{i\theta}, \theta \in [0, \pi]\}$, and let $M(R) = \max_{\theta \in [0, \pi]} |f(Re^{i\theta})|$. Then:

$$\left| \int_{\sigma} dz f(z) e^{iaz} \right| \leq \frac{\pi}{a} M(R), \quad a > 0 \tag{14.9}$$

Proof.

$$\begin{aligned} \left| \int_{\sigma} dz f(z) e^{iaz} \right| &= \left| iR \int_0^{\pi} e^{i\theta} d\theta f(Re^{i\theta}) e^{iaRe^{i\theta}} \right| \\ &\leq 2RM(R) \int_0^{\frac{\pi}{2}} d\theta e^{-Ra\sin\theta} \leq 2RM(R) \int_0^{\frac{\pi}{2}} d\theta e^{-2Ra\theta/\pi} \leq \frac{\pi}{a} M(R) \end{aligned}$$

The inequality $\sin\theta \geq 2\theta/\pi$ is used, for $0 \leq \theta \leq \pi/2$.

If $a < 0$ the semicircle σ for convergence is in the lower half plane. In any case $a \neq 0$. \square

If the maximum $M(R)$ of $|f|$ on σ vanishes for $R \rightarrow \infty$, no matter how fast, then the semicircle contribution is zero. Here's an important example:

$$\boxed{\int_{-\infty}^{\infty} dx \frac{e^{-ikx}}{x^2 + a^2} = \frac{\pi}{a} e^{-a|k|}, \quad a > 0, k \in \mathbb{R}} \quad (14.10)$$

For $k = 0$ one is free to close in the upper or lower half plane. If $k \neq 0$, since $|e^{-ik(x+iy)}| = e^{ky}$ must vanish, one is compelled to close with a semicircle in the lower half plane if $k > 0$ or in the upper half plane if $k < 0$.

Example 14.3.8. Evaluate:

$$\int_0^{\infty} dx \frac{\cos(kx)}{(x^2 + 1)^2} = \frac{\pi}{4} (|k| + 1) e^{-|k|} \quad (14.11)$$

The function is even, then the integral is 1/2 the integral on the real axis; $\cos(kx) = \cos(|k|x) = \operatorname{Re} \exp(i|k|x)$. The path is closed in the upper half plane, where it encircles the double pole $z = i$

$$= \frac{1}{2} \operatorname{Re} \left[2\pi i \lim_{z \rightarrow i} \frac{d}{dz} (z - i)^2 \frac{e^{i|k|z}}{(z^2 + 1)^2} \right] = \operatorname{Re} \left[\pi i \lim_{z \rightarrow i} \frac{d}{dz} \frac{e^{i|k|z}}{(z + i)^2} \right] = \dots$$

Exercise 14.3.9.

$$\int_0^{\infty} dx \frac{x \sin(\pi x)}{(x^2 + 1)^2} = \frac{\pi^2}{4} e^{-\pi} \quad (14.12)$$

Remark 14.3.10. Ordinary integrals on the real line are tacitly defined with limits to infinity being taken independently:

$$\int_{\mathbb{R}} f(x) dx = \lim_{u, v \rightarrow \infty} \int_{-u}^v f(x) dx$$

The examples presented above use a weaker definition (Cauchy's principal value):

$$\int_{\mathbb{R}} f(x) dx = \lim_{R \rightarrow \infty} \int_{-R}^R f(x) dx$$

where the limits are taken simultaneously. If the ordinary integral exists, it coincides with Cauchy's principal value integral.

For the important class of Fourier integrals the following statement holds:

Theorem 14.3.11 (Jordan). *Let $f(z)$ be analytic, save for isolated singularities. If $a > 0$ and if $f(z) \rightarrow 0$ as $z \rightarrow \infty$ in the upper half plane then:*

$$\int_{-\infty}^{\infty} dx f(x) e^{iax} = 2\pi i \sum_{k=1}^n \text{Res}[f(z)e^{iaz}, z_k] \quad (14.13)$$

where z_1, \dots, z_n are the singularities in the upper half plane.

If $a < 0$ and $f(z) \rightarrow 0$ as $z \rightarrow \infty$ in the lower half plane, the sum involves the poles in the lower half plane, with a change of sign.

Proof. Consider the rectangular path with corners $(-u, 0)$, $(v, 0)$, (v, iw) and $(-u, iw)$, $u, v > 0$, $w = u + v$. The rectangle is large enough to accommodate all singularities in the upper half plane. The integral of $f(z)e^{iaz}$ on this closed path is $2\pi i$ times the sum of residues. Let us show that integration on all sides but the interval $[-u, v]$ give zero for $u, v \rightarrow \infty$: the integral on the segment from v to $v + iw$ is

$$\left| \int_0^w idyf(v + iy)e^{iav - ay} \right| \leq \sup_y |f(v + iy)| \int_0^w e^{-ay} \leq \frac{1}{a} \sup_y |f(v + iy)|,$$

the sup factor vanishes for $v \rightarrow \infty$ (and u is left free). The opposite side behaves similarly for $u \rightarrow \infty$ and all v . The integral on the side from $-u + iw$ to $v + iw$ is

$$\left| \int_{-u}^v dx f(x + iw)e^{iax - aw} \right| \leq e^{-aw} (v + u) \sup_x |f(x + iw)|,$$

and vanishes in the independent limits u and $v \rightarrow \infty$.

The integral on the whole real axis is obtained by two independent limits

$$\lim_{u \rightarrow \infty} \int_{-u}^0 dx f(x) e^{iax} + \lim_{v \rightarrow \infty} \int_0^v dx f(x) e^{iax}$$

and equals the integral on the closed rectangle. □

14.3.3 Principal value integrals

When a function has one or more simple poles on the real axis, we may still give meaning to the integral as a principal value integral (Cauchy), not to be confused with the principal value integral on $[-R, R]$, $R \rightarrow \infty$.

This example illustrates the essence of it: the integral $\int_a^c (x-b)^{-1}$ is singular, for $b \in (a, c)$. However, one may isolate the singularity by removing an infinitesimal interval, and evaluate:

$$\int_a^{b-\epsilon} \frac{dx}{x-b} + \int_{b+\eta}^c \frac{dx}{x-b} = \log \frac{\epsilon}{b-a} + \log \frac{c-b}{\eta}$$

The independent limits $\epsilon, \eta \rightarrow 0$ do not exist. However, a finite result is obtained with the “principal value” prescription: $\epsilon = \eta$, i.e. a symmetric interval, and $\epsilon \rightarrow 0$. The result is the “principal value” prescription (in place of f one often writes $P f$):

$$\int_a^c \frac{dx}{x-b} \equiv \lim_{\epsilon \rightarrow 0} \left[\int_a^{b-\epsilon} \frac{dx}{x-b} + \int_{b+\epsilon}^c \frac{dx}{x-b} \right] = \log \frac{c-b}{b-a}$$

A principal value integral on the real line can be evaluated as follows:

- 1) restrict the real axis to a large enough interval $[-R, R]$ (or $[-u, v]$);
- 2) for each singularity x_i in the real line remove an interval $[x_i - \epsilon_i, x_i + \epsilon_i]$;
- 3) close the interval $[-R, R]$ (R big enough to include all gaps) with a semicircle in the appropriate half-plane (we assume that for infinite radius the contribution of the semicircle is zero);
- 4) close each gap centred in x_i by semicircles of radius ϵ_i in the same half plane as the big semicircle;
- 5) the principal part integral (real axis with gaps) is the sum of two contributions: the integral on the closed path (evaluated by residues) with $R \rightarrow \infty$, and the integrals on the semicircles (with opposite orientation that cancel the contributions that were added to close the contour) in the limits $\epsilon_i \rightarrow 0$.

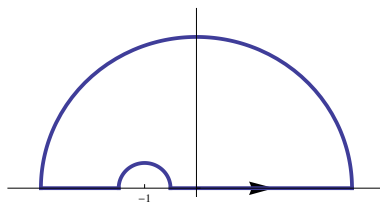


Figure 14.3 The contour for the principal part evaluation of $\int_{-\infty}^{\infty} dx(1+x^3)^{-1}$. The large semicircle of radius R is added to use the Residue theorem, the small semicircle isolates the singularity in $x = -1$.

Example 14.3.12.

$$\int_{\mathbb{R}} dx \frac{1}{1+x^3} = \lim_{\epsilon \rightarrow \infty} \lim_{R \rightarrow 0} \left[\int_{-R}^{-1-\epsilon} + \int_{-1+\epsilon}^R dx \frac{1}{1+x^3} \right]$$

The singularity $x = -1$ is a simple pole on the integration path. The integral exists as a principal part integral.

Close the path in the upper half plane (see Fig.14.3), it encircles the simple pole $e^{i\pi/3}$. The small semicircle centred in $x = -1$ is parametrized by $z = -1 + \epsilon e^{i\theta}$, $0 \leq \theta \leq \pi$. The integral is evaluated as the integral on the closed contour (residue theorem) plus the anticlockwise integral on the small semicircle:

$$\begin{aligned} &= 2\pi i \lim_{z \rightarrow e^{i\pi/3}} \frac{z - e^{i\pi/3}}{1+z^3} + \lim_{\epsilon \rightarrow 0} \int_0^\pi d\theta \frac{i\epsilon e^{i\theta}}{1+(-1+\epsilon e^{i\theta})^3} \\ &= \frac{2\pi i}{(e^{i\pi/3} + 1)(e^{i\pi/3} - e^{-i\pi/3})} + i \lim_{\epsilon \rightarrow 0^+} \int_0^\pi d\theta \frac{\epsilon e^{i\theta}}{3\epsilon e^{i\theta} + \dots} \\ &= \frac{\pi}{2} \frac{e^{-i\pi/6}}{\cos(\pi/6) \sin(\pi/3)} + i \frac{\pi}{3} = \frac{\pi}{\sqrt{3}}. \end{aligned}$$

Exercise 14.3.13.

$$\int_{\mathbb{R}} \frac{dx}{(x-a)(x-b)(x^2+1)} = \pi \frac{ab-1}{(a^2+1)(b^2+1)} \quad (14.14)$$

$$\int_{\mathbb{R}} \frac{dx}{(2+x)(x^2+4)} = \frac{\pi}{8} \quad (14.15)$$

$$\int_{\mathbb{R}} dx \frac{e^{ix}}{(x-a)(x-b)} = i\pi \frac{e^{ia} - e^{ib}}{a-b}. \quad (14.16)$$

$$\int_{\mathbb{R}} dx \frac{e^{ikx}}{x-y} = i\pi e^{iky} \text{sign } k \quad (14.17)$$

Example 14.3.14. Evaluation of the integral:

$$\boxed{\int_{-\infty}^{\infty} dx \frac{\sin x}{x} = \pi} \quad (14.18)$$

Consider the Cauchy integral $\oint_{\gamma} dz \frac{e^{iz}}{z}$ on the closed path made of segments $[-R, -\epsilon]$, $[\epsilon, R]$ and two semicircles of radii R (anticlockwise) and ϵ (clockwise) in the upper half plane,

centred in $z = 0$. The path avoids the pole $z = 0$, and the integral is zero:

$$0 = \left[\int_{-R}^{-\epsilon} + \int_{\epsilon}^R \right] \frac{e^{ix}}{x} - i \int_0^\pi d\theta e^{i\epsilon e^{i\theta}} + \int_{\sigma(R)} dz \frac{e^{iz}}{z} \rightarrow \oint_{\mathbb{R}} dx \frac{e^{ix}}{x} - i\pi$$

The integral on the large half-circle vanishes for large R (Jordan's Lemma). □

Exercise 14.3.15.

$$\int_{-\infty}^{\infty} dx \frac{\sin^2 x}{x^2} = \frac{1}{2} \operatorname{Re} \int_{-\infty}^{\infty} dx \frac{1 - e^{i2x}}{x^2} = \pi \tag{14.19}$$

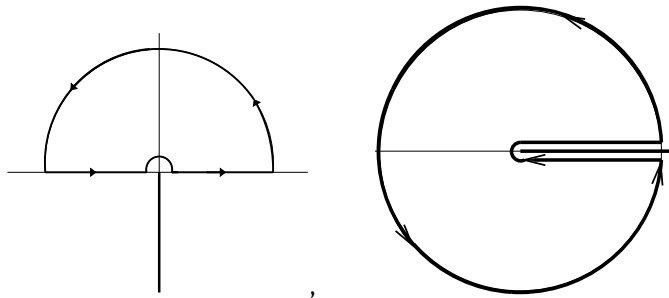


Figure 14.4 Left: Contour path with radii R and ϵ . The branch cut of the log is chosen as the negative imaginary axis. Right: the “keyhole” path, with branch cut in the positive real axis.

14.3.4 Integrals with branch cut

Certain integrals with log or non-integer powers can be evaluated by residues. We illustrate this by examples:

Example 14.3.16.

$$\int_0^\infty dx x^{a-1} \frac{\log x}{x^2 + 1}, \quad 0 < a < 2 \tag{14.20}$$

Use the contour γ shown in Fig.14.4 (left); the log function is chosen with the cut on the imaginary half-line. The integral is evaluated with the residue at the simple pole $z = i$:

$$\oint_{\gamma} dz e^{(a-1)\log z} \frac{\log z}{z^2 + 1} = 2\pi i \lim_{z \rightarrow i} (z - i) e^{(a-1)\log z} \frac{\log z}{z^2 + 1} = \frac{\pi^2}{2} e^{ia\pi/2}$$

The same integral is the sum of two integrals on the real half-lines and the integrals on the semicircles, which are zero for $R \rightarrow \infty$ and $\epsilon \rightarrow 0$. Then

$$\begin{aligned} &= \int_{-\infty}^0 dx e^{(a-1)(\log|x|+i\pi)} \frac{\log|x|+i\pi}{x^2+1} + \int_0^{\infty} dx x^{a-1} \frac{\log x}{x^2+1} \\ &= (1 - e^{i a \pi}) \int_0^{\infty} dx x^{a-1} \frac{\log x}{x^2+1} - i \pi e^{i a \pi} \int_0^{\infty} dx \frac{x^{a-1}}{x^2+1} \end{aligned}$$

Separation of real and imaginary parts gives two integrals:

$$\int_0^{\infty} dx \frac{x^{a-1}}{x^2+1} = \frac{\pi}{2 \sin(a\pi/2)}, \quad \int_0^{\infty} dx \frac{x^{a-1}}{x^2+1} \log x = -\frac{\pi^2 \cos(\pi a/2)}{4 \sin^2(\pi a/2)} \quad (14.21)$$

Example 14.3.17.

$$\int_0^{\infty} dx x^{a-1} \frac{\log x}{x+1}, \quad 0 < a < 1 \quad (14.22)$$

The path of the previous example does not help. The appropriate path is the keyhole path (see Fig.14.4), with the log cut chosen as the real positive half-line. The integral is evaluated with the residue at the simple pole $z = -1$:

$$\oint_{\gamma} dz e^{(a-1)\log z} \frac{\log z}{z+1} = 2\pi i \lim_{z \rightarrow -1} (z+1) e^{(a-1)\log z} \frac{\log z}{z+1} = 2\pi^2 e^{i a \pi}$$

The same integral is the sum of two integrals on two half-lines: the first one is just above the branch cut ($z = x + i\epsilon$, $\arg z = 0$), the second one is just below the branch cut and with opposite orientation ($z = x - i\epsilon$, $\arg z = i2\pi$). The large and small circles do not contribute. Then:

$$\begin{aligned} &= \int_0^{\infty} dx x^{a-1} \frac{\log x}{x+1} - \int_0^{\infty} dx e^{(a-1)(\log|x|+i2\pi)} \frac{\log|x|+i2\pi}{x+1} \\ &= (1 - e^{i2a\pi}) \int_0^{\infty} dx x^{a-1} \frac{\log x}{x+1} - i2\pi e^{i2a\pi} \int_0^{\infty} dx \frac{x^{a-1}}{x+1} \end{aligned}$$

By separating real and imaginary parts we obtain two integrals:

$$\int_0^{\infty} dx \frac{x^{a-1}}{x+1} = \frac{\pi}{\sin(a\pi)}, \quad (14.23)$$

$$\int_0^{\infty} dx \frac{x^{a-1}}{x+1} \log x = -\pi^2 \frac{\cos(\pi a)}{\sin^2(\pi a)} \quad (14.24)$$

Note that the integral with the log (and powers of the log) may be obtained by derivatives in the parameter a of the first integral. \square

Exercise 14.3.18.

$$1) \int_0^{\infty} dx \frac{\sqrt{x}}{x^3+1} = \frac{\pi}{3}, \quad \int_0^{\pi/2} dx (\tan x)^p = \frac{\pi}{2 \cos(p\frac{\pi}{2})}, \quad |p| < 1$$

$$2) \int_0^{\infty} dx \frac{x^{-1/3}}{x+1} = \frac{2\pi}{\sqrt{3}}, \quad \int_0^{\infty} dx \frac{x^{3/4}}{(x+1)^3} = \frac{3\sqrt{2}}{32} \pi$$

$$3) \int_0^{\infty} dx \frac{x^{1/4}}{(x+1)^2} = \frac{\pi}{2\sqrt{2}}, \quad \int_0^{\infty} dx \frac{x^{-1/n}}{(x+1)^2} = \frac{\pi/n}{\sin(\pi/n)}$$

$$4) \int_0^{\infty} dx \frac{\sqrt{x}}{x^3+x^2+x+1} = \frac{\pi}{2}(\sqrt{2}-1)$$

$$5) \int_0^{\infty} dx \frac{x^{\mu}}{x^2-2x \cos \theta + 1} = \pi \frac{\sin \mu(\pi-\theta)}{\sin \theta \sin(\mu\pi)}, \quad |\mu| < 1.$$

14.3.5 Integrals of exponential, hyperbolic functions

The exponential and the hyperbolic functions are periodic on the imaginary axis, so the trick of closing $[-R, R]$ with a semicircle at infinity does not work (the extra integral does not vanish). One rather exploits periodicity to close the path by a rectangle, such that the function on the new side $[-R + ih, R + ih]$ has a simple relation with the function on the real interval. The trick was used for the Fourier transform of the Gaussian function, (8.2). Here is another example:

Example 14.3.19.

$$\int_{-\infty}^{+\infty} dx \frac{e^{\alpha x}}{1+e^x} = \frac{\pi}{\sin(\pi\alpha)} \quad 0 < \operatorname{Re} \alpha < 1 \quad (14.25)$$

The integral is well defined. The denominator is unchanged when x is replaced by $x + i2\pi$. We then consider the rectangular path of corners $\pm R, \pm R + i2\pi$. It surrounds a simple pole

at $i\pi$. The residue theorem gives:

$$\oint_{\partial R} dz \frac{e^{\alpha z}}{1+e^z} = -2\pi i e^{i\alpha\pi}$$

For $R \rightarrow \infty$ the same integral evaluated on the contour is:

$$(1 - e^{i2\alpha\pi}) \int_{-\infty}^{+\infty} dx \frac{e^{\alpha x}}{1+e^x}$$

The equality of the two evaluations gives the integral.

Example 14.3.20.

$$\int_{\mathbb{R}} dx \frac{\cos(xy)}{\cosh x} = \frac{\pi}{\cosh(\frac{\pi}{2}y)} \quad (14.26)$$

The integral on $[-R, R]$ is closed by the rectangle with vertices $(\pm R, 0)$, $(\pm R, i\pi)$, where $\cosh(x+i\pi) = -\cosh x$ and the integrals on the short sides vanish for $R \rightarrow \infty$. The rectangle encloses the simple pole $i\pi/2$. The residue gives:

$$2\pi i \lim_{z \rightarrow i\frac{\pi}{2}} \left(z - i\frac{\pi}{2} \right) \frac{\cos(zy)}{\cosh z} = 2\pi \cosh\left(\frac{\pi}{2}y\right)$$

the same integral evaluated on the boundary is:

$$\begin{aligned} &= \int_{\mathbb{R}} dx \frac{\cos xy}{\cosh x} - \int_{\mathbb{R}} dx \frac{\cos y(x+i\pi)}{\cosh(x+i\pi)} \\ &= [1 + \cosh(\pi y)] \int_{\mathbb{R}} dx \frac{\cos xy}{\cosh x} - i \sinh(\pi y) \int_{\mathbb{R}} dx \frac{\sin xy}{\cosh x} \end{aligned}$$

The last integral is zero (odd function on symmetric domain), then the integral is $2\pi \cosh(\frac{\pi}{2}y) / [1 + \cosh(\pi y)]$, use the identity $2 \cosh^2(z) = \cosh(2z) + 1$. \square

Exercise 14.3.21.

$$\int_{-\infty}^{+\infty} dx \frac{x^2}{\cosh x} = \frac{\pi^3}{4}, \quad \int_0^{\infty} dx \frac{\cos(2xy)}{\cosh^2 x} = \frac{\pi y}{\sinh(\pi y)} \quad (14.27)$$

Example 14.3.22.

$$\int_{-\infty}^{\infty} dk \frac{\sinh(ky)}{\sinh k} e^{ikx} = \pi \frac{\sin(\pi y)}{\cosh(\pi x) + \cos(\pi y)} \quad (0 < y < 1). \quad (14.28)$$

The integral, with the change $k \rightarrow -k$, becomes:

$$\int_{-\infty}^{\infty} \frac{dk}{2} \left[\frac{e^{k(y+ix)}}{\sinh k} + \frac{e^{k(y-ix)}}{\sinh k} \right] = \operatorname{Re} \int_{-\infty}^{\infty} dk \frac{e^{k(y+ix)}}{\sinh k}.$$

Since $\sinh(z + i\pi) = -\sinh z$, one considers a rectangle with corners $-u$, v , $v + i\pi$, $-u + i\pi$, where $u, v \rightarrow \infty$. Two sides are deformed by small half-circles of radius ϵ to exclude the singular points $k = 0, i\pi$ from the interior of the rectangle. By Cauchy's formula the loop-integral is zero, and the integrals on the sides parallel to the imaginary axis vanish in the limit. Then:

$$\begin{aligned} 0 &= \left[1 + e^{i\pi(y+ix)} \right] \int_{-\infty}^{\infty} dk \frac{e^{k(y+ix)}}{\sinh k} - \int_0^{\pi} i\epsilon e^{i\theta} d\theta \frac{e^{\epsilon e^{i\theta}(y+ix)}}{\sinh(\epsilon e^{i\theta})} \\ &\quad - \int_{\pi}^{2\pi} i\epsilon e^{i\theta} d\theta \frac{e^{(i\pi + \epsilon e^{i\theta})(y+ix)}}{\sinh(i\pi + \epsilon e^{i\theta})} \end{aligned}$$

Therefore:

$$\int_{-\infty}^{\infty} dk \frac{e^{k(y+ix)}}{\sinh k} = i\pi \frac{e^{\pi x} - e^{i\pi y}}{e^{\pi x} + e^{i\pi y}} \quad (14.29)$$

The real part gives the integral. □

14.3.6 Other examples

Example 14.3.23.

$$\int_0^{\infty} dx \frac{1}{x^5 + 1} = \frac{\pi/5}{\sin(\pi/5)}, \quad \int_0^{\infty} dx \frac{\log x}{x^5 + 1} = -\left(\frac{\pi}{5}\right)^2 \frac{\cos(\pi/5)}{\sin^2(\pi/5)} \quad (14.30)$$

The denominator remains unchanged if x is replaced by $x e^{i2\pi/5}$. This suggests to close the real positive line with an arc of amplitude $2\pi/5$ and the radial line $z = x e^{i2\pi/5}$ (the second integral requires the first one).

Exercise 14.3.24.

$$\int_0^{\infty} dx \frac{x^3}{x^8 + 1} = \frac{\pi}{8} \quad (14.31)$$

Example 14.3.25.

$$\int_0^{\infty} dx \frac{\log x}{x^2 - 1} = \frac{\pi^2}{4} \quad (14.32)$$

The cut is chosen away from the real positive axis, and the point $x = 1$ is a removable singularity. If x is replaced by ix the integral is simple to evaluate. Therefore, integrate on the closed path formed by $[0, R]$, the circle $\text{Re}^{i\theta}$ $0 < \theta < \frac{\pi}{2}$ and the segment $[iR, 0]$, $R \rightarrow \infty$.

Example 14.3.26.

$$\int_0^{\infty} dx \frac{\log(x^2 + 1)}{x^2 + 1} = \pi \log 2 \quad (14.33)$$

Evaluate $\oint_{\gamma} dz \log(z + i)/(z^2 + 1)$ where γ is the real axis closed by a semicircle in the upper half plane. The cut of $\log(z + i)$ is any line connecting $-i$ to infinity, for example the line $[-i, -i\infty)$.

Example 14.3.27.

$$\int_0^{\infty} dx \frac{\log x}{(x + a)(x + b)} = \frac{1}{2} \frac{(\log b)^2 - (\log a)^2}{b - a} \quad (14.34)$$

If the keyhole path is considered, the integral is cancelled by the integral on the other side of the cut. The trick here is to evaluate the keyhole integral of the function $(\log z)^2/(z + a)(z + b)$ (see P. Nahin, *Inside interesting integrals*, Springer 2015).

The Mathematics Stack Exchange is a website devoted to questions and answers at any level. This link addresses to hundreds of questions on contour integrals: <http://math.stackexchange.com/questions/tagged/contour-integration>.

14.4 Enumeration of zeros and poles*

Theorem 14.4.1. Let $f(z)$ be meromorphic in D and γ a Jordan curve in D . If z_1, \dots, z_n are the zeros (of order k_1, \dots, k_n) and p_1, \dots, p_m are the poles (of order q_1, \dots, q_m) of f encircled by γ , then:

$$\oint_{\gamma} \frac{dz}{2\pi i} \frac{f'(z)}{f(z)} = \sum_i k_i - \sum_j q_j. \quad (14.35)$$

Proof. A zero or a pole of f is a pole for f'/f . In a neighbourhood of a zero z_i , $f(z) = A_i(z - z_i)^{k_i} \varphi_i(z)$ with φ_i analytic. Then

$$\frac{f'(z)}{f(z)} = \frac{k_i}{(z - z_i)} + \frac{\varphi_i'(z)}{\varphi_i(z)}$$

with residue k_i . In a neighbourhood of a pole, $f(z) = (z - p_j)^{-q_j} \phi_j(z)$ with ϕ_j analytic. Then

$$\frac{f'(z)}{f(z)} = \frac{-q_j}{(z - p_j)} + \frac{\phi_j'(z)}{\phi_j(z)}$$

and the residue is $-q_j$. The integral is the sum of the residues of all zeros and singular points encircled by γ . \square

Exercise 14.4.2. Show that: $\int_{|z|=k\pi} \frac{dz}{2\pi i} \tan z = -2k$.

This beautiful theorem is useful for the location of zeros of analytic functions:

Theorem 14.4.3 (Rouché). *Let f and g be holomorphic functions on and inside a simple closed curve γ . If $|g(z)| < |f(z)|$ for all $z \in \gamma$, then f and $f + g$ have the same number of zeros inside γ .*

Proof. Since $|f| > |g|$ on γ it is $|f| \neq 0$ on γ and the variable $w = [f(z) + g(z)]/f(z)$ is well defined on γ . By the inequality $|w(z) - 1| < 1$, $z \in \gamma$, the image of the curve γ does not encircle the origin. By eq.(14.35)

$$\#(\text{zeros of } f + g) - \#(\text{zeros of } f) = \oint_{\gamma} \frac{dz}{2\pi i} \frac{w'(z)}{w(z)} = \frac{\Delta \arg w}{2\pi} = 0$$

(the zeros and poles of w are respectively the zeros of $f + g$ and of f). \square

Example 14.4.4. How many solutions of $e^z - 3z^4 + 5z = 0$ are in the disk $|z| < 2$?

Choose $f(z) = -3z^4 + 5z$ and $g(z) = e^z$. On the boundary $|g(z)| = e^{2\cos\theta}$, $|f(z)| = |48e^{4i\theta} - 10e^{i\theta}| > 38$. Since $|f| > |g|$, the number of solutions equals that of $3z^4 - 5z = 0$ in $|z| < 2$, which is 4.

14.5 Evaluation of sums*

The theorem of residues can be used to evaluate infinite sums by reducing them to sums on a finite number of residues.

The functions $\pi \cot(\pi z)$ and $\pi \operatorname{cosec}(\pi z)$ are meromorphic with simple poles on the real

axis at $z_n = n \in \mathbb{Z}$, and residues respectively equal to 1 and $(-1)^n$. If $f(z)$ is analytic in the neighbourhood of the integer n , then:

$$\operatorname{Res}[f(z)\pi \cot(\pi z), n] = f(n), \quad \operatorname{Res}[f(z)\pi \operatorname{cosec}(\pi z), n] = (-1)^n f(n).$$

Proposition 14.5.1. *Let $f(z)$ be meromorphic with a finite set of poles $\mathcal{P} = \{p_1, \dots, p_m\}$ and suppose that there is $K > 0$ such that $|z^2 f(z)| < K$ for all z with $|z|$ larger than some constant R . Then*

$$0 = \sum_{n \in \mathbb{Z} \setminus \mathcal{P}} f(n) + \sum_{k=1}^n \operatorname{Res}[f(z)\pi \cot(\pi z), p_k] \quad (14.36)$$

$$0 = \sum_{n \in \mathbb{Z} \setminus \mathcal{P}} (-1)^n f(n) + \sum_{k=1}^m \operatorname{Res}[f(z)\pi \operatorname{cosec}(\pi z), p_k] \quad (14.37)$$

Proof. To apply the theorem of residues, consider a square path \square with corners $\pm[n + \frac{1}{2} \pm i(n + \frac{1}{2})]$ big enough to include all poles p_k . Then:

$$\oint_{\square} \frac{d\zeta}{2\pi i} f(\zeta)g(\zeta) = \sum_a \operatorname{Res}[f(z)g(z), a]$$

where $a \in \{0, \pm 1, \dots, \pm n\} \cup \{p_1, \dots, p_m\}$, and $g(z)$ is either $\pi \cot(\pi z)$ or $\pi \operatorname{cosec}(\pi z)$. On the sides of the squares it is $|\cot(\pi z)| \leq 1$ and $|\operatorname{cosec}(\pi z)| < 1$. Then Darboux's inequality and the bound on f ensure that the contour integral vanishes for $n \rightarrow \infty$:

$$\left| \oint_{\square} \frac{d\zeta}{2\pi i} f(\zeta)g(\zeta) \right| \leq \frac{4(2n+1)}{2\pi} \frac{K}{(n+1/2)^2}$$

□

Corollary 14.5.2. *If f is meromorphic with poles in $p_1, \dots, p_m \notin \mathbb{Z}$, then*

$$\sum_{n=-\infty}^{\infty} f(n) = - \sum_{k=1}^m \operatorname{Res}[f(z)\pi \cot(\pi z), p_k] \quad (14.38)$$

$$\sum_{n=-\infty}^{\infty} (-1)^n f(n) = - \sum_{k=1}^m \operatorname{Res}[f(z)\pi \operatorname{cosec}(\pi z), p_k] \quad (14.39)$$

Example 14.5.3. *The function $f(\zeta) = 1/(\zeta^2 + z^2)$ has simple poles $\pm iz$. Then*

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + z^2} = \sum_{p=\pm iz} \operatorname{Res} \left[\frac{\pi \cot(\pi \zeta)}{\zeta^2 + z^2}, p \right] = \frac{\pi}{z} \coth(\pi z)$$

The result gives a representation for $\coth(\pi z)$:

$$\coth(\pi z) = \frac{1}{\pi z} + 2 \frac{z}{\pi} \sum_{n=1}^{\infty} \frac{1}{z^2 + n^2} \quad (14.40)$$

For $|z| < 1$ one may expand in geometric series: $\frac{1}{n^2 + z^2} = \sum_{\ell} (-1)^{\ell} \frac{z^{2\ell}}{n^{2+2\ell}}$. The exchange of sums is allowed because the series are absolutely convergent:

$$\coth(\pi z) = \frac{1}{\pi z} + \frac{2}{\pi} \sum_{\ell=0}^{\infty} (-1)^{\ell} z^{2\ell+1} \zeta(2+2\ell) \quad (14.41)$$

Comparison with eq.(11.12) reveals the relationship of Riemann's Zeta at even positive integers with Bernoulli numbers:

$$\zeta(2\ell) = \frac{1}{2} \frac{(2\pi)^{2\ell}}{(2\ell)!} |B_{2\ell}| \quad (14.42)$$

The replacement $z \rightarrow iz$ gives:

$$\cot(\pi z) = \frac{1}{\pi z} + 2 \frac{z}{\pi} \sum_{n=1}^{\infty} \frac{1}{z^2 - n^2}. \quad (14.43)$$

As $\cot(\pi z) = \frac{1}{\pi} \frac{d}{dz} \log \sin(\pi z)$ and $\frac{2z}{z^2 - n^2} = \frac{d}{dz} \log(z^2 - n^2)$, the famous product formula for the sine function results (Euler, 1734):

$$\sin(\pi z) = \pi z \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2} \right) \quad (14.44)$$

Example 14.5.4. Consider $f(z) = z^{-2}$, with a double pole at the origin.

$\sum_{n \neq 0} n^{-2} = -\text{Res}[\frac{\pi \cot(\pi z)}{z^2}, 0]$. The residue is evaluated with the rule for poles of order 3:

$$2\zeta(2) = -\frac{1}{2!} \lim_{z \rightarrow 0} \frac{d^2}{dz^2} \frac{\pi z \cos(\pi z)}{\sin(\pi z)}$$

A different way to evaluate the residue is to produce the Laurent series directly, from known series, and read c_{-1} : $\frac{\pi \cos(\pi z)}{z^2 \sin(\pi z)} = \frac{\pi [1 - (\pi z)^2/2! + \dots]}{z^3 \pi [1 - (\pi z)^2/3! + \dots]} = \frac{1}{z^3} - \frac{\pi^2}{3z} + \dots$. Then $c_{-1} = -\pi^2/3$ and

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

Chapter 15

Elliptic Functions*

The theory of elliptic functions, shaped by the masters Abel, Jacobi and Weierstrass, *is a treasurehouse of results whose variety, aesthetic appeal, and capacity of arousing our astonishment, has not since been equaled by research in any other area. But the circumstance that this theory can be applied to solve problems arising in many departments of science and engineering graces the topic with an additional aura ...*¹.

This is a short list of problems: pendulum, asymmetric top², geodesics in Schwarzschild metric³, Korteweg de Vries equation⁴, area of ellipsoid⁵, potential of a homogeneous ellipsoid, motion on ellipsoid⁶, the equation for $\lambda\varphi^4$ in $1d^7$, conformal mapping⁸ and related problems of electrostatics⁹, hydraulics; solitary waves¹⁰.

Before entering this realm of complex analysis, let us linger on related functions of real variable. As circular functions are first studied on the unit circle, extended to the real line, and then to the complex plane, let us introduce the angular “elliptic” sine and cosine, as Cayley named them. Later, they will be extended to the real line and to the complex plane.

¹ from the preface of Derek F. Lawden, *Elliptic Functions and Applications*, Springer-Verlag 1989. Other books: J. V. Armitage and W. F. Eberlein, *Elliptic Functions*, London Math. Soc. Student text 67, Cambridge 2006; A. L. Markushevich, *Theory of functions*, Chelsea 1985.

² L. D. Landau and E. M. Lifshitz, *Mechanics*, Pergamon Press 1976

³ G. Scharf, <https://doi.org/10.4236/jmp.2011.24036>

⁴ B. G. Dimitrov, <https://arxiv.org/abs/2301.00643>

⁵ NIST Handbook of Mathematical Functions, <https://dlmf.nist.gov/19.33>

⁶ P. Erdős, <https://aapt.scitation.org/doi/10.1119/1.1285882>

⁷ M. Frasca, <https://doi.org/10.1140/epjc/s10052-014-2929-9>

⁸ Z. Nehari, *Conformal mapping*, Dover Ed.

⁹ F Bowman, *Introduction to elliptic functions with applications*, Dover

¹⁰ S. Liu et al., [https://doi.org/10.1016/S0375-9601\(01\)00580-1](https://doi.org/10.1016/S0375-9601(01)00580-1)

15.1 The elliptic sine and cosine

The equation of the ellipse with semiaxes $b \leq a$

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$

has parametric representation $x = a \cos \theta$ and $y = b \sin \theta$.

The eccentricity $k = \sqrt{1 - (b/a)^2}$, is hereafter named the *modulus*, $0 \leq k < 1$. The distance of (x, y) from the origin is $r = \sqrt{x^2 + y^2} = a\sqrt{1 - k^2 \sin^2 \theta}$.

A function of the angle is now introduced (it is an elliptic integral):

$$u(\theta, k) = \int_0^\theta \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}} \quad (15.1)$$

A special value is $K = u(\frac{\pi}{2}, k)$ (a complete elliptic integral):

$$K = \int_0^{\frac{\pi}{2}} \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}} = \int_0^1 \frac{dx}{\sqrt{1 - x^2} \sqrt{1 - k^2 x^2}} \quad (15.2)$$

Both K and u depend on the modulus k . It is simple to show that

$$u\left(\theta + \frac{\pi}{2}, k\right) = K + u(\theta, k) \quad (15.3)$$

Then $u(\theta + 2\pi) = 4K + u(\theta)$. Modulo $4K$ and 2π , there is a one-to-one correspondence between u and θ , i.e. u and points $(x, y) = (a \cos \theta, b \sin \theta)$ of the ellipse. Special points are:

u	θ	(x, y)
0	0	$(a, 0)$
K	$\frac{\pi}{2}$	$(0, b)$
$2K$	π	$(-a, 0)$
$3K$	$\frac{3\pi}{2}$	$(0, -b)$
$4K$	2π	$(a, 0)$

By virtue of this correspondence, the elliptic cosine and sine are introduced as a new parametrization of the ellipse with eccentricity k :

$$x = a \operatorname{cn}(u|k), \quad y = b \operatorname{sn}(u|k)$$

$$\boxed{\operatorname{cn}(u|k) = \cos \theta, \quad \operatorname{sn}(u|k) = \sin \theta} \quad (15.4)$$

where now u is a parameter and $\theta = \theta(u, k)$ is obtained by inversion of eq.(15.1). They coincide with the circular functions if $k = 0$. One has the first property:

$$\boxed{\text{cn}^2(u|k) + \text{sn}^2(u|k) = 1} \tag{15.5}$$

A useful function, with no circular analogue, is

$$\text{dn}(u|k) = \sqrt{1 - k^2 \text{sn}^2(u|k)} \tag{15.6}$$

Some values of the functions are simply obtained by the trigonometric identification.

u	sn	cn	dn
0	0	1	1
K	1	0	$\sqrt{1 - k^2}$
$2K$	0	-1	1
$3K$	-1	0	$\sqrt{1 - k^2}$
$4K$	0	1	1

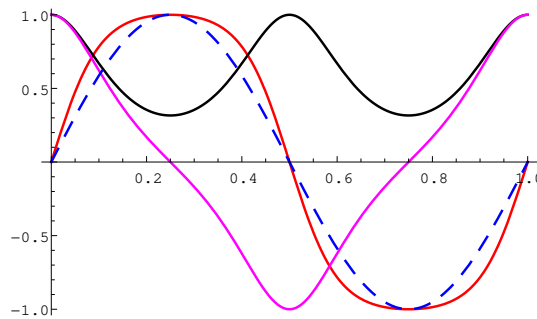


Figure 15.1 The functions $\text{sn}(4Kx|k)$ (red), $\text{cn}(4Kx|k)$ (fuchsia), $\text{dn}(4Kx|k)$ (black) with $k = 0.9$ and, for comparison, the function $\sin(2\pi x)$ (dashed). As k increases, the maxima and minima of sn become more rounded.

The property (15.3) reflects in the relation

$$\text{cn}(u + K|k) = \cos\left(\theta + \frac{\pi}{2}\right) = -\sin\theta = -\text{sn}(u|k)$$

and similarly: $\text{sn}(u + K|k) = \text{cn}(u|k)$, $\text{dn}(u + 2K|k) = \text{dn}(u|k)$. In particular, cn and sn have period $4K$ and dn has period $2K$.

15.1.1 Derivatives

Derivatives are easily obtained from $\text{sn}(u|k) = \sin \theta(u)$ etc.

$$\frac{d}{du} \text{sn}(u|k) = \frac{d\theta}{du} \cos \theta = \sqrt{1 - k^2 \sin^2 \theta} \cos \theta = \text{dn}(u|k) \text{cn}(u|k) \quad (15.7)$$

$$\frac{d}{du} \text{cn}(u|k) = -\text{dn}(u|k) \text{sn}(u|k) \quad (15.8)$$

$$\frac{d}{du} \text{dn}(u|k) = -k^2 \text{sn}(u|k) \text{cn}(u|k) \quad (15.9)$$

They imply the non-linear second-order differential equations:

$$\frac{d^2}{du^2} \text{sn}(u|k) = -(1 + k^2) \text{sn}(u|k) + 2k^2 \text{sn}^3(u|k) \quad (15.10)$$

$$\frac{d^2}{du^2} \text{cn}(u|k) = -(1 - 2k^2) \text{cn}(u|k) - 2k^2 \text{cn}^3(u|k) \quad (15.11)$$

$$\frac{d^2}{du^2} \text{dn}(u|k) = (2 - k^2) \text{dn}(u|k) - 2 \text{dn}^3(u|k) \quad (15.12)$$

Other equations are obtained by squaring the first derivatives; for example:

$$\left[\frac{d}{du} \text{sn}(u|k) \right]^2 = 1 - (1 + k^2) \text{sn}^2(u|k) + k^2 \text{sn}^4(u|k) \quad (15.13)$$

15.1.2 Summation formulae

The elliptic functions have summation rules, more involved than their circular cousins ($k = 0$). The specification of the modulus k is omitted for brevity.

$$\text{sn}(x_1 \pm x_2) = \frac{\text{sn}(x_1) \text{cn}(x_2) \text{dn}(x_2) \pm \text{sn}(x_2) \text{cn}(x_1) \text{dn}(x_1)}{1 - k^2 \text{sn}^2(x_1) \text{sn}^2(x_2)} \quad (15.14)$$

$$\text{cn}(x_1 \pm x_2) = \frac{\text{cn}(x_1) \text{cn}(x_2) \mp \text{sn}(x_1) \text{sn}(x_2) \text{dn}(x_1) \text{dn}(x_2)}{1 - k^2 \text{sn}^2(x_1) \text{sn}^2(x_2)} \quad (15.15)$$

$$\text{dn}(x_1 \pm x_2) = \frac{\text{dn}(x_1) \text{dn}(x_2) \mp k^2 \text{sn}(x_1) \text{sn}(x_2) \text{cn}(x_1) \text{cn}(x_2)}{1 - k^2 \text{sn}^2(x_1) \text{sn}^2(x_2)} \quad (15.16)$$

Proof. Let $s_1 = \text{sn}(x+x_1|k)$, $s_2 = \text{sn}(x+x_2|k)$, etc. A prime denotes a derivative in x . Multiply (15.10) for s_1 by s_2 , and subtract from it the equation with labels exchanged:

$$(s_2 s_1' - s_1 s_2')' = 2k^2 s_1 s_2 (s_1^2 - s_2^2)$$

Multiply (15.13) for s_1 by s_2^2 and subtract from it the equation with labels exchanged:

$$s_2^2(s_1')^2 - s_1^2(s_2')^2 = -(s_1^2 - s_2^2)(1 - k^2 s_1^2 s_2^2)$$

Divide the two equations and obtain:

$$\frac{(s_2 s_1' - s_1 s_2')'}{s_2 s_1' - s_1 s_2'} = -2k^2 \frac{s_1 s_2 (s_2 s_1' + s_1 s_2')}{1 - k^2 s_1^2 s_2^2} = \frac{(1 - k^2 s_1^2 s_2^2)'}{1 - k^2 s_1^2 s_2^2}$$

An integration gives $s_2 s_1' - s_1 s_2' = C(1 - k^2 s_1^2 s_2^2)$, where C is independent of x . With $s_i' = c_i d_i$ we obtain the algebraic relation valid for any x : $s_2 c_1 d_1 - s_1 c_2 d_2 = C(1 - k^2 s_1^2 s_2^2)$. For $x = -x_2$, it is $s_2 = 0$ and the identity gives $C = -\operatorname{sn}(x_1 - x_2|k)$. Eq.(15.14) follows, the others are similarly obtained. \square

Exercise 15.1.1. With $x_1 = x_2 = \frac{K}{2}$, obtain the special values:

$$\operatorname{sn}\left(\frac{K}{2} \middle| k\right) = \frac{1}{\sqrt{1+k'}}, \quad \operatorname{cn}\left(\frac{K}{2} \middle| k\right) = \frac{\sqrt{k'}}{\sqrt{1+k'}}, \quad \operatorname{dn}\left(\frac{K}{2} \middle| k\right) = \sqrt{k'}. \quad (15.17)$$

where $k' = \sqrt{1-k^2}$ is the complementary modulus.

15.2 Elliptic integrals

Elliptic integrals frequently arise in physics. They have the form

$$\int dx R\left(x, \sqrt{P(x)}\right)$$

where R is a rational function of the real variable x and of the square root of a cubic or quartic polynomial with real coefficients (a higher degree defines hyperelliptic integrals). Legendre showed that any elliptic integral may be expressed as a combination of three canonical elliptic integrals, introduced in the following examples¹¹.

• **Elliptic integrals of the first kind.** A pendulum of length L oscillates with maximal angle ϕ_0 from the vertical. Energy conservation poses:

$$\frac{1}{2}L^2\dot{\phi}^2 = gL(\cos\phi - \cos\phi_0) = 2gL\left[\sin^2\left(\frac{\phi_0}{2}\right) - \sin^2\left(\frac{\phi}{2}\right)\right]$$

¹¹ A specialized book is P. F. Byrd and M. D. Friedman, *Handbook of Elliptic Integrals for Engineers and Scientists*, 2nd ed. 1971, Springer-Verlag. A different treatment is based on the symmetric integrals of the I, II, III kind; see NIST: <https://dlmf.nist.gov/19>.

The time to swing from 0 to ϕ is:

$$t(\phi) = \frac{1}{2} \sqrt{\frac{L}{g}} \int_0^\phi \frac{d\phi'}{\sqrt{\sin^2(\phi_0/2) - \sin^2(\phi'/2)}},$$

The period of the pendulum is $T = 4t(\phi_0)$. For small oscillations the period is independent of the amplitude, $T_0 = 2\pi\sqrt{L/g}$.

The change of variable $\sin(\phi/2) = k \sin \theta$ with $k = \sin(\phi_0/2)$, gives

$$t = \sqrt{\frac{L}{g}} \int_0^\theta \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}}, \quad T = T_0 \frac{2}{\pi} \int_0^{\pi/2} \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}}$$

The two integrals are the incomplete and the complete elliptic integrals of the first kind:

$$F(\theta, k) = \int_0^\theta \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}}, \quad K(k) = \int_0^{\pi/2} \frac{d\theta'}{\sqrt{1 - k^2 \sin^2 \theta'}} \quad (15.18)$$

Note that the incomplete integral $F(\theta, k)$ is exactly the function $u(\theta, k)$ in eq.(15.1). Then $t = \sqrt{\frac{L}{g}} u(\theta, k)$. The period of the pendulum $T = T_0 \frac{2}{\pi} K(k)$ depends on the amplitude through $k = \sin \frac{\phi_0}{2}$. If ϕ_0 nears π the period diverges.

The angle as a function of time is

$$\sin \frac{\phi}{2} = k \sin \theta = k \operatorname{sn}(u|k) = \sin \frac{\phi_0}{2} \operatorname{sn} \left(\frac{2\pi t}{T_0} \middle| k \right)$$

• **Elliptic integrals of the second kind.** They arise in the evaluation of the arc-length of the ellipse. If $x = a \cos \theta$, $y = b \sin \theta$, then $ds^2 = dx^2 + dy^2 = a^2(1 - k^2 \cos^2 \theta) d\theta^2$ (k is the eccentricity). The length of the elliptic arc with an extremum in $(0, b)$ is the integral

$$L(\theta) = a \int_{\pi/2}^{\pi/2+\theta} d\theta' \sqrt{1 - k^2 \cos^2 \theta'} = a \int_0^\theta d\theta' \sqrt{1 - k^2 \sin^2 \theta'}$$

The incomplete and complete elliptic integrals of the second kind are:

$$E(\theta, k) = \int_0^\theta d\theta' \sqrt{1 - k^2 \sin^2 \theta'}, \quad E(k) = \int_0^{\pi/2} d\theta' \sqrt{1 - k^2 \sin^2 \theta'} \quad (15.19)$$

Then $L(\theta) = aE(\theta, k)$. The perimeter is $4L(\frac{\pi}{2}) = 4aE(k)$.

• **Elliptic integral of the third kind:**

$$\Pi(\theta, \alpha, k) = \int_0^\theta \frac{d\theta'}{(1 + \alpha^2 \sin^2 \theta') \sqrt{1 - k^2 \sin^2 \theta'}} \quad (15.20)$$

The complete elliptic integrals K , E , $K' \equiv K(k')$ and $E' \equiv E(k')$ are linked by Legendre's relation:

$$KE' + K'E - KK' = \frac{\pi}{2} \quad (15.21)$$

The change of variable $x = \sin \theta'$ transforms the integrals F , E and Π into:

$$F(u|k) = \int_0^u \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}}, \quad E(u|k) = \int_0^u dx \sqrt{\frac{1-k^2x^2}{1-x^2}},$$

$$\Pi(u|\alpha, k) = \int_0^u \frac{dx}{(1+\alpha^2x^2)\sqrt{(1-x^2)(1-k^2x^2)}}$$

15.2.1 Reduction of elliptic integrals

Example 15.2.1. *In these examples $a < x < b < c$. The reduction to the Legendre forms is obtained with the replacement $x' = a + (b-a)\sin^2 \theta'$.*

$$1) \int_a^x \frac{dx'}{\sqrt{(x'-a)(b-x')(c-x')}} = \frac{2}{\sqrt{c-a}} F\left(\theta, \sqrt{\frac{b-a}{c-a}}\right), \quad \sin^2 \theta = \frac{x-a}{b-a}$$

$$2) \int_a^x \frac{x' dx'}{\sqrt{(x'-a)(b-x')(c-x')}}$$

$$= \int_a^x dx' \left[\frac{c}{\sqrt{(x'-a)(b-x')(c-x')}} - \sqrt{\frac{c-x'}{(x'-a)(b-x')}} \right]$$

$$= \frac{2c}{\sqrt{c-a}} F\left(\theta, \sqrt{\frac{b-a}{c-a}}\right) - 2\sqrt{c-a} E\left(\theta, \sqrt{\frac{b-a}{c-a}}\right)$$

Example 15.2.2. *Elliptic functions are useful to evaluate elliptic integrals.*

$$\int_0^x \frac{dx'}{\sqrt{x'(1-x')(c-x')(d-x')}} \quad x \leq 1 \leq c \leq d$$

We make the standard change of variable

$$x = \frac{A_1 + A_2 \operatorname{sn}^2(u|k)}{A_3 + A_4 \operatorname{sn}^2(u|k)}, \quad 0 \leq u \leq K$$

where parameters are chosen in order that $dx/\sqrt{P(x)} = du$ up to a constant.

As $0 \leq x' \leq 1$, we require $x = 0$ for $u = 0$ and $x = 1$ for $u = K$. Then $A_1 = 0$ and $A_2 = A_3 + A_4$. $q = A_4/A_3$ is still a

free parameter.

$$x = \frac{(1+q)\operatorname{sn}^2(u|k)}{1+q\operatorname{sn}^2(u|k)}, \quad dx = 2(1+q) \frac{\operatorname{sn}(u|k)\operatorname{cn}(u|k)\operatorname{dn}(u|k)}{[1+q\operatorname{sn}^2(u|k)]^2}$$

$$\frac{dx}{\sqrt{P(x)}} = 2\sqrt{\frac{1+q}{cd}} \frac{\operatorname{dn}(u|k) du}{\sqrt{1-(1/c+q/c-q)\operatorname{sn}^2(u|k)} \sqrt{1-(1/d+q/d-q)\operatorname{sn}^2(u|k)}}$$

Set $q = 1/(d-1)$ and $k^2 = 1/c + q/c - q = (d-c)/[c(d-1)]$ to eliminate one of the square roots and cancel the other with $\operatorname{dn}(u|k)$. Then:

$$\int_0^x \frac{dx}{\sqrt{P(x)}} = 2 \frac{1}{\sqrt{c(d-1)}} u = 2 \frac{1}{\sqrt{c(d-1)}} F\left(\sqrt{\frac{x(d-1)}{d-x}} \middle| \sqrt{\frac{d-c}{c(d-1)}}\right)$$

15.3 Jacobi Elliptic functions

The functions sn , cn and dn are extended from real to complex variable. Their properties illustrate the general theory of elliptic functions.

The purely imaginary argument is introduced as follows. In the integral (15.1) with $\theta < \pi/2$, put $k^2 = 1 - k'^2$:

$$u = \int_0^\theta \frac{d\theta'}{\sqrt{\cos^2\theta' + k'^2 \sin^2\theta'}} = \int_0^\theta \frac{d\theta'}{\cos\theta'} \frac{1}{\sqrt{1 + k'^2 \tan^2\theta'}}$$

Now make the change $\sinh x' = \tan\theta'$, and obtain another integral for u :

$$u = \int_0^x \frac{dx'}{\sqrt{1 + k'^2 \sinh^2 x'}}, \quad \sinh x = \tan\theta = \frac{\operatorname{sn}(u|k)}{\operatorname{cn}(u|k)}$$

On noting that $\sinh x = -i \sin(ix)$,

$$iu = \int_0^{ix} \frac{dx'}{\sqrt{1 - k'^2 \sin^2 x'}}, \quad \sin(ix) = i \frac{\operatorname{sn}(u|k)}{\operatorname{cn}(u|k)}$$

The last relation defines the Jacobi elliptic function with imaginary argument, where we exchange k' with k :

$$\boxed{\operatorname{sn}(iu|k) = i \frac{\operatorname{sn}(u|k')}{\operatorname{cn}(u|k')}} \quad (15.22)$$

Accordingly, the other functions with imaginary argument are:

$$\operatorname{cn}(iu|k) = \cosh x = \frac{1}{\operatorname{cn}(u|k')}, \quad (15.23)$$

$$\operatorname{dn}(iu|k) = \sqrt{1 - k^2 \operatorname{sn}^2(iu|k)} = \frac{\operatorname{dn}(u|k')}{\operatorname{cn}(u|k')} \quad (15.24)$$

The Jacobi functions $\operatorname{sn}(u|k')$ and $\operatorname{cn}(u|k')$ change sign for a shift $u \rightarrow u + 2K'$, and have period $2K'$. It follows that $\operatorname{sn}(iu + i2K'|k) = \operatorname{sn}(iu|k)$, $\operatorname{cn}(iu + i2K'|k) = -\operatorname{cn}(iu|k)$, $\operatorname{dn}(iu + i2K'|k) = \operatorname{dn}(iu|k)$.

As one may check, they obey the same differential equations and addition rules as the functions with real argument.

The Jacobi elliptic functions with argument $z = x + iy$ are *defined* through the summation formulae:

$$\begin{aligned} \operatorname{sn}(z|k) &= \frac{\operatorname{sn}(x|k)\operatorname{cn}(iy|k)\operatorname{dn}(iy|k) + \operatorname{cn}(x|k)\operatorname{dn}(x|k)\operatorname{sn}(iy|k)}{1 - k^2 \operatorname{sn}^2(x|k)\operatorname{sn}^2(iy|k)} \\ &= \frac{\operatorname{sn}(x|k)\operatorname{dn}(y|k') + i \operatorname{cn}(x|k)\operatorname{dn}(x|k)\operatorname{sn}(y|k')\operatorname{cn}(y|k')}{1 - \operatorname{dn}^2(x|k)\operatorname{sn}^2(y|k')} \end{aligned} \quad (15.25)$$

$$\operatorname{cn}(z|k) = \frac{\operatorname{cn}(x|k)\operatorname{cn}(y|k') - i \operatorname{sn}(x|k)\operatorname{dn}(x|k)\operatorname{sn}(y|k')\operatorname{dn}(y|k')}{1 - \operatorname{dn}^2(x|k)\operatorname{sn}^2(y|k')} \quad (15.26)$$

$$\operatorname{dn}(z|k) = \frac{\operatorname{dn}(x|k)\operatorname{cn}(y|k')\operatorname{dn}(y|k') - i k^2 \operatorname{sn}(x|k)\operatorname{cn}(x|k)\operatorname{sn}(y|k')}{1 - \operatorname{dn}^2(x|k)\operatorname{sn}^2(y|k')} \quad (15.27)$$

The summation formulae (15.14), (15.15), (15.16), derivatives and the differential equations remain valid when z replaces x .

Some useful properties are listed:

$$\overline{\operatorname{sn}(z|k)} = \operatorname{sn}(\bar{z}|k), \quad \overline{\operatorname{cn}(z|k)} = \operatorname{cn}(\bar{z}|k), \quad \overline{\operatorname{dn}(z|k)} = \operatorname{dn}(\bar{z}|k) \quad (15.28)$$

w	$\operatorname{sn}(w k)$	$\operatorname{cn}(w k)$	$\operatorname{dn}(w k)$
$z + K$	$\frac{\operatorname{cn}(z k)}{\operatorname{dn}(z k)}$	$-k' \frac{\operatorname{sn}(z k)}{\operatorname{dn}(z k)}$	$k' \frac{1}{\operatorname{dn}(z k)}$
$z + 2K$	$-\operatorname{sn}(z k)$	$-\operatorname{cn}(z k)$	$\operatorname{dn}(z k)$
$z + iK'$	$\frac{1}{k \operatorname{sn}(z k)}$	$-i \frac{\operatorname{dn}(z k)}{k \operatorname{sn}(z k)}$	$-i \frac{\operatorname{cn}(z k)}{\operatorname{sn}(z k)}$
$z + 2iK'$	$\operatorname{sn}(z k)$	$-\operatorname{cn}(z k)$	$-\operatorname{dn}(z k)$

Proposition 15.3.1. *The Jacobi elliptic functions are doubly periodic. For all integers n_1, n_2 :*

$$\operatorname{sn}(z + n_1 4K + n_2 2iK' | k) = \operatorname{sn}(z | k), \quad (15.29)$$

$$\operatorname{cn}(z + n_1 4K + n_2 (2K + i2K') | k) = \operatorname{cn}(z | k), \quad (15.30)$$

$$\operatorname{dn}(z + n_1 2K + n_2 4iK' | k) = \operatorname{dn}(z | k). \quad (15.31)$$

- In the rectangle $0 \leq \operatorname{Re} z < 4K, 0 \leq \operatorname{Im} z < 2K'$, the function $\operatorname{sn}(z|k)$ has two simple zeros at $z = 0, z = 2K$, and two simple poles at $z = iK', z = 2K + iK'$ with residues $1/k, -1/k$.
- In the parallelogram with vertices $0, 4K, 6K + i2K', 2K + i2K'$ the function $\operatorname{cn}(z|k)$ has two simple zeros at $z = K, z = 3K$, and two simple poles at $z = K + iK', z = 3K + iK'$ with residues $1/k, -1/k$.
- In the rectangle $0 \leq \operatorname{Re} z < 2K, 0 \leq \operatorname{Im} z < 4K'$ the function $\operatorname{dn}(z|k)$ has two simple zeros at $z = K + iK', z = K + i3K'$, and two simple poles at $z = iK', z = 2K + iK'$ with residues $-i, i$.

It turns out that for the three elliptic functions:

- 1) the sum of the residues is zero,
- 2) the number of zeros equals the number of poles,
- 3) the sum of the zeros equals the sum of the poles modulo a lattice vector.

15.3.1 Conformal map for the rectangle

Jacobi Elliptic functions define useful conformal transformations, the basic one being *the map of the rectangle onto the upper half or quarter plane*.

Proposition 15.3.2. *The analytic function $w \rightarrow z = \operatorname{sn}(w|k)$ maps the rectangle $\mathcal{R} = \{w : 0 < \operatorname{Re} w < K, 0 < \operatorname{Im} w < K'\}$ conformally on the first quadrant of the z plane.*

Proof. Let $w = u + iv$ and $z = x + iy$. In components the map is:

$$x = \frac{\operatorname{sn}(u|k) \operatorname{dn}(v|k')}{1 - \operatorname{dn}^2(u|k) \operatorname{sn}^2(v|k')}, \quad y = \frac{\operatorname{cn}(u|k) \operatorname{dn}(u|k) \operatorname{sn}(v|k') \operatorname{cn}(v|k')}{1 - \operatorname{dn}^2(u|k) \operatorname{sn}^2(v|k')}$$

If $w \in \mathcal{R}$ then: $x \geq 0, y \geq 0$, and $\operatorname{sn}'(w|k) = \operatorname{cn}(w|k) \operatorname{dn}(w|k) \neq 0$; therefore \mathcal{R} is mapped in the first quadrant, and the map is injective.

It is sufficient to obtain the image of the boundary of the rectangle.

- 1) $\{(u, 0), 0 < u < K\}$, is mapped to $\{(x, 0), 0 < x < 1\}$ where $x = \operatorname{sn}(u|k)$;
- 2) $\{(K, v), 0 < v < K'\}$ is mapped to $\{(x, 0), 1 < x < 1/k^2\}$ where $x = 1/\operatorname{dn}(v|k')$;
- 3) $\{(u, K'), 0 < u < K\}$ is mapped to $\{(x, 0), 1/k^2 < x < \infty\}$ where $x = 1/[k^2 \operatorname{sn}(u|k)]$.

Three sides of the rectangle are mapped to the positive real axis. As the point ∞ is reached, the image of the rectangle's boundary descends to the origin along the imaginary axis:

- 4) $\{(0, v), 0 < v < K'\}$ is mapped to $\{(0, y), 0 < y < \infty\}$ where $y = \operatorname{sn}(v|k')/\operatorname{cn}(v|k')$. \square

The corners of \mathcal{R} : $0, K, K + iK'$ and iK' , are mapped to $0, 1, 1/k^2$ and ∞ . At the corner $\omega = 0$ the map is analytic with nonzero derivative; therefore the right angle of the rectangle is mapped to the right angle at $z = 0$.

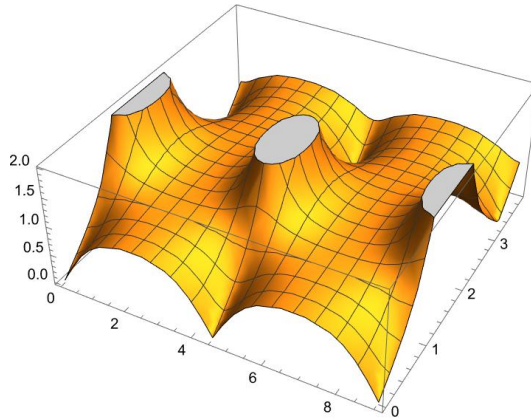


Figure 15.2 The function $|\operatorname{sn}(z|k)|$ for z in the fundamental rectangle of sides $4K \times 2K'$, for $k = 0.8$ ($K = 2.5721, K' = 1.94957$). The quarter-rectangle $K \times K'$ is mapped to the half-plane: $0 \rightarrow 0, K \rightarrow 1, iK' \rightarrow \infty, K + iK' \rightarrow 1/k^2$. (Mathematica)

15.4 Doubly periodic functions

A complex function f is *periodic* if there is a complex number ω (the period) such that $f(z + \omega) = f(z)$ for all z . The exponential and the hyperbolic functions are periodic with $\omega = 2\pi i$, the trigonometric functions are periodic with $\omega = 2\pi$.

A function is *doubly periodic* if there are *two* periods ω and ω' , not proportional by a real number, such that¹²:

$$f(z + \omega) = f(z) \quad \text{and} \quad f(z + \omega') = f(z), \quad \forall z \in \mathbb{C}$$

Although Gauss was aware of doubly periodic functions, the subject was disclosed in 1827 by Niels H. Abel, and developed further by Jacobi and Weierstrass.

The points $n\omega + n'\omega'$, $n, n' \in \mathbb{Z}$, form a lattice in \mathbb{C} , and the cell with corners $0, \omega, \omega + \omega', \omega'$ is a fundamental parallelogram. The values of f in it determine the function everywhere.

A doubly periodic entire function is necessarily constant (being continuous on the parallelogram - a compact set- it is bounded, but then it is bounded on \mathbb{C} by periodicity, i.e. it is constant by Liouville's theorem). We then have to allow for isolated poles.

¹² Jacobi proved that a non-constant single-valued analytic function whose singularities do not have limit points at finite distance cannot have more than two periods, not proportional by a real factor

Definition 15.4.1. An elliptic function is a doubly periodic meromorphic function. The number of poles (counted with their order) inside a fundamental parallelogram, is the order of the elliptic function.

A famous example is the Weierstrass elliptic function (1872):

$$\wp(z) = \frac{1}{z^2} + \sum_{m,n \neq 0} \left[\frac{1}{(z - m\omega - n\omega')^2} - \frac{1}{(m\omega - n\omega')^2} \right] \quad (15.32)$$

It has a second order pole at each site of the lattice $m\omega + n\omega'$. For a review and applications see <https://arxiv.org/pdf/1706.07371.pdf>.

These properties hold for elliptic functions:

Proposition 15.4.2. Let $f(z)$ be an elliptic function with poles p_k and zeros z_k inside a fundamental parallelogram:

- 1) the sum of the residues is zero;
- 2) the number of zeros equals the number of poles (both counted with their order), i.e. an elliptic function takes each complex value a number of times equal to its order;
- 3) the sum of the zeros minus the sum of the poles is a lattice point;
- 4) If two elliptic functions f and g have the same periods, then there is a polynomial $P(z, z')$ with constant coefficients such that $P(f(z), g(z)) = 0$. In particular, f satisfies a differential equation of the type $P(f(z), f'(z)) = 0$.

Chapter 16

Quaternions and Beyond*

16.1 Quaternions and vector calculus.

After the successful axiomatic construction of \mathbb{C} as the set of pairs of real numbers $(a, b) = a + ib$, with vector sum and distributive product with the rule $i^2 = -1$, W. R. Hamilton eagerly tried to construct of a new number field with triplets (a, b, c) . After years of efforts, in 1843, he realized that a consistent multiplication could be defined for quadruplets (a, b, c, d) , which he called *quaternions*.

With three units $I = (0, 1, 0, 0)$, $J = (0, 0, 1, 0)$, $K = (0, 0, 0, 1)$, a quaternion is a number $q = a + bI + cJ + dK$, where a, b, c, d are real numbers. Besides the vector sum, multiplications are done with the rules $I^2 = J^2 = K^2 = -1$ and

$$IJ = -JI = K, \quad JK = -KJ = I, \quad KI = -IK = J$$

The set \mathbb{H} of quaternions is a non-commutative algebra with conjugation $q^\dagger = a - bI - cJ - dK$ and $(q_1 q_2)^\dagger = q_2^\dagger q_1^\dagger$. \mathbb{H} has the inner product $(q|p) = \frac{1}{2}(q^\dagger p + p^\dagger q)$. The norm of a quaternion is $\|q\| = \sqrt{(q|q)} = \sqrt{a^2 + b^2 + c^2 + d^2}$, with the property $\|qp\| = \|q\| \|p\|$ ¹.

A realization of the quaternion basis is given with the 2×2 complex Pauli matrices: $1 = \sigma_0$ (the unit 2×2 matrix), $I = i\sigma_3$, $J = i\sigma_2$ and $K = i\sigma_1$, where the Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (16.1)$$

¹ The rule implies a nontrivial identity: given integers m_i and n_i there are integers p_i ($i = 1, 2, 3, 4$) such that $(m_1^2 + m_2^2 + m_3^2 + m_4^2)(n_1^2 + n_2^2 + n_3^2 + n_4^2) = p_1^2 + p_2^2 + p_3^2 + p_4^2$. For example: $(1 + 2I + 3J + 4K)(5 + 6I + 7J + 8K) = -60 + 12I + 30J + 24K$, then it is: $(1^2 + 2^2 + 3^2 + 4^2)(5^2 + 6^2 + 7^2 + 8^2) = 60^2 + 12^2 + 30^2 + 24^2$.

The algebra of sigma matrices is summarized by the matrix identity²

$$\sigma_i \sigma_j = \delta_{ij} \sigma_0 + i \sum_{k=1}^3 \epsilon_{ijk} \sigma_k \quad (16.2)$$

Quaternions are then represented by complex matrices, with the ordinary matrix operations:

$$q = \begin{pmatrix} a + ib & c + id \\ -c + id & a - ib \end{pmatrix}$$

Quaternions with unit norm correspond to SU(2) matrices (see 3.3.4).

It is interesting to note that modern 3D vector calculus stemmed from quaternions (but also from the works of Hermann Grassmann, less known at the time). The inauguration was made independently by Josiah Gibbs³, professor of chemical physics at Yale's university, and Oliver Heaviside, the engineer who formulated Maxwell's equations in the present vector form⁴.

In modern language, a quaternion $q = a$ with $b = c = d = 0$ is a scalar, and a purely imaginary quaternion $bI + cJ + dK$ is a vector. Therefore a quaternion can be viewed as a pair (a, \mathbf{v}) . It is $(0, \mathbf{u})(0, \mathbf{v}) = (-\mathbf{u} \cdot \mathbf{v}, \mathbf{u} \times \mathbf{v})$.

Hamilton introduced the operator $\nabla = I\partial_x + J\partial_y + K\partial_z$, and named it *nabla*⁵. If $q = (a, 0)$ then ∇q is a vector. If $q = (0, \mathbf{v})$, $\nabla q = (-\text{div} \mathbf{v}, \text{rot} \mathbf{v})$.

Quaternions influenced James Clerk Maxwell in the formulation of his fundamental *Treatise on Electricity and Magnetism* (1873), though he preferred the Cartesian form⁶.

A natural approach to quaternions is to define them as pairs of complex numbers (z_1, z_2) with sum, multiplication and conjugation

$$\begin{aligned} (z_1, z_2) + (w_1, w_2) &= (z_1 + w_1, z_2 + w_2), \\ (z_1, z_2)(w_1, w_2) &= (z_1 w_1 - \bar{w}_2 z_2, z_2 \bar{w}_1 + w_2 z_1), \\ \overline{(z_1, z_2)} &= (\bar{z}_1, -z_2). \end{aligned} \quad (16.3)$$

² ϵ_{ijk} is the totally antisymmetric symbol; $\epsilon_{123} = -\epsilon_{213} = 1$ and cyclic permutations, zero otherwise.

³ J. Gibbs and E. Wilson, *Vector analysis*, 1901.

⁴ A detailed account is in M. J. Crowe, *A history of vector analysis*, Dover reprint of Notre Dame University Press, 1967.

⁵ The symbol ∇ recalls the nabla, an ancient Hebrew musical instrument.

⁶ *I am convinced, however, that the introduction of the ideas, as distinguished from the operations and methods of Quaternions, will be of great use ... especially in electrodynamics ... can be expressed far more simply by a few words of Hamilton's, than the ordinary equations. One of the most important features of Hamilton's method is the division of quantities into Scalars and Vectors.*

A pair $(a+ib, c+id)$ identifies with the real combination $a+Ib+cJ+dK$ with units $I = (i, 0)$, $J = (0, 1)$ and $K = (0, i)$.

Exercise 16.1.1. Find the inverse of a quaternion.

16.2 Octonions

The generalization of quaternions are the *octonions* \mathbb{O} or Cayley numbers⁷. They can be defined as pairs of quaternions (q_1, q_2) with sum, multiplication and conjugation defined as above, for the pairs of complex numbers. The octonion algebra is both non commutative and non associative (because of non associativity, octonions cannot be represented as matrices).

In alternative, one can introduce 8 units I_j with multiplication table $I_i I_j = f_{ijk} I_k$ (not given here), and write $O = \sum_j o_j I_j$. The norm

$$\|O\|^2 = O^\dagger O = o_0^2 + o_1^2 + \dots + o_7^2$$

has the property $\|O_1 O_2\| = \|O_1\| \|O_2\|$. This makes \mathbb{O} a division algebra (see below). Octonions enter in the construction of certain exceptional Lie algebras.

Quaternions and Octonions are examples of Clifford algebras⁸, which are relevant in the study of Dirac's equation for odd spin particles (fermions).

Continuation of the process with pairs of octonions brings to *Sedenions*, of dimension 16, with weaker algebraic properties.

Remark 16.2.1. $\mathbb{R}, \mathbb{C}, \mathbb{H}, \mathbb{O}$ are real division algebras of dimensions 1, 2, 4 and 8, i.e. the equations $ax = b$ and $ya = b$ (where $a \neq 0$ and b are elements of the algebra) have unique solutions x and y in the algebra (for commutative algebras $x = y$).

Theorem 16.2.2 (Bott-Milnor (1958), Kervair (1958)). *The only possible dimensions of a real division algebra are 1, 2, 4, 8.*

The proofs (for 2, 4, 8) are based on the topological assertion that the only spheres $S^n = \{x \in \mathbb{R}^{n+1} : \|x\| = 1\}$ that admit n linearly independent vector fields (parallelizable spheres) are S^1 , S^3 and S^7 . No algebraic proof of the theorem is known.

Algebras with anticommuting units $\theta_i \theta_j + \theta_j \theta_i = 0$ were developed since 1844 by Hermann Grassmann (see the last chapter).

⁷ John Baez, *Octonions*, Bull. Am. Math. Soc. 39 (2001) 145-205.

⁸ V. V. Prasolov, *Problems and theorems in linear algebra*, translations of mathematical monographs 134, Am. Math. Soc.

Part 2

FUNCTIONAL ANALYSIS



Figure 16.1 Maurice Fréchet (Maligny 1878, Paris 1973) had the fortunate chance of having the eminent mathematician Jacques Hadamard as teacher in secondary school. Hadamard noticed him and started an individual tutorship. In 1900 Maurice enrolled in mathematical studies at the *École Normale Supérieure*. His doctorate dissertation *Sur quelques points du calcul fonctionnelle*, with Hadamard, contains the new concept of metric space. Fréchet served several institutions in France and abroad, with a period near the front-line during world war I.

Figure 16.2 Stefan Banach (Kraków 1892, Lviv 1945). The turn in his life happened in Kraków when the mathematician Hugo Steinhaus, during an evening walk, heard by chance the young engineer Banach and Otto Nikodym talking about Lebesgue measure. The three founded, with others, Kraków's (now Polish) *Mathematical Society*. The doctorate dissertation *Sur les opérations dans les ensembles abstraits et leur application aux équations intégrales* (1920) contains the axioms of what Fréchet coined "Banach spaces". In 1924 he became full professor. His monograph *Théorie des Opérations linéaires* (1931) was very influential. After the German invasion in 1941 several colleagues were murdered. He survived feeding lice in Weigl's institute for infectious diseases, but his health paid the toll. He died of cancer one year after the Soviets entered Lviv. Banach's main achievements are in functional analysis, measure theory, topological spaces, orthogonal series.

Chapter 17

Metric Spaces

There are many contexts in mathematics where, given two items x and y (functions, matrices, sequences, operators, ...), one wishes to quantify how much they differ. In 1906 Maurice Fréchet, in his doctorate thesis, gave the axioms of a very general structure, the Metric Space, that allows to discuss topological concepts that arise in most situations of analysis. Soon after, in 1914, Felix Hausdorff gave the axioms for Topological Spaces, the most general conceptualization of “nearness”.

This is a brief summary of useful facts.

17.1 Metric spaces and completeness

Definition 17.1.1. A **Metric Space** (X, d) is a set X equipped with a distance between pairs of elements. A distance is characterized by the natural requirements of being symmetric, non negative, and constrained by the triangle inequality:

$$d(x, y) = d(y, x); \tag{17.1}$$

$$d(x, y) \geq 0, \quad d(x, y) = 0 \text{ iff } x = y; \tag{17.2}$$

$$d(x, y) \leq d(x, z) + d(z, y) \quad \forall x, y, z. \tag{17.3}$$

The distance defines a *topology* on X , i.e. a family of *neighbourhoods* at each point x . Such a family is the set of disks centred in x

$$D(x, r) = \{y \in X : d(x, y) < r\}.$$

With this definition, a metric space is a *Topological Hausdorff Space*.

The following definitions are of great relevance:

Definition 17.1.2. A sequence x_n in X converges to $x \in X$ if the sequence $d(x_n, x)$ converges to zero, i.e. $\forall \epsilon > 0 \exists N_\epsilon$ such that $d(x_n, x) < \epsilon \forall n > N_\epsilon$.

Definition 17.1.3. A sequence x_n is a **Cauchy sequence** (or a fundamental sequence) if $\forall \epsilon \exists N_\epsilon$ such that $d(x_m, x_n) < \epsilon \forall m, n > N_\epsilon$.

Exercise 17.1.4. Prove that if x_n is a Cauchy sequence in a metric space, and x_{n_j} is a subsequence with limit x , then $x_n \rightarrow x$.

Hint: use the triangle inequality $d(x_n, x) \leq d(x_n, x_{n_j}) + d(x_{n_j}, x)$.

Every convergent sequence is a Cauchy sequence (by the triangle inequality), but a Cauchy sequence may not converge. We are thus led to the important definition:

Definition 17.1.5. A metric space (X, d) is **complete** if every Cauchy sequence is convergent in X .

Completeness is a fundamental property: once a metric space is established to be complete, the Cauchy criterion ensures convergence of a sequence without knowledge of the limit.

A metric space that is not complete may be completed, in a manner similar to the construction of \mathbb{R} as the completion of \mathbb{Q} .

Theorem 17.1.6. If a metric space X is not complete, it is always possible to construct a metric space \overline{X} , the completion of X , which is complete.

Proof. Consider the set of Cauchy sequences x_n in X . Two sequences are equivalent, $x_n \sim x'_n$, if they definitely approach:

$$\forall \epsilon \exists N_\epsilon : d(x_n, x'_m) < \epsilon \quad \forall m, n > N_\epsilon$$

The reflexive and symmetric properties are obvious, the transitive property is true by the triangle inequality: if $x_n \sim x'_n$ and $x'_n \sim x''_n$ then: $d(x_n, x''_m) \leq d(x_n, x'_p) + d(x'_p, x''_m) \leq 2\epsilon$ for all $m, n, p > \max(N_\epsilon, N'_\epsilon)$, i.e. $x_n \sim x''_n$.

Define \overline{X} as the set of equivalence classes of Cauchy sequences in X . Such classes are of two types: the first one are the classes $[x]$ of Cauchy sequences in X that converge to $x \in X$ (in particular one selects the representative $\{x, x, \dots\}$), the others are the classes $[x_n]$ of Cauchy sequences with no limit in X .

\overline{X} is a linear space with $[x_n + y_n] = [x_n] + [y_n]$ and $[\lambda x_n] = [\lambda x_n]$.

It is a metric space with the distance

$$d([x_n], [y_n]) = \lim_{n \rightarrow \infty} d(x_n, y_n)$$

A finite limit exists because $d(x_n, y_n)$ is a Cauchy sequence in \mathbb{R} : $|d(x_n, y_n) - d(x_m, y_m)| \leq |d(x_n, y_n) - d(x_n, y_m)| + |d(x_n, y_m) - d(x_m, y_m)| \leq d(y_n, y_m) + d(x_m, x_n) < 2\epsilon$ for $m, n > N_\epsilon$ because x_n and y_n are Cauchy sequences.

\bar{X} is complete: let $[x_n]_p$ be a Cauchy sequence in \bar{X} (a Cauchy sequence of equivalent Cauchy sequences):

$$\forall \epsilon \exists N_\epsilon \text{ s.t. } d([x_n]_p, [x_n]_q) = \lim_{n \rightarrow \infty} d(x_{n,p}, x_{n,q}) < \epsilon \quad \forall p, q > N_\epsilon$$

The sequence $z_n = x_{n,n}$ is a Cauchy sequence: $d(z_n, z_m) = d(x_{n,n}, x_{m,m}) \leq d(x_{n,n}, x_{n,p}) + d(x_{n,p}, x_{m,p}) + d(x_{m,m}, x_{m,p}) < 3\epsilon$ for large enough n, m, p . The class $[z_n]$ is the limit in \bar{X} of the Cauchy sequence $[x_n]_p$: $d([x_n]_m, [z_n]) = \lim_{n \rightarrow \infty} d(x_{n,m}, x_{n,n}) \rightarrow 0$. \square

17.2 Maps between metric spaces

Let $f : X \rightarrow Y$ be a map between metric spaces, with domain $\text{Dom} f$. The image of the domain is the range: $\text{Ran} f = \{y \in Y : y = f(x), x \in \text{Dom} f\}$.

Definition 17.2.1 (Continuity).

- A map f is continuous at $x \in \text{Dom} f$ if:

$$\forall \epsilon \exists \delta_{\epsilon, x} \text{ such that } d(f(x'), f(x))_Y < \epsilon \quad \forall x' \in \text{Dom} f \text{ with } d(x', x)_X < \delta_{\epsilon, x}$$

- A map f is sequentially continuous at $x \in \text{Dom} f$ if:

$$x_n \rightarrow x \text{ in } \text{Dom} f \Rightarrow f(x_n) \rightarrow f(x) \text{ in } Y$$

Theorem 17.2.2. f is continuous at $x \iff f$ is sequentially continuous at x .

Proof. \implies Suppose that f is continuous and $x_n \rightarrow x$ in $\text{Dom} f$. Then $\forall \epsilon > 0 \exists \delta_{\epsilon, x}$ such that $d(f(x_n), f(x)) < \epsilon$ for all x_n such that $d(x_n, x) < \delta_{\epsilon, x}$ i.e. for all $n > N_\delta$. This means precisely that $f(x_n) \rightarrow f(x)$.

\impliedby By hypothesis all sequences that converge to x are mapped by f to sequences that converge to $f(x)$. This implies continuity of f at x : $\lim_{x' \rightarrow x} f(x') = f(x)$ (otherwise a sequence of points x'_n belonging to disks $d(x'_n, x) < (1/n)$ for n large enough, would be mapped to a different limit). \square

17.3 Contractive maps

Definition 17.3.1. A map $A : X \rightarrow X$ is a **contraction** if there is a constant $\alpha < 1$ such that $d(Ax, Ax') \leq \alpha d(x, x')$ for every pair in X .

Exercise 17.3.2. Show that a contraction is a continuous map.

A point $x \in X$ is a fixed point for a map $A : X \rightarrow X$ if $Ax = x$. Contractions have this fundamental property:

Theorem 17.3.3 (Fixed point theorem). *Every contraction on a complete metric space has a unique fixed point.*

Proof. Given an initial point x_0 , let $x_k = A^k x_0$ be the sequence generated by iteration of the map. Let's show that x_k is a Cauchy sequence. For $n > m$:

$$\begin{aligned} d(x_n, x_m) &= d(Ax_{n-1}, Ax_{m-1}) \leq \alpha d(x_{n-1}, x_{m-1}) \leq \dots \leq \alpha^m d(x_{n-m}, x_0) \\ &\leq \alpha^m [d(x_{n-m}, x_{n-m-1}) + \dots + d(x_2, x_1) + d(x_1, x_0)] \\ &\leq \alpha^m [\alpha^{n-m-1} + \dots + \alpha + 1] d(x_1, x_0) \leq \frac{\alpha^m}{1-\alpha} d(x_1, x_0) \end{aligned}$$

If m is large enough the estimate can be made smaller than any prefixed ϵ . Because of completeness, the Cauchy sequence converges to a limit \bar{x} . Since A is continuous: $A\bar{x} = A\lim_n x_n = \lim_n Ax_n = \lim_n x_{n+1} = \bar{x}$. Then \bar{x} is a fixed point, and is the limit of the sequence of iterates of a point.

Unicity is now proven. Suppose that a different fixed point \bar{y} exists. The equality $d(\bar{x}, \bar{y}) = d(A\bar{x}, A\bar{y}) \leq \alpha d(\bar{x}, \bar{y})$ implies $d(\bar{x}, \bar{y}) = 0$. \square

Example 17.3.4 (Kepler equation). *The elliptic orbit of a planet $(x/a)^2 + (y/b)^2 = 1$ ($a \geq b$) has eccentricity $e = \sqrt{1 - (b/a)^2}$. The Sun is in the focus $(ae, 0)$. The position of the planet can be parameterized as $x = a \cos E$, $y = b \sin E$, where $0 \leq E \leq 2\pi$ is named eccentric anomaly ($E = 0$ at perihelion and $E = \pi$ at aphelion). The distance from the Sun is $r = a(1 - e \cos E)$. Since the areal velocity is constant, the area swept at time t after the passage at perihelion ($E = 0$ at $t = 0$) is $\pi ab(t/T)$, where T is the orbital period. The evaluation of the same area in terms of E gives Kepler's law:*

$$E - e \sin E = M, \quad M = \frac{2\pi}{T} t \quad (17.4)$$

It is an equation for $E(M)$, where M is the "mean anomaly"; $E(M + 2\pi) = E(M)$. At each time one solves Kepler's equation to obtain E and the position of the planet. The transcendental equation can be solved as a fixed point problem $E = K(E)$ where $K(E) = M + e \sin E$ is a contraction on $[0, 2\pi]$:

$$|K(E) - K(E')| = e |\sin E - \sin E'| = e |\cos E^*| |E - E'| \leq e |E - E'|$$

The solution $E(t)$ is the limit of a sequence $E_{k+1} = K(E_k)$, with e.g. initial value $E_0 = M$. Convergence is faster the smaller is the eccentricity e (Earth $e_{\oplus} = 0.01671$, Ceres $e = 0.0789$, Halley's comet $e = 0.967$).

Example 17.3.5 (Volterra equation). Consider the integral equation, with real λ , $g \in \mathcal{C}[0, 1]$, and k (the “kernel”) a continuous function on the unit square:

$$u(x) = g(x) + \lambda \int_0^x dy k(x, y) u(y), \quad x \in [0, 1] \quad (17.5)$$

It can be written as a fixed point equation in $\mathcal{C}[0, 1]$ equipped with the sup norm: $Tu = u$ with $(Tu)(x) = g(x) + \lambda \int_0^x dy k(x, y) u(y)$. Let us evaluate:

$$\begin{aligned} |(Tu_1)(x) - (Tu_2)(x)| &\leq |\lambda| \int_0^x dy |k(x, y)| |u_1(y) - u_2(y)| \\ &\leq |\lambda| \sup_{y \in [0, 1]} |u_1(y) - u_2(y)| \int_0^x dy |k(x, y)| \\ &\leq |\lambda| K \|u_1 - u_2\|, \quad K = \sup_{x \in [0, 1]} \int_0^x dy |k(x, y)| \end{aligned}$$

The sup $x \in [0, 1]$ of the inequality gives $\|Tu_1 - Tu_2\| \leq |\lambda| K \|u_1 - u_2\|$. If $|\lambda| K < 1$, T is a contraction and the equation $u = Tu$ has a unique solution in $\mathcal{C}[0, 1]$, which may be obtained by convergent iteration of u_0 , $u_{k+1} = Tu_k$.

Chapter 18

Banach Spaces

18.1 Normed and Banach spaces

Definition 18.1.1. A linear space X equipped with a *norm* is a **normed space**. A norm is defined by the properties ($x \in X, \lambda \in \mathbb{C}$):

$$\|\lambda x\| = |\lambda| \|x\|; \tag{18.1}$$

$$\|x\| \geq 0, \quad \|x\| = 0 \Leftrightarrow x = 0; \tag{18.2}$$

$$\|x_1 + x_2\| \leq \|x_1\| + \|x_2\|. \tag{18.3}$$

The definition of abstract normed space was given in the years 1920 - 22 by various authors, the most influential being the Polish mathematician Stefan Banach. It is straightforward to check that *a normed space is a metric space* with distance $d(x_1, x_2) = \|x_1 - x_2\|$.

A sequence $\{x_n\}$ converges to x if $\|x_n - x\| \rightarrow 0$.

Definition 18.1.2. A **Banach space** is a complete normed space (every Cauchy sequence is convergent).

Example 18.1.3. *The set $\mathcal{C}[a, b]$ of continuous functions $f : [a, b] \rightarrow \mathbb{C}$ is a Banach space with the sup-norm:*

$$\|f\|_\infty = \sup_{a \leq x \leq b} |f(x)|$$

Proof. Completeness: let f_n be a Cauchy sequence: $\forall \epsilon > 0 \exists N_\epsilon$ such that for all $n, m > N_\epsilon$ it is $\sup_x |f_n(x) - f_m(x)| < \epsilon$. This implies that for each $x \in [a, b]$, the sequence $f_n(x)$ is a Cauchy sequence in \mathbb{C} . Then it converges to a complex number which we name $f(x)$. This defines a function f . As $m \rightarrow \infty$, the Cauchy condition becomes $\sup_x |f_n(x) - f(x)| < \epsilon$, i.e. $f_n \rightarrow f$ in the sup-norm. It remains to show that f belongs to $\mathcal{C}[a, b]$. This amounts to

prove that a uniformly convergent sequence of continuous functions converges to a continuous function. Continuity of f is proven as follows: $|f(x) - f(y)| \leq |f(x) - f_n(x)| + |f(y) - f_n(y)| + |f_n(x) - f_n(y)| \leq 3\epsilon$ for $|x - y|$ small and n large enough. \square

The following linear spaces are Banach spaces in the sup norm:

$\mathcal{C}(\mathbb{R})$ (the set of continuous and bounded complex functions),

$\mathcal{C}_\infty(\mathbb{R})$ (the set of continuous functions that vanish at infinity). It is the completion of the normed space $\mathcal{C}_0(\mathbb{R})$ (the set of continuous functions with compact support).

18.2 The Banach spaces $L^p(\Omega)$

Let Ω be \mathbb{R}^n or a measurable subset, and consider the set of complex valued Lebesgue measurable functions $f: \Omega \rightarrow \mathbb{C}$. The sum of two functions and the product by a complex number λ are defined pointwise: $(f + g)(x) = f(x) + g(x)$ and $(\lambda f)(x) = \lambda f(x)$, and give measurable functions.

18.2.1 $L^1(\Omega)$ (Lebesgue integrable functions)

Consider the measurable functions on Ω such that

$$\int_{\Omega} dx |f(x)| < \infty \quad (18.4)$$

Since $|f(x) + g(x)| \leq |f(x)| + |g(x)|$ and $|\lambda f(x)| = |\lambda| |f(x)|$, it turns out that $f + g$ and λf are in $\mathcal{L}^1(\Omega)$ if f and g are. Then $\mathcal{L}^1(\Omega)$ is a linear space.

The integral (18.4) cannot define a norm because $\int |f| dx = 0$ implies $f = 0$ a.e. (almost everywhere) i.e. infinitely many functions, not the single null element $f = 0$ of the linear space. The remedy is to identify these functions in equivalence classes: two functions $f, g \in \mathcal{L}^1$ are equivalent if $f = g$ a.e.

Let $[f]$ be the equivalence class containing f and all functions that differ from it on sets of measure zero. The equivalence classes of functions in $\mathcal{L}^1(\Omega)$ form a linear space with: $[f] + [g] = [f + g]$ and $\lambda[f] = [\lambda f]$. The linear space is $L^1(\Omega)$, and it is a normed space with the norm¹

$$\|f\|_1 = \int_{\Omega} |f(x)| dx \quad (18.5)$$

Now comes the beautiful proof of completeness:

Theorem 18.2.1 (Riesz - Fisher). $L^1(\Omega)$ is complete (it is a Banach space).

¹ as f can be any function in $[f]$, purists avoid writing $f(x)$, which can be any value by changing f within its class.

Proof. Let $\{f_n\}$ be a Cauchy sequence in L^1 : $\forall \epsilon$ it is $\|f_n - f_m\|_1 < \epsilon$ for $n, m > N_\epsilon$. To prove convergence of the Cauchy sequence, it is sufficient to prove convergence of a subsequence, which is now produced.

For the choices $\epsilon = 1, 1/2, 1/2^2, \dots, 1/2^k, \dots$ the Cauchy condition is satisfied for $N_\epsilon = N_0, N_1, \dots, N_k, \dots$. The subsequence $f_{N_0}, \dots, f_{N_k}, \dots$ has the property $\|f_{N_{k+1}} - f_{N_k}\|_1 < 2^{-k}$.

Consider the sequence:

$$S_m(x) = \sum_{k=0}^{m-1} |f_{N_{k+1}}(x) - f_{N_k}(x)|$$

It is $S_{m+1}(x) \geq S_m(x) \geq 0$ and $\|S_m\|_1 = \sum_{k=0}^{m-1} \frac{1}{2^k} \leq 2$.

By Beppo Levi's theorem² the sequence S_m converges a.e. pointwise to a function S in $L^1(\Omega)$ and $\int S_m dx \rightarrow \int S dx$.

Convergence of $S_m(x)$ is the absolute convergence of the sequence

$$s_m(x) = \sum_{k=0}^{m-1} (f_{N_{k+1}}(x) - f_{N_k}(x)) \rightarrow f(x) - f_{N_0}(x)$$

The telescopic sum is $s_m(x) = f_{N_m}(x) - f_{N_0}(x)$, then $f_{N_m}(x) \rightarrow f(x)$ a.e.

Since $|f_{N_m}(x) - f_{N_0}(x)| = |s_m(x)| \leq S_m(x) \leq S(x)$ and S is integrable, it follows that $f - f_{N_0}$ is integrable and $f_{N_m} \rightarrow f$ in L^1 (dominated convergence theorem)³. \square

18.2.2 $L^p(\Omega)$ spaces

The generalization of L^p spaces is due to the Hungarian mathematician Frigyes Riesz (1880-1956). Consider the set $\mathcal{L}^p(\Omega)$ of measurable functions such that

$$\|f\|_p = \left(\int_{\Omega} |f|^p dx \right)^{\frac{1}{p}} < \infty \quad (18.6)$$

where $p \geq 1$. To show that \mathcal{L}^p is a linear space one must show that it is closed for the sum of two functions. This follows from Minkowski's inequality, whose proof requires Hölder's inequality.

² Monotone Convergence Theorem (B. Levi): Let f_n be a sequence of real integrable functions such that $0 \leq f_1(x) \leq f_2(x) \leq \dots$ a.e. in Ω and $\int_{\Omega} f_n dx \leq K$. Then the sequence $f_n(x)$ converges a.e. in Ω , $f_n(x) \rightarrow f(x)$, with $f \in \mathcal{L}^1(\Omega)$ and $\int_{\Omega} f_n dx \rightarrow \int_{\Omega} f dx$.

³ Dominated Convergence Theorem: Given a sequence of measurable functions such that $f_n(x) \rightarrow f(x)$ a.e. $x \in \Omega$, and a function $g \in \mathcal{L}^1(\Omega)$ such that $|f_n(x)| \leq g(x)$ a.e. in Ω and for all n , then $f \in \mathcal{L}^1(\Omega)$ and $\int_{\Omega} f_n dx \rightarrow \int_{\Omega} f dx$.

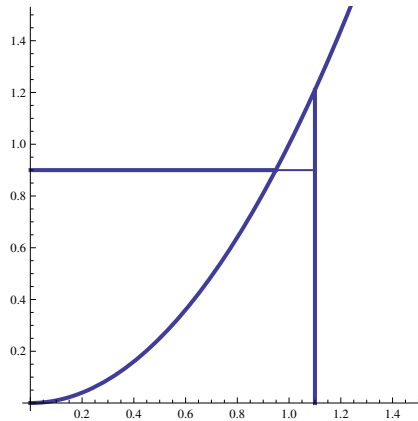


Figure 18.1 Construction for Hölder's inequality. The curve is $y = x^2$.

Proposition 18.2.2 (Hölder's inequality). If $f \in \mathcal{L}^p(\Omega)$ and $g \in \mathcal{L}^q(\Omega)$, where $p, q > 1$ and $p^{-1} + q^{-1} = 1$ then: $fg \in \mathcal{L}^1(\Omega)$ and

$$\|fg\|_1 \leq \|f\|_p \|g\|_q \quad 1 = \frac{1}{p} + \frac{1}{q} \tag{18.7}$$

Proof. Consider the curve $y = x^{p-1}$ in the positive quadrant. Inversion gives $x = y^{q-1}$. The area of the rectangle $0 < x < u$ and $0 < y < v$, is (see fig.18.1)

$$uv \leq \int_0^u dx x^{p-1} + \int_0^v dy y^{q-1} = \frac{u^p}{p} + \frac{v^q}{q} \tag{18.8}$$

Put $u = |f(x)|/\|f\|_p$ and $v = |g(x)|/\|g\|_q$ and integrate x on Ω :

$$\int_{\Omega} dx \frac{|fg|}{\|f\|_p \|g\|_q} \leq \frac{1}{p} \int_{\Omega} dx \frac{|f|^p}{\|f\|_p^p} + \frac{1}{q} \int_{\Omega} dx \frac{|g|^q}{\|g\|_q^q} = \frac{1}{p} + \frac{1}{q}.$$

The inequality is obtained. □

Remark 18.2.3. If $m(\Omega) < \infty$, one may take $g = 1$ in Hölder's inequality, and note that if $f \in \mathcal{L}^p(\Omega)$ then $f \in \mathcal{L}^1(\Omega)$, i.e. $\mathcal{L}^p(\Omega) \subseteq \mathcal{L}^1(\Omega)$, for any $p > 1$.

Proposition 18.2.4 (Minkowski's inequality). If f, g in $\mathcal{L}^p(\Omega)$ then:

$$\|f + g\|_p \leq \|f\|_p + \|g\|_p \tag{18.9}$$

Proof. Inequality (18.8) with $u > 0$ and $v = z^{p-1}$, $\frac{1}{p} + \frac{1}{q} = 1$, is

$$uz^{p-1} \leq \frac{u^p}{p} + \frac{z^p}{q}$$

Put $u = |f(x)|/\|f\|_p$, $z = |f(x) + g(x)|/\|f + g\|_p$ and integrate:

$$\int_{\Omega} dx |f(x)| |f(x) + g(x)|^{p-1} \leq \|f\|_p \|f + g\|_p^{p-1}$$

Add the inequality with f and g exchanged:

$$\int_{\Omega} dx (|f(x)| + |g(x)|) |f(x) + g(x)|^{p-1} \leq (\|f\|_p + \|g\|_p) \|f + g\|_p^{p-1}$$

Since $|f(x) + g(x)| \leq |f(x)| + |g(x)|$, the inequality becomes:

$$\int_{\Omega} dx |f(x) + g(x)|^p \leq (\|f\|_p + \|g\|_p) \|f + g\|_p^{p-1}$$

i.e. $\|f + g\|_p^p \leq (\|f\|_p + \|g\|_p) \|f + g\|_p^{p-1}$, and the result follows. \square

The inequality implies that $\mathcal{L}^p(\Omega)$ is a linear space. To promote $\|f\|_p$ to a norm one must switch to the set of equivalence classes. Minkowski's inequality proves the triangle inequality, and $L^p(\Omega)$ is a normed space. The Riesz-Fisher theorem states that it is complete (a Banach space) for all $p \geq 1$.

Hölder' inequality shows that the functions of $L^q(\Omega)$ define linear continuous functionals on $L^p(\Omega)$ if $1/p + 1/q = 1$. One actually proves that a space is the dual of the other. The dual of $L^1(\Omega)$ is the space $L^\infty(\Omega)$, but the dual of L^∞ contains L^1 (see Reed and Simon, Functional Analysis, Academic Press).

18.2.3 $L^\infty(\Omega)$ space

$\mathcal{L}^\infty(\Omega)$ is the space of measurable functions $f : \Omega \rightarrow \mathbb{C}$ that are a.e. bounded: given f , there is a constant M_f such that the set where $|f(x)| > M_f$ has Lebesgue measure zero. The inf of such bounds M_f is $\|f\|_\infty$, which becomes a norm for the equivalence classes of functions that are equal a.e.

The space $L^\infty(\Omega)$ is a Banach space.

$\mathcal{C}(\mathbb{R})$ is a subspace of $\mathcal{L}^\infty(\mathbb{R})$. The norm coincides with the sup-norm.

18.3 Continuous and bounded maps

Hereafter $\hat{A} : X \rightarrow Y$ is a map (the term “operator” will be used) between normed spaces, with domain $\mathcal{D}(\hat{A})$. The image of the domain is the range $\text{Ran } \hat{A} = \{y \in Y : y = \hat{A}x, x \in \mathcal{D}(\hat{A})\}$, the kernel is the set $\text{Ker } \hat{A} = \{x \in X : \hat{A}x = 0\}$.

We recall definitions and results exported from the more general context of metric spaces:

- \hat{A} is continuous at $x \in \mathcal{D}(\hat{A})$ if:

$$\forall \epsilon \exists \delta_{\epsilon, x} \text{ such that } \|\hat{A}x' - \hat{A}x\|_Y < \epsilon \quad \forall x' \in \mathcal{D}(\hat{A}) \text{ with } \|x' - x\|_X < \delta_{\epsilon, x}.$$

- \hat{A} is sequentially continuous at $x \in \mathcal{D}(\hat{A})$ if $x_n \rightarrow x$ in $\mathcal{D}(\hat{A}) \Rightarrow \hat{A}x_n \rightarrow \hat{A}x$.
- \hat{A} is continuous at x if and only if \hat{A} is sequentially continuous at x .

Proposition 18.3.1. *The kernel of a continuous operator is a closed set.*

Proof. Suppose that x_n is a sequence in $\text{Ker } \hat{A}$ and $x_n \rightarrow x \in \mathcal{D}(\hat{A})$. Then $\hat{A}x = \lim_Y \hat{A}x_n = 0$ i.e. $x \in \text{Ker } \hat{A}$. \square

Definition 18.3.2. \hat{A} is **bounded** if there is a constant $C_A > 0$ such that $\|\hat{A}x\|_Y < C_A \|x\|_X$ for all $x \in \mathcal{D}(\hat{A})$.

18.3.1 Linear operators

Definition 18.3.3. \hat{A} is **linear** if $\mathcal{D}(\hat{A})$ is a linear subspace and $\hat{A}(x + \lambda x') = \hat{A}x + \lambda \hat{A}x'$ for all $x, x' \in \mathcal{D}(\hat{A})$, $\lambda \in \mathbb{C}$.

Remark 18.3.4. *If \hat{A} is linear, then \hat{A} is continuous if and only if it is continuous at $x = 0$.*

Theorem 18.3.5. *A linear map $\hat{A} : \mathcal{D}(\hat{A}) \rightarrow Y$ is bounded if and only if it is continuous.*

Proof. Suppose that \hat{A} is bounded and $x_n \rightarrow 0$ in $\mathcal{D}(\hat{A})$. Then $\|\hat{A}x_n\| \leq C_A \|x_n\| \rightarrow 0$ i.e. \hat{A} is sequentially continuous in the origin i.e. \hat{A} is continuous.

Let \hat{A} be continuous. Then for $\epsilon = 1$ there is $\delta > 0$ such that $\|\hat{A}x\| < 1$ for all x in the domain with $\|x\| < \delta$. For any $y \in \mathcal{D}(\hat{A})$, put $x = y\delta / (2\|y\|)$. Then $\|x\| \leq \delta$ so that $1 \geq \|\hat{A}x\| = \|\hat{A}y\| / \|y\| (\delta/2)$ i.e. \hat{A} is bounded. \square

Theorem 18.3.6. *Let X be a normed space and Y a Banach space. A linear bounded operator $\hat{A} : \mathcal{D}(\hat{A}) \subset X \rightarrow Y$ extends uniquely to a linear bounded operator on the closure of the domain: $\bar{A} : \overline{\mathcal{D}(\hat{A})} \rightarrow Y$.*

Proof. If $x \in \overline{\mathcal{D}}$ there is a convergent sequence x_n in \mathcal{D} with limit x . A convergent sequence is Cauchy, therefore $\|\hat{A}x_n - \hat{A}x_m\|_Y \leq C_A \|x_n - x_m\|_X \leq \epsilon$ for $n, m > N_\epsilon$ i.e. $\hat{A}x_n$ is Cauchy in Y . Since Y is Banach, $\hat{A}x_n \rightarrow y$.

Define $\bar{A}x = y$. The domain $\mathcal{D}(\bar{A})$ is a linear space: if $x_n \rightarrow x$ and $x'_n \rightarrow x'$ in $\overline{\mathcal{D}(\bar{A})}$, then

$x_n + x'_n \rightarrow x + x'$ and $\lambda x_n \rightarrow \lambda x$. \bar{A} is linear: $\bar{A}(x + x') = \lim_n \hat{A}x_n + \lim_n \hat{A}x'_n = \bar{A}x + \bar{A}x'$. \bar{A} is bounded: since the norm is continuous, $\|\bar{A}x\| = \lim_n \|\hat{A}x_n\| \leq C_A \lim_n \|x_n\| = C_A \|x\|$. \square

18.3.2 The inverse operator

If $\hat{A} : X \rightarrow Y$ is an operator with domain $\mathcal{D}(\hat{A})$, the inverse operator $\hat{A}^{-1} : Y \rightarrow X$ exists if \hat{A} is injective, i.e. $\hat{A}x = \hat{A}x'$ implies $x = x'$. Then, if $\hat{A}x = y$ it is $\hat{A}^{-1}y = x$, with $\mathcal{D}(\hat{A}^{-1}) = \text{Ran } \hat{A}$, and $\text{Ran } \hat{A}^{-1} = \mathcal{D}(\hat{A})$.

Proposition 18.3.7. *If \hat{A} is linear, \hat{A}^{-1} exists if and only if $\text{Ker } \hat{A} = \{0\}$. If \hat{A}^{-1} exists, it is linear.*

Proof. The condition $\hat{A}x = \hat{A}y$ if and only if $x = y$ is equivalent to $\hat{A}(x - y) = 0$ iff $x - y = 0$ i.e. $\text{Ker } (\hat{A}) = \{0\}$.

If $\hat{A}x = y$ and $\hat{A}x' = y'$ then $\hat{A}(\lambda x + x') = \lambda y + y'$. The inverse is such that $x = \hat{A}^{-1}y$, $x' = \hat{A}^{-1}y'$ and $\lambda x + x' = \hat{A}^{-1}(\lambda y + y')$, i.e. $\lambda \hat{A}^{-1}y + \hat{A}^{-1}y' = \hat{A}^{-1}(\lambda y + y')$, i.e. \hat{A}^{-1} is linear. \square

18.4 Linear bounded operators on X

The set $\mathcal{L}(X, Y)$ of linear operators on a normed space X , with domain X , to a normed space Y , is a linear space with the definitions

$$(\hat{A} + \hat{B})x = \hat{A}x + \hat{B}x, \quad (\lambda \hat{A})x = \lambda(\hat{A}x), \quad x \in X, \lambda \in \mathbb{C}.$$

If two operators are bounded, their sum is bounded:

$$\|(\hat{A} + \hat{B})x\|_Y \leq \|\hat{A}x\|_Y + \|\hat{B}x\|_Y \leq (C_A + C_B)\|x\|_X, \quad \forall x \in X \quad (18.10)$$

$\mathcal{B}(X, Y)$ is the linear space of *linear and bounded* operators from X to Y .

To be bounded is a very strong property of an operator \hat{A} . The best bound is the least constant C_A such that $\|\hat{A}x\|_Y / \|x\|_X \leq C_A$ for all $x \in X$, $x \neq 0$. This constant is the **operator norm** of \hat{A} :

$$\|\hat{A}\| = \sup_{x \in X, x \neq 0} \frac{\|\hat{A}x\|_Y}{\|x\|_X} = \sup_{\|x\|_X=1} \|\hat{A}x\|_Y \quad (18.11)$$

As a consequence the best inequality is

$$\|\hat{A}x\|_Y \leq \|\hat{A}\| \|x\|_X, \quad \forall x \in X$$

If an element \bar{x} can be found that saturates the inequality, then $\|\hat{A}\| = \|\hat{A}\bar{x}\|_Y / \|\bar{x}\|_X$.

Eq.(18.11) defines a norm and makes $\mathcal{B}(X, Y)$ a normed space:

- $\|\hat{A}\| \geq 0$. If $\|\hat{A}\| = 0$ it is $\|\hat{A}x\|_Y = 0$ for all x , i.e. $\hat{A} = 0$;
- $\|\lambda \hat{A}\| = |\lambda| \|\hat{A}\|$ is obvious;
- the triangle inequality is obtained with (18.10): divide by $\|x\|_X \neq 0$ and take the sup: $\|\hat{A} + \hat{B}\| \leq \|\hat{A}\| + \|\hat{B}\|$.

Theorem 18.4.1. *If Y is a Banach space, then $\mathcal{B}(X, Y)$ is a Banach space.*

Proof. Let \hat{A}_n be a Cauchy sequence in $\mathcal{B}(X, Y)$:

$$\forall \epsilon \quad \exists N_\epsilon \text{ s.t. } \|\hat{A}_n - \hat{A}_m\| < \epsilon \quad \forall n, m \geq N_\epsilon$$

It follows that, for any x , also $\hat{A}_n x$ is a Cauchy sequence in Y by the inequality

$$\|\hat{A}_n x - \hat{A}_m x\|_Y \leq \|\hat{A}_n - \hat{A}_m\| \|x\|_X \quad (18.12)$$

- 1) The sequence $\|\hat{A}_n\|$ is Cauchy by the inequality $|\|\hat{A}_n\| - \|\hat{A}_m\|| \leq \|\hat{A}_n - \hat{A}_m\|$. Then $\|\hat{A}_n\|$ converges to a real number A .
- 2) Since Y is complete, the sequence $\hat{A}_n x$ converges to a unique element y_x in Y . This correspondence defines the operator $\hat{A}x = y_x$.
- 3) \hat{A} is linear: $\hat{A}(x + \lambda x') = \lim_n \hat{A}_n(x + \lambda x') = \lim_n \hat{A}_n x + \lambda \lim_n \hat{A}_n x' = \hat{A}x + \lambda \hat{A}x'$.
- 4) \hat{A} is bounded: $\|\hat{A}_n x - \hat{A}_m x\| \leq (\|\hat{A}_n\| + \|\hat{A}_m\|) \|x\|$ for all x, m implies the limit case $\|\hat{A}_n x - \hat{A}x\| \leq (\|\hat{A}_n\| + A) \|x\|$ for all x , i.e. $\hat{A}_n - \hat{A}$ is bounded, i.e. \hat{A} is bounded.
- 5) The Cauchy condition implies $\hat{A}_n \rightarrow \hat{A}$ in the sup-norm: $\|\hat{A}_n - \hat{A}\| = \sup_{\|x\|=1} \|(\hat{A}_n - \hat{A})x\| < \epsilon$ for all $n > N_\epsilon$. □

Remark 18.4.2. *Convergence $\hat{A}_n \rightarrow \hat{A}$ in $\mathcal{B}(X, Y)$ implies $\hat{A}_n x \rightarrow \hat{A}x$ in Y , for any x (norm convergence implies strong convergence).*

18.4.1 The dual space

In 1929 Banach introduced the important notion of **dual space** X^* of a Banach space X : it is the space of bounded linear functionals $\mathcal{B}(X, \mathbb{C})$. Since \mathbb{C} is complete, X^* is a Banach space.

There are two ways by which a sequence may converge in X :

- 1) $x_n \rightarrow x$ *strongly* if $\|x_n - x\|_X \rightarrow 0$;
- 2) $x_n \rightarrow x$ *weakly* if $Fx_n \rightarrow Fx$ in \mathbb{C} for all $F \in X^*$.

There are three ways by which a sequence of operators in $\mathcal{B}(X, Y)$ converges:

- 1) \hat{A}_n converges in norm to \hat{A} if $\|\hat{A}_n - \hat{A}\| \rightarrow 0$;
- 2) \hat{A}_n converges strongly if $\hat{A}_n x$ converges in Y -norm for all $x \in X$;
- 3) \hat{A}_n converges weakly if $F\hat{A}_n x$ converges in \mathbb{C} for all $x \in X, F \in Y^*$.

18.5 The Banach algebra $\mathcal{B}(X)$

If $X = Y$, the space $\mathcal{B}(X) \equiv \mathcal{B}(X, X)$ is closed for the product.

If $\hat{A}, \hat{B} \in \mathcal{B}(X)$, the operator $\hat{A}\hat{B}$ is defined by $(\hat{A}\hat{B})x = \hat{A}(\hat{B}x)$. The product is linear and bounded: $\|(\hat{A}\hat{B})x\| \leq \|\hat{A}\| \|\hat{B}x\| \leq (\|\hat{A}\| \|\hat{B}\|) \|x\|$. Therefore:

$$\boxed{\|\hat{A}\hat{B}\| \leq \|\hat{A}\| \|\hat{B}\|} \quad (18.13)$$

$\mathcal{B}(X)$ is an *associative algebra* (associative and distributive properties) with unit (the identity operator).

This statement is interesting for quantum mechanics:

Proposition 18.5.1 (Helmut Wielandt (1949)). *If $[\hat{A}, \hat{B}] = cI$ then \hat{A} and \hat{B} cannot be both bounded.*

Proof. Suppose that both \hat{A}, \hat{B} are in $\mathcal{B}(X)$. By induction one proves that $[\hat{A}^n, \hat{B}] = n c \hat{A}^{n-1}$. Now take the sup norm and use the triangular inequality

$$n|c| \|\hat{A}^{n-1}\| = \|\hat{A}^n \hat{B} - \hat{B} \hat{A}^n\| \leq 2 \|\hat{A}^n\| \|\hat{B}\| \leq 2 \|\hat{A}^{n-1}\| \|\hat{A}\| \|\hat{B}\|$$

Simplify and obtain $n|c| \leq 2 \|\hat{A}\| \|\hat{B}\|$. This tells that the product of the two norms is never bounded. \square

18.5.1 The inverse of a linear operator

Suppose that $\hat{A} \in \mathcal{B}(X)$ is invertible, and that $\text{Ran } \hat{A} = X$, so that $\mathcal{D}(\hat{A}^{-1}) = X$. The inverse operator need not be bounded. From $\|x\|_X = \|\hat{A}\hat{A}^{-1}x\|_X \leq \|\hat{A}\| \|A^{-1}x\|_X$ for all x , it is

$$\frac{\|\hat{A}^{-1}x\|}{\|x\|} \geq \frac{1}{\|\hat{A}\|} \quad (18.14)$$

If A^{-1} is bounded, then the sup of the ratio gives $\|A^{-1}\| \geq \|A\|^{-1}$.

18.6 Power series of operators

Several important complex functions that are expressed as power series may be extended to functions of operators. Consider the two power series

$$f(z) = \sum_{n=0}^{\infty} c_n z^n, \quad f(\hat{A}) = \sum_{n=0}^{\infty} c_n \hat{A}^n$$

where $\hat{A} \in \mathcal{B}(X)$. If \hat{S}_N are the operator partial sums, it is $\|\hat{S}_{N+p} - \hat{S}_N\| = \|\sum_{n=N+1}^{N+p} c_n \hat{A}^n\| \leq \sum_{n=N+1}^{N+p} |c_n| \|\hat{A}\|^n$. The partial sums form a Cauchy sequence in $\mathcal{B}(X)$ if the partial sums of the power series $f(\|\hat{A}\|)$ are a Cauchy sequence in \mathbb{C} . A sufficient condition is $\|\hat{A}\| < R$ where R is the radius of convergence of the power series $f(z)$.

Exercise 18.6.1. Show that $\|f(\hat{A})\| \leq f(\|\hat{A}\|)$ if $c_n > 0$ for all n .

Exercise 18.6.2. Show that if \hat{A} and $f(\hat{A})$ are in $\mathcal{B}(X)$, and if $\hat{A}x = \lambda x$, where $x \in X$, then $f(\hat{A})x = f(\lambda)x$.

Example 18.6.3 (Neumann series). If $\hat{A} \in \mathcal{B}(X)$, and $\|\hat{A}\| < 1$, then $(1 - \hat{A})^{-1}$ exists in $\mathcal{B}(X)$ and is given by the Neumann series:

$$(1 - \hat{A})^{-1} = \sum_{k=0}^{\infty} \hat{A}^k \quad (18.15)$$

For $\|\hat{A}\| < 1$ the partial sum $\hat{S}_n = I + \hat{A} + \hat{A}^2 + \dots + \hat{A}^n$ converges in $\mathcal{B}(X)$ and defines the geometric series.

Since $\|(1 - \hat{A})\hat{S}_n - 1\| = \|\hat{A}^{n+1}\| \leq \|\hat{A}\|^{n+1} \rightarrow 0$ for $n \rightarrow \infty$, (18.15) is true.

Example 18.6.4 (The exponential series).

If $\hat{A} \in \mathcal{B}(X)$, then $\forall z \in \mathbb{C}$ the exponential series

$$e^{z\hat{A}} = \sum_{k=0}^{\infty} \frac{(z\hat{A})^k}{k!} \quad (18.16)$$

converges in the operator norm to a bounded operator, and $\|e^{z\hat{A}}\| \leq e^{|z|\|\hat{A}\|}$.

Proposition 18.6.5. If \hat{A} and \hat{B} are commuting operators in $\mathcal{B}(X)$ then

$$(\exp \hat{A})(\exp \hat{B}) = \exp(\hat{A} + \hat{B}) \quad (18.17)$$

Proof. Consider the product of partial sums:

$$\begin{aligned} S_n(\hat{A}) \cdot S_n(\hat{B}) &= (1 + \hat{A} + \frac{1}{2}\hat{A}^2 + \dots + \frac{1}{n!}\hat{A}^n)(1 + \hat{B} + \frac{1}{2}\hat{B}^2 + \dots + \frac{1}{n!}\hat{B}^n) \\ &= 1 + (\hat{A} + \hat{B}) + \frac{1}{2}(\hat{A} + \hat{B})^2 + \dots + \frac{1}{n!}(\hat{A} + \hat{B})^n + R_n(\hat{A}, \hat{B}) \\ R_n(\hat{A}, \hat{B}) &= \frac{\hat{A}\hat{B}^n}{n!} + \frac{\hat{A}^2}{2!}(\frac{\hat{B}^n}{n!} + \frac{\hat{B}^{n-1}}{(n-1)!}) + \frac{\hat{A}^3}{3!}(\frac{\hat{B}^n}{n!} + \frac{\hat{B}^{n-1}}{(n-1)!} + \frac{\hat{B}^{n-2}}{(n-2)!}) + \dots \\ &\quad + \frac{\hat{A}^n}{n!}(\frac{\hat{B}^n}{n!} + \frac{\hat{B}^{n-1}}{(n-1)!} + \dots + \hat{B}) \end{aligned}$$

$S_n(\hat{A})S_n(\hat{B}) - S_n(\hat{A} + \hat{B}) = R_n(\hat{A}, \hat{B})$. We prove that $\|R_n(\hat{A}, \hat{B})\| \rightarrow 0$ in $\mathcal{B}(X)$ as $n \rightarrow \infty$. The triangle inequality and $\|\hat{A}\hat{B}\| \leq \|\hat{A}\| \cdot \|\hat{B}\|$ give:

$$\begin{aligned} \|R_n(\hat{A}, \hat{B})\| &\leq \frac{\|\hat{A}\| \|\hat{B}\|^n}{1} + \frac{\|\hat{A}\|^2}{2!} \left(\frac{\|\hat{B}\|^n}{n!} + \frac{\|\hat{B}\|^{n-1}}{(n-1)!} \right) + \frac{\|\hat{A}\|^3}{3!} \left(\frac{\|\hat{B}\|^n}{n!} + \frac{\|\hat{B}\|^{n-1}}{(n-1)!} + \frac{\|\hat{B}\|^{n-2}}{(n-2)!} \right) \\ &\quad + \dots + \frac{\|\hat{A}\|^n}{n!} \left(\frac{\|\hat{B}\|^n}{n!} + \frac{\|\hat{B}\|^{n-1}}{(n-1)!} + \dots + \frac{\|\hat{B}\|}{1} \right) = R_n(\|A\|, \|B\|) \end{aligned}$$

Note that $R_n(\|A\|, \|B\|) = S_n(\|A\|)S_n(\|B\|) - S_n(\|A\| + \|B\|)$. Since $S_n(\|A\|)$ converges to $\exp \|A\|$ in \mathbb{R} , then $R_n(\|A\|, \|B\|) \rightarrow 0$ as $n \rightarrow \infty$. \square

In particular:

$$\boxed{(\exp z \hat{A})(\exp z' \hat{A}) = \exp(z + z') \hat{A} \quad (\exp z \hat{A})^{-1} = \exp(-z \hat{A})} \quad (18.18)$$

The following formula applies to non-commuting bounded operators. It is useful, for example, in the path-integral formulation of quantum mechanics.

Proposition 18.6.6 (Lie-Trotter*). \hat{A} and \hat{B} are bounded operators:

$$\exp(\hat{A} + \hat{B}) = \lim_{n \rightarrow \infty} \left[\exp\left(\frac{\hat{A}}{n}\right) \exp\left(\frac{\hat{B}}{n}\right) \right]^n \quad (18.19)$$

Proof. Let $S_n = \exp \frac{\hat{A} + \hat{B}}{n}$, and $T_n = \exp \frac{\hat{A}}{n} \exp \frac{\hat{B}}{n}$.

$S_n^n - T_n^n = \sum_{k=0}^{n-1} S_n^k (S_n - T_n) T_n^{n-k-1}$. Use $\|\hat{A}\|^n \leq \|\hat{A}\|^n$, $\|\exp \hat{A}\| \leq \exp \|\hat{A}\|$:

$$\begin{aligned} \|S_n^n - T_n^n\| &\leq \|S_n - T_n\| \sum_{k=0}^{n-1} \|S_n\|^k \|T_n\|^{n-k-1} \\ &\leq \|S_n - T_n\| \sum_{k=0}^{n-1} \exp \left[\frac{k}{n} (\|\hat{A} + \hat{B}\|) \right] \exp \left[\frac{n-k-1}{n} (\|\hat{A}\| + \|\hat{B}\|) \right] \end{aligned}$$

Now use the triangular inequality, and obtain

$$\|S_n^n - T_n^n\| \leq n \|S_n - T_n\| \exp(\|\hat{A}\| + \|\hat{B}\|)$$

For large n it is $\|S_n - T_n\| = \mathcal{O}(1/n^2)$, then the limit is zero. \square

Let us report the Baker - Campbell - Hausdorff (BCH) formula,

$$e^{\hat{A} + \hat{B}} = e^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}([\hat{A}, [\hat{A}, \hat{B}]] + [[\hat{A}, \hat{B}], \hat{B}]) - \frac{1}{24}[\hat{A}, [\hat{B}, [\hat{A}, \hat{B}]]] + \dots} \quad (18.20)$$

The infinite sum truncates if both \hat{A} and \hat{B} commute with $[\hat{A}, \hat{B}]$, or in more complicated cases.

Chapter 19

Hilbert Spaces

The theory of Hilbert spaces originates in the studies of David Hilbert and his student Erhard Schmidt on integral equations. Their relevance for the mathematical foundation of quantum mechanics led John von Neumann to give them an axiomatic setting, in the years 1929-30.

19.1 Inner product spaces

Definition 19.1.1 (Inner product). A linear space \mathcal{H} (on \mathbb{C}) is a Inner Product Space (or pre-Hilbert space) if there is a map (the inner product) $(\cdot | \cdot) : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ such that for all $x, y, z \in \mathcal{H}$ and $\lambda \in \mathbb{C}$:

$$(x|x) \geq 0 \quad \text{and} \quad (x|x) = 0 \quad \text{iff} \quad x = 0 \quad (19.1)$$

$$(x|y+z) = (x|y) + (x|z) \quad (19.2)$$

$$(x|\lambda y) = \lambda(x|y) \quad (19.3)$$

$$\overline{(x|y)} = (y|x). \quad (19.4)$$

The properties imply antilinearity in the first argument¹:

$$(x + \lambda y|z) = (x|z) + \bar{\lambda}(y|z).$$

For real spaces the rule (19.4) is replaced by $(x|y) = (y|x)$, which implies bi-linearity (linearity in both arguments of the inner product).

It will be shown that the inner product induces a norm; we begin by introducing the notation $\|x\| = \sqrt{(x|x)}$.

¹ In the mathematical literature the inner product is often defined to be linear in the first and antilinear in the second argument. Physicists prefer the converse.

Exercise 19.1.2. Show that: 1) $(x|0) = 0$; 2) if $(x|y) = 0 \forall y$ then $x = 0$.

Definition 19.1.3. Two vectors x and x' are *orthogonal*, $x \perp x'$, if $(x|x') = 0$. A set of vectors u_1, \dots, u_n is an *orthonormal set* if $(u_i|u_j) = \delta_{ij}$.

Pythagoras' relation holds: if $x \perp x'$ then $\|x + x'\|^2 = \|x\|^2 + \|x'\|^2$.

Theorem 19.1.4 (Bessel's inequality²). Let $\{u_k\}_{k=1}^n$ be an orthonormal set, then for any x :

$$\|x\|^2 \geq \sum_{k=1}^n |(u_k|x)|^2 \quad (19.5)$$

Proof. Set $x' = \sum_k (u_k|x)u_k$; since it is the sum of orthonormal vectors, $\|x'\|^2 = \sum_k |(u_k|x)|^2$. Next, let's show that x' and $x - x'$ are orthogonal: $(x'|x - x') = (x'|x) - \|x'\|^2 = \sum_k \overline{(u_k|x)}(u_k|x) - \|x'\|^2 = 0$. Then $\|x\|^2 = \|(x - x') + x'\|^2 = \|x - x'\|^2 + \|x'\|^2 \geq \|x'\|^2$. \square

Bessel's inequality for $n = 1$ is $\|x\| \geq |(u|x)|$. With $u = y/\|y\|$ it gives a famous and fundamental inequality:

Proposition 19.1.5 (Schwarz inequality). $\forall x, y \in \mathcal{H}$:

$$\boxed{|(x|y)| \leq \|x\| \|y\|} \quad (19.6)$$

Exercise 19.1.6.

1) Let $\|x\| = \|y\| = 1$. Show that if $(x|y) = 1$ then $x = y$; if $|(x|y)| = 1$ then $x = (x|y)y$.

2) Show that $|(x|y)| = \|x\| \|y\|$ if and only if $y = \lambda x$, $\lambda \in \mathbb{C}$.

19.1.1 The Hilbert norm

Proposition 19.1.7. A inner product space is a normed space, with norm

$$\boxed{\|x\| = \sqrt{(x|x)}} \quad (19.7)$$

Proof. We prove the triangle inequality: $\|x + y\|^2 = (x + y|x + y) = (x|x) + 2\text{Re}(x|y) + (y|y) \leq \|x\|^2 + 2|(x|y)| + \|y\|^2 \leq \|x\|^2 + 2\|x\|\|y\| + \|y\|^2 = (\|x\| + \|y\|)^2$. \square

² Atle Selberg gave an extension of Bessel's inequality to non orthonormal vectors $y_1 \dots y_n$ (for a proof see: *Inequalities in Hilbert spaces*, J. Wigstrand, 2008, <https://ntnuopen.ntnu.no/ntnu-xmlui/handle/11250/258406>):

$$\|x\|^2 \geq \sum_{k=1}^n \frac{|(y_k|x)|^2}{\sum_{j=1..n} |(y_j|y_k)|}$$



Figure 19.1 **David Hilbert** (Königsberg 1862, Göttingen 1943) continued the glorious tradition in mathematics of his predecessors Gauss, Dedekind and Riemann at the University of Göttingen, until the racial laws in 1933 dissolved his group. In 1899 he published the *Grundlagen der Geometrie* (*The Foundations of Geometry*) which contains the definitive set of axioms of Euclidean geometry. In his lecture on The problems of mathematics at the International Mathematical Congress in Paris (1900) he set forth a famous list of 23 problems for the mathematicians of the XX century. His studies on integral equations prepared for the important developments in functional analysis and quantum mechanics. He got interested in general relativity and derived the field equations from a variational principle. A partial list of famous students: Felix Bernstein, Richard Courant, Max Dehn, Erich Hecke, Alfréd Haar, Wallie Hurwitz, Hugo Steinhaus, Hermann Weyl, Ernst Zermelo.

Figure 19.2 **János von Neumann** (Budapest 1903, Washington 1957). Only few persons in XX century contributed to so many different fields. He made advances in axiomatic set theory, logic, theory of operators, measure theory, ergodic theory, the mathematical formulation of quantum mechanics, fluid dynamics, nuclear science, and is a founder of computer science. He started as a prodigious child: at the age of 15 he was tutored by the analyst Szegő; by the age of 19 he already published two major papers (providing the modern definition of ordinal numbers, which supersedes G. Cantor's definition). At 22 he received a PhD in mathematics and a diploma in chemical engineering (from ETH Zurich, to comply with his father's desire of a more practical orientation). He taught as Privatdozent at the University of Berlin, the youngest in its history. Since 1933 he was professor in mathematics at the Institute for Advanced Studies in Princeton. He worked in the Manhattan Project.

The existence of a norm implies notions such as continuity, convergent sequences, Cauchy sequences, etc.

Proposition 19.1.8. Fix $x \in \mathcal{H}$, the function $(x|\cdot) : \mathcal{H} \rightarrow \mathbb{C}$ is continuous.

Proof. Let $\{y_n\}$ be a convergent sequence, $y_n \rightarrow y$; we show that $(x|y_n) \rightarrow (x|y)$: $|(x|y_n) - (x|y)| = |(x|y_n - y)| \leq \|x\| \|y_n - y\| \rightarrow 0$. \square

The following *Polarization formulae* express the inner product in terms of the Hilbert norm:

$$\operatorname{Re}(x|y) = \frac{1}{4}(\|x + y\|^2 - \|x - y\|^2) \quad (19.8)$$

$$\operatorname{Im}(x|y) = \frac{1}{4}(\|x - iy\|^2 - \|x + iy\|^2) \quad (19.9)$$

The Hilbert norm has the *parallelogram property*, which can be directly checked out of its definition:

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2 \quad (19.10)$$

Proposition 19.1.9. *A norm is a Hilbert norm (i.e. there is a inner product such that the norm descends from it) if and only if it fulfils the parallelogram condition.³*

Proof. We only need proving that a norm with the parallelogram property descends from a inner product. The formulae (19.8) and (19.9) suggest the following expression as a candidate for the inner product (for a real space the last two terms are absent):

$$(x|y) = \frac{1}{4}\|x + y\|^2 - \frac{1}{4}\|x - y\|^2 - \frac{i}{4}\|x + iy\|^2 + \frac{i}{4}\|x - iy\|^2 \quad (19.11)$$

The difficult task is to prove linearity in the second argument, the other properties being easy to prove. By repeated use of the parallelogram property,

$$\begin{aligned} \operatorname{Re}(x|y + z) &= \frac{1}{4}\|x + y + z\|^2 - \frac{1}{4}\|x - y - z\|^2 \\ &= \left(\frac{1}{2}\|x + y\|^2 + \frac{1}{2}\|z\|^2 - \frac{1}{4}\|x + y - z\|^2\right) - \frac{1}{4}\|x - y - z\|^2 \\ &= \frac{1}{2}\|x + y\|^2 + \frac{1}{2}\|z\|^2 - \frac{1}{2}\|x - z\|^2 - \frac{1}{2}\|y\|^2 \end{aligned}$$

Now sum to it the expression with y and z exchanged, divide by 2 and obtain

$$\begin{aligned} \operatorname{Re}(x|y + z) &= \frac{1}{4}\|x + y\|^2 - \frac{1}{4}\|x - z\|^2 + \frac{1}{4}\|x + z\|^2 - \frac{1}{4}\|x - y\|^2 \\ &= \operatorname{Re}(x|y) + \operatorname{Re}(x|z). \end{aligned}$$

The same procedure works for the imaginary part: $\operatorname{Im}(x|y + z) = \operatorname{Im}(x|y) + \operatorname{Im}(x|z)$. Hence the additive property is proven.

Linearity for scalar multiplication: for $p \in \mathbb{N}$, additivity implies $(x|py) = p(x|y)$. For $q \in \mathbb{N}$: $p(x|y) = p(x|q(y/q)) = pq(x|y/q) = q(x|p(y/q)) \Rightarrow \frac{p}{q}(x|y) = (x|\frac{p}{q}y)$. Since the inner product is continuous and $(x|-y) = -(x|y)$ (see (19.11)), the property extends from rationals

³ see *Analysis for Applied Mathematics*, Ward Cheney (Springer, 2001)

p/q to real numbers. Moreover, since $(x|iy) = i(x|y)$ (see (19.11)), the property holds for complex numbers. \square

Exercise 19.1.10. *In a normed space, a vector x is orthogonal to y in the sense of Birkhoff-James if and only if $\|x\| \leq \|x + \lambda y\|$ for all $\lambda \in \mathbb{C}$. Prove that in a inner-product space the definition coincides with $(x|y) = 0$.*

19.2 Hilbert space

Definition 19.2.1. A **Hilbert space** is a inner product space which is complete in the Hilbert norm topology.

Example 19.2.2. *The linear space \mathbb{C}^n is a Hilbert space with the scalar product $(\mathbf{z}|\mathbf{w}) = \sum_{k=1}^n \overline{z_k} w_k$.*

Example 19.2.3. *The linear space $\mathbb{C}^{n \times n}$ of complex $n \times n$ matrices is a Hilbert space with the inner product*

$$(A|B) = \text{tr}(A^\dagger B) \quad (19.12)$$

where $(A^\dagger)_{ij} = \overline{A_{ji}}$. The corresponding norm is the Frobenius norm:

$$\|A\| = \sqrt{\text{tr}(A^\dagger A)} = \sqrt{\sum_{ij} |A_{ij}|^2}$$

Exercise 19.2.4. *A square matrix is strictly positive, $P > 0$, if and only if $P = M^\dagger M$, with M invertible. Show that $(A|B) = \text{tr}(PA^\dagger B)$ is a inner product in $\mathbb{C}^{n \times n}$.*

Example 19.2.5. *The set $\mathcal{C}[-1, 1]$ of continuous complex-valued functions on $[-1, 1]$ is a inner product space with $(f|g) = \int_{-1}^1 dx \overline{f(x)} g(x)$, but it is not a Hilbert space as this counter-example shows:*

$$f_n(x) = \begin{cases} -1 & -1 \leq x \leq -1/n \\ nx & -1/n < x < 1/n \\ 1 & 1/n \leq x \leq 1 \end{cases} \quad (19.13)$$

is a Cauchy sequence (i.e. $\forall \epsilon$ there is N such that $\int_{-1}^1 dx |f_n(x) - f_m(x)|^2 < \epsilon^2$ for all $n, m > N$) but the limit function (the step function) is not continuous.

19.2.1 Isomorphism of Hilbert spaces

Definition 19.2.6. Two Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 are *isomorphic* if there is a linear operator $\hat{U} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ that is a bijection among the two spaces, and conserves the norm $\|\hat{U}x\|_2 = \|x\|_1 \forall x$. \hat{U} is a **unitary** operator.

Remark. By the polarization formula (19.11), norm conservation and linearity imply the conservation of inner products: $(\hat{U}x|\hat{U}y)_2 = (x|y)_1 \forall x, y \in \mathcal{H}_1$.

Any complex n -dimensional Hilbert space \mathcal{H}_n is isomorphic to \mathbb{C}^n : given an orthonormal basis $\{u_k\}_{k=1}^n$ in \mathcal{H}_n , the expansion $x = \sum_{k=1}^n x_k u_k$ has coefficients $x_k = (u_k|x)$ that define a vector $\mathbf{x} \in \mathbb{C}^n$. The map $\hat{U}x = \mathbf{x}$ is a unitary operator from \mathcal{H}_n to \mathbb{C}^n .

Is there a canonical isomorphism for infinite-dimensional Hilbert spaces? The answer is affirmative for Hilbert spaces with the following property:

Definition 19.2.7. A Hilbert space is **separable** if it has a countable dense subset.

19.2.2 Square summable sequences

In 1906 David Hilbert introduced the important set $\ell^2(\mathbb{C})$ of complex sequences $\{a_k\}_{k=1}^\infty$ such that

$$\sum_{k=1}^{\infty} |a_k|^2 < \infty$$

This set is the infinite-dimensional analogue of \mathbb{C}^n (\mathbb{R}^n for real sequences).

- $\ell^2(\mathbb{C})$ is a linear space. If $\mathbf{a} = \{a_k\}$ and $\mathbf{b} = \{b_k\}$, define:

$$\mathbf{a} + \mathbf{b} = \{a_k + b_k\}, \quad \lambda \mathbf{a} = \{\lambda a_k\}$$

The inequality $|a_k + b_k|^2 \leq |a_k|^2 + |b_k|^2 + 2|a_k b_k| \leq 2|a_k|^2 + 2|b_k|^2$ (use $0 < (x - y)^2 = x^2 + y^2 - 2xy$) implies that $\mathbf{a} + \mathbf{b} \in \ell^2(\mathbb{C})$.

- $\ell^2(\mathbb{C})$ is an inner product space with

$$(\mathbf{a}|\mathbf{b}) = \sum_{k=1}^{\infty} \overline{a_k} b_k \tag{19.14}$$

The series converges absolutely: $2|a_k b_k| \leq |a_k|^2 + |b_k|^2$. The formal properties of inner product are easily checked.

- $\ell^2(\mathbb{C})$ is complete (it is a Hilbert space).

Proof. Let $\{\mathbf{a}_\nu\}$ be a Cauchy sequence of elements in ℓ^2 (a sequence of sequences $\{a_{\nu k}\}$), i.e. for any $\epsilon > 0$ there is N_ϵ such that for all $\nu, \mu > N_\epsilon$ it is

$$\|\mathbf{a}_\nu - \mathbf{a}_\mu\|^2 = \sum_{k=1}^{\infty} |a_{\nu k} - a_{\mu k}|^2 < \epsilon^2 \quad (19.15)$$

We show that \mathbf{a}_ν converges in $\ell^2(\mathbb{C})$. The Cauchy condition implies that $|a_{\nu k} - a_{\mu k}| < \epsilon$ for all k and $\nu, \mu > N_\epsilon$, then each sequence $\{a_{\nu 1}\}, \{a_{\nu 2}\}, \dots$ is Cauchy and converges in \mathbb{C} to limits a_1, a_2, \dots . Let $\mathbf{a} = \{a_1, a_2, \dots\}$ be the sequence of such limits.

Eq.(19.15) holds for all $\nu, \mu > N_\epsilon$; now let $\mu = \infty: \sum_k |a_{\nu k} - a_k|^2 < \epsilon^2$, i.e. $\mathbf{a}_\nu - \mathbf{a} \in \ell^2(\mathbb{C})$. Since \mathbf{a}_ν belongs to the linear space, also \mathbf{a} does. Moreover, $\|\mathbf{a}_\nu - \mathbf{a}\| \leq \epsilon$, i.e. $\mathbf{a}_\nu \rightarrow \mathbf{a}$ in the ℓ^2 topology. \square

- $\ell^2(\mathbb{C})$ is separable.

Proof. Consider the subset of sequences $\mathbf{q} = \{q_0, q_1, \dots, q_k, 0, \dots\}$, where $\text{Re } q_j$ and $\text{Im } q_j$ are rational numbers for $j < k$, and $q_j = 0$ for $j \geq k$ (where each sequence has its own k). The set is countable. We show that it is dense in $\ell^2(\mathbb{C})$, i.e. for any element \mathbf{a} and any $\epsilon > 0$ there is an element \mathbf{q} such that $\|\mathbf{a} - \mathbf{q}\| < \epsilon$.

Fix ϵ and choose n such that $\sum_{k=n+1}^{\infty} |a_k|^2 < \frac{1}{2}\epsilon^2$ and $\mathbf{q} = \{q_1, \dots, q_n, 0, \dots\}$ such that $|a_k - q_k|^2 \leq \epsilon^2/2n$ for all $k \leq n$ (the numbers q_k are dense in \mathbb{C}). Then: $\|\mathbf{a} - \mathbf{q}\|^2 = \sum_{k=1}^n |a_k - q_k|^2 + \sum_{k>n} |a_k|^2 < n \frac{\epsilon^2}{2n} + \frac{1}{2}\epsilon^2 = \epsilon^2$. \square

This is an example of non-separable Hilbert space⁴.

Consider the set $\mathcal{E} = \{e_\omega\}_{\omega \in \mathbb{R}}$ of functions $e_\omega(t) = \exp(i\omega t)$, $t \in \mathbb{R}$. The finite linear combinations $f = \sum_\omega f_\omega e_\omega$ with complex numbers f_ω form a linear space. The following “time average” is always well defined, and is a inner product:

$$(f|g) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} \overline{f(t)} g(t) dt \quad (19.16)$$

The completion of the linear space with respect to the norm is a Hilbert space. As $(e_\omega | e_{\omega'}) = \delta_{\omega, \omega'}$, it is $\|e_\omega - e_{\omega'}\|^2 = 2$ if $\omega \neq \omega'$. Since \mathcal{E} is uncountable, with elements separated by a finite distance, there cannot exist a countable set of functions such that any e_ω is approximated by a linear combination of such functions (we'd need an uncountable set of approximating functions!). Then the Hilbert space is non-separable.

19.3 Orthogonal systems

Given n linearly independent elements x_1, \dots, x_n it is always possible to produce linear combinations u_1, \dots, u_n that form an orthonormal set.

⁴ N.I.Akhiezer and I.M.Glazman, "Theory of linear operators in Hilbert spaces", vol 1, par.13 (1961) (Dover reprint).

The (Gram - Schmidt) orthonormalization procedure is:

$$\begin{aligned}
 y_1 &= x_1, & \Rightarrow u_1 &= y_1 / \|y_1\|, \\
 y_2 &= x_2 - (u_1|x_2)u_1, & \Rightarrow u_2 &= y_2 / \|y_2\|, \\
 y_3 &= x_3 - (u_1|x_3)u_1 - (u_2|x_3)u_2, & \Rightarrow u_3 &= y_3 / \|y_3\|, \\
 \dots & & & \dots
 \end{aligned}$$

Exercise 19.3.1. With x_1, \dots, x_n introduce the Gram matrix $G_{ij} = (x_i|x_j)$. Show that:

- 1) the vectors are linearly dependent iff $\det G = 0$;
- 2) the matrix is non-negative ($G \geq 0$) i.e. $u^\dagger G u \geq 0 \forall u \in \mathbb{C}^n$;
- 3) $\det G \leq \|x_1\|^2 \cdots \|x_n\|^2$ (use Hadamard's inequality for positive matrices).

Exercise* 19.3.2. In \mathbb{C}^n , given n linearly independent vectors x_1, \dots, x_n , a vector has expansion $y = \sum_{i=1}^n c_i x_i$. The coefficients c_i solve the linear system $(x_i|y) = \sum_j G_{ij} c_j$ where G is Gram's matrix. Show that (Cramer):

$$c_i = \frac{(-1)^{i+1} \det \begin{bmatrix} 0 & x_1 & \cdots & x_n \\ (x_1|y) & (x_1|x_1) & \cdots & (x_1|x_n) \\ \vdots & \vdots & & \vdots \\ (x_n|y) & (x_n|x_1) & \cdots & (x_n|x_n) \end{bmatrix}}{\det G} \tag{19.17}$$

19.4 The Hilbert space $L^2(\Omega)$

The norm of the Banach space of Lebesgue square integrable functions,

$$\|f\|_2 = \sqrt{\int_{\Omega} |f|^2 dx}$$

descends from the inner product

$$(f|g) = \int_{\Omega} \bar{f} g dx \tag{19.18}$$

Then L^2 spaces are Hilbert spaces. They are among the most important spaces in functional analysis.

Exercise 19.4.1. Evaluate the norm in $L^2(0, \infty)$ of the function

$$h(x) = \frac{1}{\sqrt{x+a} \sqrt[4]{x/a}} \quad a > 0$$

Exercise 19.4.2 (Hilbert’s inequality). *If $f > 0$ and $g > 0$ belong to $\mathcal{L}^2(0, \infty)$:*

$$\int_0^\infty dx \int_0^\infty dy \frac{f(x)g(y)}{x+y} \leq \pi \|f\|_2 \|g\|_2$$

For a simple derivation⁵ set $x = u^2$, $y = v^2$ and then $u = r \cos \theta$, $v = r \sin \theta$. Next, use the Schwarz inequality. The constant π is optimal.

19.4.1 Orthogonal polynomials

On the real line, or half-line, or intervals, one introduces important families of orthogonal functions (see also the chapter on trigonometric series). An important case are the orthogonal polynomials.

Let p_0, p_1, \dots be a sequence of real *polynomials* of degree $0, 1, \dots$, that satisfy the *orthogonality condition*

$$\int_\sigma dx \omega(x) p_i(x) p_j(x) = h_j \delta_{ij} \tag{19.19}$$

$\omega(x) \geq 0$ is a weight function, σ is a real (possibly unbounded) interval, $h_j > 0$ are constants.

The table lists some important sets of orthogonal polynomials, that may be obtained by orthogonalization of the monomials $1, x, x^2, \dots$:

σ	$\omega(x)$	p_k	
\mathbb{R}	$\exp(-x^2)$	H_k	Hermite
$[0, \infty)$	$\exp(-x)$	L_k	Laguerre
$[-1, 1]$	1	P_k	Legendre
$[-1, 1]$	$(1 - x^2)^{-\frac{1}{2}}$	T_k	Chebyshev
$[-1, 1]$	$(1 - x^2)^{\alpha - \frac{1}{2}}$	C_k^α	Gegenbauer

Proposition 19.4.3. *Orthogonal polynomials satisfy a three-term recursion relation with real constants a_k, b_k and c_k :*

$$x p_k(x) = a_k p_{k+1}(x) + b_k p_k(x) + c_k p_{k-1}(x) \tag{19.20}$$

Proof. Suppose that the recursion contains the term $d_k p_{k-2}(x)$. Multiply the recursion by $\omega(x) p_{k-2}(x)$ and integrate. All terms but two vanish by orthogonality:

$$\int_\sigma dx \omega(x) x p_k(x) p_{k-2}(x) = d_k h_{k-2}.$$

⁵ D. C. Ullrich, *A simple elementary proof of Hilbert’s Inequality*, Amer. Math. Monthly, 120 n.2 (2013) p.161-4.

Since it is $x p_{k-2} = a_{k-2} p_{k-1} + \dots$, also the left integral vanishes by orthogonality. Therefore $d_k = 0$. In the same way one proves the absence of all lower order terms in the recurrence. \square

The recursion starts with the pair $p_0(x) = p_0$, $p_1(x) = (p_0/a_0)(x - b_0)$ where p_0 is arbitrary, b_0 results from $(p_0|p_1) = 0$ i.e. $\int_{\sigma} dx(x - b_0) = 0$, and a_0 is yet unspecified. The coefficient of the highest power is

$$p_k(x) = x^k \frac{p_0}{a_{k-1} \dots a_0} + \dots$$

The constants p_0 and a_k are chosen to be positive (for monic orthogonal polynomials⁶ p_0 and all a_k in (19.20) are equal to 1).

The relations $c_k h_{k-1} = \int_{\sigma} dx \omega x p_k p_{k-1}$ and $x p_{k-1} = a_{k-1} p_k + \dots$ give

$$c_k h_{k-1} = a_{k-1} h_k \tag{19.21}$$

It implies that the coefficients c_k are non negative if the a_k are positive.

The recursion of polynomials may be written in multiplicative form:

$$\begin{bmatrix} p_{k+1}(x) \\ p_k(x) \end{bmatrix} = \begin{bmatrix} (x - b_k)/a_k & -c_k/a_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_k(x) \\ p_{k-1}(x) \end{bmatrix}$$

Iteration provides p_k in terms of p_1 and p_0 via a product of k matrices (transfer matrix). In a different guise, the recursion corresponds to the evaluation of the determinant of a symmetric tridiagonal matrix. For monic polynomials:

$$p_{k+1}(x) = \det \begin{bmatrix} x - b_k & \sqrt{c_k} & & & \\ \sqrt{c_k} & \ddots & \ddots & & \\ & \ddots & x - b_1 & \sqrt{c_1} & \\ & & \sqrt{c_1} & x - b_0 & \end{bmatrix}$$

This has an important implication: the zeros of orthogonal polynomials are real.

⁶ A polynomial is monic if the coefficient of the leading power is unity

Proposition 19.4.4 (Christoffel-Darboux summation formulae).

$$\sum_{k=0}^n \frac{p_k(x)p_k(y)}{h_k} = \frac{a_n}{h_n} \frac{p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)}{x-y} \quad (19.22)$$

$$\sum_{k=0}^n \frac{p_k(x)^2}{h_k} = \frac{a_n}{h_n} [p'_{n+1}(x)p_n(x) - p'_n(x)p_{n+1}(x)] \quad (19.23)$$

Proof. Multiply the recursion (19.20) by $p_k(y)$, and subtract the same expression with x and y exchanged. Divide by h_k and sum on k . Cancellation of all but two terms occurs, because of (19.21). The second formula is the limit $y \rightarrow x$ of the first one. \square

Exercise 19.4.5. If $\sigma = [a, b]$, show that $a \leq b_k \leq b$ for all k .

Exercise 19.4.6. Show that $p_k(x)$ and $p'_k(x)$ cannot be zero at the same point, i.e. the zeros of orthogonal polynomials are simple⁷.

Two important sets of orthogonal polynomials are discussed below⁸ (see also Chebyshev polynomials in 11.3.2).

Legendre polynomials

Legendre's polynomials $P_k(x)$ (see the generating function in 11.3.3) result from the orthogonalization of $1, x, x^2, \dots$ in $L^2(-1, 1)$:

$$\int_{-1}^1 dx P_i(x)P_j(x) = h_j \delta_{ij}$$

The constants h_j are determined by the conditions $P_j(1) = 1$. Then $P_0(x) = 1$ and $P_1(x) = x$ (they are orthogonal).

P_2 has no linear term to ensure orthogonality with P_1 : $P_2(x) = C_2(x^2 + A_2)$; the conditions $1 = P_2(1)$ and $0 = \int_{-1}^1 dx P_0 P_2$ give $P_2(x) = (3x^2 - 1)/2$.

The odd polynomial $P_3(x) = C_3(x^3 + A_3x)$ is orthogonal to even polynomials, with $P_3(1) = 1$ and $0 = \int_{-1}^1 dx P_3(x)P_1(x)$. The next one is even: $P_4(x) = C_4(x^4 + A_4x^2 + B_4)$, with parameters determined by three conditions: $P_4(1) = 1$, $P_4 \perp P_2$ and $P_4 \perp P_0$... the process is tedious

⁷ Besides being real and simple, the zeros of orthogonal polynomials are all in the interval of orthogonality σ . Moreover, any zero of $p_k(x)$ is between two consecutive zeros of $p_{k+1}(x)$ (interlacing property).

⁸ The books *Orthogonal Polynomials* by Szego, *Polynomials* by V. Prasolov, and *Polynomials and polynomial inequalities* by P. Bowman and T. Erdélyi are useful references, together with books on special functions (NIST, Askey). Orthogonal polynomials arise in the theory of Jacobi operators (infinite Hermitian tridiagonal matrices), Sturm-Liouville differential equations, approximation theory, soluble models of statistical mechanics. They arise unexpectedly and beautifully in random matrix theory (see the books by Mehta, or Deift, or Forrester).

to continue. Instead one can succeed in obtaining the recursive relation (where parity of polynomials is accounted for):

$$xP_k(x) = a_k P_{k+1}(x) + c_k P_{k-1}(x)$$

by evaluating h_k , a_k and c_k .

For $x = 1$ it is $1 = a_k + c_k$, moreover $(1 - a_k)h_{k-1} = a_{k-1}h_k$, by (19.21). Another equation is obtained by taking the derivative of the recursion, $P_k + xP'_k = a_k P'_{k+1} + c_k P'_{k-1}$, multiplication by P_k and integration on $[-1, 1]$,

$$h_k + \frac{1}{2} \int_{-1}^1 x \frac{d}{dx} P_k^2 dx = a_k \int_{-1}^1 P_k P'_{k+1} dx$$

and integration by parts: $\frac{1}{2}h_k + 1 = 2a_k$. The two equations for a_k and h_k give $h_k h_{k-1} + h_k - h_{k-1} = 0$ i.e. $h_k^{-1} = h_{k-1}^{-1} + 1$, with initial condition $h_0 = 2$. The solution is $h_k^{-1} = k + h_0^{-1}$ i.e. $h_k = \frac{2}{2k+1}$. Therefore, the orthogonality and recursive relations are:

$$\int_{-1}^1 dx P_m(x) P_n(x) = \frac{2}{2n+1} \delta_{mn} \quad (19.24)$$

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \quad (19.25)$$

Hermite polynomials

Hermite polynomials are obtained by orthogonalization of the functions $1, x, x^2, \dots$ on the real line, with weight $\omega(x) = e^{-x^2}$:

$$\int_{-\infty}^{+\infty} dx e^{-x^2} H_i(x) H_j(x) = h_j \delta_{ij}$$

They are determined by fixing the leading coefficient: $H_k(x) = 2^k x^k + \dots$. Because weight and domain are symmetric for $x \rightarrow -x$, Hermite polynomials have definite parity:

$$H_k(-x) = (-1)^k H_k(x).$$

This simplifies the recursion relation: $xH_k(x) = \frac{1}{2}H_{k+1}(x) + c_k H_{k-1}(x)$. To evaluate c_k and h_k note that $c_k h_{k-1} = \frac{1}{2}h_k$. The derivative of the recursion is multiplied by H_k and integrated with the weight:

$$h_k + \frac{1}{2} \int_{\mathbb{R}} dx e^{-x^2} x \frac{d}{dx} H_k^2(x) = \frac{1}{2} \int_{\mathbb{R}} dx e^{-x^2} H_k(x) H'_{k+1}(x)$$

Integrate by parts, $\frac{1}{2}h_k + \int_{\mathbb{R}} dx e^{-x^2} [xH_k(x)]^2 = \int_{\mathbb{R}} dx e^{-x^2} xH_k(x)H_{k+1}(x)$. Use the recursion to obtain $\frac{1}{2}h_k + \frac{1}{4}h_{k+1} + c_k^2 h_{k-1} = \frac{1}{2}h_{k+1}$, i.e. $\frac{h_{k+1}}{h_k} = \frac{h_k}{h_{k-1}} + 2$ with solution $\frac{h_{k+1}}{h_k} = 2k + \frac{h_1}{h_0}$. Since $h_1 = \int_{\mathbb{R}} dx 4x^2 e^{-x^2} = 2\sqrt{\pi}$ and $h_0 = \int_{\mathbb{R}} dx e^{-x^2} = \sqrt{\pi}$, one obtains $h_{k+1} = 2(k+1)h_k$ i.e. $h_k = 2^k k! \sqrt{\pi}$ and $c_k = k$. Therefore:

$$\int_{\mathbb{R}} dx e^{-x^2} H_i(x)H_k(x) = 2^k k! \sqrt{\pi} \delta_{ik} \quad (19.26)$$

$$H_{k+1}(x) = 2xH_k(x) - 2kH_{k-1}(x) \quad (19.27)$$

The large- n distribution of the zeros of $H_n(x)$ is discussed in subsection 25.4.

Hermite polynomials are related to *Hermite functions*, that are an orthonormal basis in $L^2(\mathbb{R})$:

$$h_k(x) = \frac{1}{\sqrt{2^k k! \sqrt{\pi}}} e^{-\frac{1}{2}x^2} H_k(x) \quad (19.28)$$

A proof of completeness will be given in theorem 27.2.1.

The differential equation (11.20) solved by Hermite polynomials gives the following second-order equation solved by Hermite functions (Weber's equation):

$$-h_n''(x) + x^2 h_n(x) - (2n+1)h_n(x) = 0 \quad (19.29)$$

19.4.2 Gauss quadrature formula*

A nice application of orthogonal polynomials is a method by Gauss to approximately evaluate weighted integrals on a set σ . The formula is

$$\int_{\sigma} dx w(x) f(x) = \sum_{k=1}^n w_k f(x_k) + R_n \quad (19.30)$$

$$w_k = \frac{1}{p_n'(x_k)} \int_{\sigma} dx \frac{p_n(x)}{x - x_k} \quad (19.31)$$

$\{x_k\}$ are the zeros of the monic polynomial $p_n(x)$, belonging to an orthogonal set on the interval σ with weight function w . The weights w_k and the roots x_k are tabulated (for the frequently used Chebyshev polynomials they are the zeros of $\cos n\theta$, with $x = \cos\theta$). The remainder R_n is here given for a smooth f , and ξ is a point in σ .

Proof. The integral is equal to:

$$\begin{aligned} \int_{\sigma} dx w(x) \frac{f(x)}{p_n(x)} p_n(x) &= \sum_{k=1}^n \frac{1}{p'_n(x_k)} \int_{\sigma} dx w(x) \frac{f(x)}{x-x_k} p_n(x) \\ &= \sum_{k=1}^n \frac{1}{p'_n(x_k)} \int_{\sigma} dx w(x) \frac{f(x_k) + f(x) - f(x_k)}{x-x_k} p_n(x) \end{aligned}$$

where (9.1) was used for $1/p_n(z)$. One reads the quadrature approximation, and the remainder:

$$R_n = \sum_{k=1}^n \frac{1}{p'_n(x_k)} \int_{\sigma} dx w(x) \frac{f(x) - f(x_k)}{x-x_k} p_n(x)$$

f is Taylor-expanded in the powers $(x-x_k)^p$, that are further expanded with Newton's formula. There are two facts that yield zero contribution:

- powers x^j , $j < n$, are orthogonal to p_n ,
- $\sum_k x_k^m / p'_n(x_k) = 0$ for $m = 0, \dots, n-2$ (see (9.2)).

The lowest degree for a non-zero result is $x^n x_k^{n-1}$. This occurs in the Taylor term with power $2n$. The remainder is then approximated as

$$\begin{aligned} R_n &\approx \frac{f^{(2n)}(\xi)}{(2n)!} \sum_{k=1}^n \frac{1}{p'_n(x_k)} \int_{\sigma} dx w(x) (x-x_k)^{2n-1} p_n(x) \\ &= \frac{f^{(2n)}(\xi)}{(2n)!} (-1)^{n-1} \binom{2n-1}{n} \sum_{k=1}^n \frac{x_k^{n-1}}{p'_n(x_k)} \int_{\sigma} dx w(x) x^n p_n(x) \\ &= \frac{h_n}{2(n!)^2} (-1)^{n-1} f^{(2n)}(\xi) \end{aligned}$$

because the sum is 1 and $\int_{\sigma} dx w(x) x^n p_n(x) = h_n$. Here R_n differs in the denominator from the expression in textbooks (which is $(2n)!$). \square

19.5 Linear subspaces and projections

Definition 19.5.1. A linear subspace M is *closed* if any sequence in M that is convergent has limit in M .

The *closure* \overline{M} of a linear subspace is a linear subspace.

Definition 19.5.2. If M is a linear subspace of \mathcal{H} , the *orthogonal complement* of M is the set M^{\perp} of points that are orthogonal to M .

Proposition 19.5.3. M^{\perp} is a linear closed subspace.

Proof. M^\perp is a linear space: if x_1 and x_2 are in M^\perp , then $(z|x_1 + \lambda x_2) = (z|x_1) + \lambda(z|x_2) = 0$ if $z \in M$, i.e. $x_1 + \lambda x_2 \in M^\perp$. If x_n is a sequence in M^\perp , and $x_n \rightarrow x$ then, by the continuity of the inner product, $0 = (z|x_n) \rightarrow (z|x)$ for all $z \in M$, i.e. $x \in M^\perp$. \square

Exercise 19.5.4. Show that if $M_1 \subset M_2$ then $M_2^\perp \supseteq M_1^\perp$.

The linear subspaces of \mathbb{R}^3 are planes and straight lines through the origin. A point \mathbf{x} external to a line r of parametric equation $\mathbf{x}(t) = \mathbf{a}t$ has a unique projection $\mathbf{p} \in r$ that corresponds to the point of minimal distance of \mathbf{x} from r . Moreover, \mathbf{x} has a unique decomposition as $\mathbf{p} \in r$ and a vector $\mathbf{x} - \mathbf{p}$ orthogonal to r . These geometric facts (existence of a point of minimal distance and the orthogonal decomposition) is shared by Hilbert spaces.

The first non-trivial step is to prove that, given a *closed* linear subspace and a point x , there exists one and only one point p belonging to it, whose distance from x is minimal (the *set distance* of x)⁹.

Definition 19.5.5. The *distance* of a point x from a set M is $d(x, M) = \inf_{y \in M} \|x - y\|$.

Lemma 19.5.6. Let M be a linear closed subspace in \mathcal{H} . Then, given $x \in \mathcal{H}$, $x \notin M$, there is a unique $p \in M$ such that $d(x, M) = \|x - p\|$.

Proof. Let d be the distance of x from M . By definition, there is a sequence y_n in M such that $\|y_n - x\| \rightarrow d$; we show that it is a Cauchy sequence.

By the parallelogram law:

$$\|y_n - y_m\|^2 = \|(y_n - x) - (y_m - x)\|^2 = 2\|y_n - x\|^2 + 2\|y_m - x\|^2 - \|2x - (y_n + y_m)\|^2$$

The vector $\frac{1}{2}(y_n + y_m)$ belongs to M , then $\|x - \frac{1}{2}(y_n + y_m)\| \geq d$ and

$$\|y_n - y_m\|^2 \leq 2\|y_n - x\|^2 + 2\|y_m - x\|^2 - 4d^2$$

By hypothesis, for any $\epsilon > 0$ there is N_ϵ such that $\|y_n - x\|^2 - d^2 \leq \epsilon$ for all $n \geq N_\epsilon$. Then it is $\|y_n - y_m\|^2 \leq 4\epsilon$ for all $n, m \geq N_\epsilon$. The Cauchy sequence $\{y_n\}$ has a limit point $p \in M$ (M is closed); as the norm is a continuous map of \mathcal{H} to \mathbb{R} , it follows that $\|x - p\| = \lim_n \|x - y_n\| = d$.

Suppose that there is another $p' \in M$ such that $\|x - p'\| = d$, then for the given x : $\|p - p'\|^2 = \|(p - x) - (p' - x)\|^2 = -\|p + p' - 2x\|^2 + 4d^2$. The mid-point $p'' = (p + p')/2$ belongs to M and $\|x - p''\| \geq d$. Therefore $\|p - p'\|^2 \leq 0$. \square

⁹ The theorem extends to uniformly convex Banach spaces, introduced by J. A. Clarkson (Trans. Amer. Math. Soc. 40, 1936, 396–414). L^p spaces with $1 < p < \infty$ are such.

Theorem 19.5.7 (Projection theorem). Let M be a closed subspace in a Hilbert space \mathcal{H} . A vector in \mathcal{H} has the unique decomposition

$$x = p + w, \quad p \in M, \quad w \in M^\perp \quad (19.32)$$

Proof. Given x there is a unique vector p in M such that $\|x - p\| = d$. We have to show that $w \equiv x - p \in M^\perp$. For any λ and $y \in M$ it is $p + \lambda y \in M$ and

$$d^2 \leq \|x - (p + \lambda y)\|^2 = d^2 - 2\operatorname{Re}[\lambda(w|y)] + |\lambda|^2 \|y\|^2.$$

$-2\operatorname{Re}[\lambda(w|y)] + |\lambda|^2 \|y\|^2 \geq 0$ for all complex λ if $(w|y) = 0$ for all y , i.e. $w \perp M$.

Suppose that $x = p + w = p' + w'$ with p, p' in M and w, w' in M^\perp . Then $(p - p') + (w - w') = 0$ with $p - p' \in M$ and $w - w' \in M^\perp$. The vanishing of the norm, $\|p - p'\|^2 + \|w - w'\|^2 = 0$, implies $p = p'$ and $w = w'$. \square

Proposition 19.5.8. If M is a linear subspace, then $M^{\perp\perp} = \overline{M}$.

Proof. The statements: $x \in M^{\perp\perp} \Leftrightarrow (x|y) = 0 \forall y \in M^\perp \Rightarrow x \in M$ imply that $M \subseteq M^{\perp\perp}$, and $\overline{M} \subseteq M^{\perp\perp}$. The other way, suppose that there is a vector $x \in M^{\perp\perp}$ with $x \notin \overline{M}$. Then $x \in M^\perp$: this means $x = 0$, as M^\perp and $M^{\perp\perp}$ are orthogonal sets. \square

Definition 19.5.9 (Orthogonal sum). Given two orthogonal closed subspaces M_1 and M_2 in \mathcal{H} , their orthogonal sum is

$$M_1 \oplus M_2 = \{x_1 + x_2, x_1 \in M_1, x_2 \in M_2\}.$$

Exercise 19.5.10. Prove that $M_1 \oplus M_2$ is closed.

(Hint: show that if $x_{1j} + x_{2j} \rightarrow x$ then x_{1j} and x_{2j} are Cauchy sequences in M_1 and M_2).

The projection theorem states that if M is closed then

$$\mathcal{H} = M \oplus M^\perp \quad (19.33)$$

Suppose that a linear subspace M is spanned by the orthonormal vectors $\{u_k\}_{k=1}^n$. Given a point x it is $x = p + r$ where $p = \sum_{k=1}^n p_k u_k$ is the projection of x in M and $r \in M^\perp$ is the remainder. Because $(u_k|r) = 0$, one immediately gets $p_k = (u_k|x)$. The same result is obtained by minimizing the squared distance of x from M :

$$d^2 = \|x - p\|^2 = \|x\|^2 - \sum_{k=1}^n \left[p_k(x|u_k) + \overline{p_k}(u_k|x) - \overline{p_k} p_k \right]$$

Minimization in the coefficients p_k and $\overline{p_k}$ again gives $p_k = (u_k|x)$.

The projection of x is

$$p = \sum_{k=1}^n (u_k | x) u_k \quad (19.34)$$

Example 19.5.11. Consider the function

$$f(x) = \frac{1}{a-x}, \quad x \in [-1, 1], |a| > 1$$

and the problem of finding its "best approximation" in terms of real polynomials of order n . In $L^2(-1, 1)$, this means to find the polynomial A_n of degree n with least $L^2(-1, 1)$ -norm deviation from the function, i.e. to minimize the squared error

$$\|f - A_n\|^2 = \int_{-1}^{+1} dx \left[\frac{1}{a-x} - (a_n x^n + \dots + a_1 x + a_0) \right]^2$$

with respect to the coefficients $a_n \dots a_0$. The minimal norm is realized by the distance of the function from the (closed) subspace \mathcal{P}_n of polynomials of degree n , and the "best approximation" is precisely the projection of the function on \mathcal{P}_n . The Legendre polynomials P_k form an orthogonal basis of $L^2(-1, 1)$, and any polynomial of order n is a linear combination of them with $k \leq n$. Taking into account normalization, the best polynomial of order n is:

$$A_n(x) = \sum_{k=0}^n C_k P_k(x), \quad C_k = \frac{2k+1}{2} \int_{-1}^{+1} dx \frac{P_k(x)}{a-x}$$

From the recursive relation (19.25) of the polynomials, one may obtain a recursion scheme for C_k (in this case $C_k = (2k+1)Q_k(a)$, where $Q_k(x)$ is a Legendre functions of the second kind).

Other norms give different approximations. In $L^2([-1, 1], dx/\sqrt{1-x^2})$ the Chebyshev polynomials are orthogonal (see also 2.5.2, 11.3.2). The projection on the subspace of polynomials of order n is:

$$\tilde{A}_n(x) = \sum_{k=0}^n \tilde{C}_k T_k(x), \quad \tilde{C}_k = \frac{1}{h_k} \int_{-1}^1 \frac{dx}{\sqrt{1-x^2}} \frac{T_k(x)}{a-x}$$

with $h_0 = \pi$, and $h_k = \pi/2$. The coefficients may be evaluated with the Residue Theorem:

$$\tilde{C}_k = \frac{2}{\pi} \int_0^\pi d\theta \frac{\cos(k\theta)}{a - \cos\theta} = e^{-(k+1)\xi}$$

where $a = \cosh \xi$. The error can be computed exactly with the Christoffel-Darboux formula:

$$\left| \frac{1}{\cosh \xi - x} - \tilde{A}_n(x) \right| = \frac{e^\xi T_{n+1}(x) - T_n(x)}{(\cosh \xi - x) \sinh \xi} e^{-(n+1)\xi}$$

The property $|T_k(x)| \leq 1$ on $[-1, 1]$ allows for a uniform upper bound of the error:

$$\left| \frac{1}{a-x} - \tilde{A}_n(x) \right| \leq \frac{e^\xi + 1}{(a-1) \sinh \xi} e^{-(n+1)\xi}, \quad -1 < x < 1.$$

Exercise 19.5.12. Show that the best approximation for $\sin x$ with cubic polynomials in $L^2(-1, 1)$ is $\sin x = 0.9981x - 0.1576x^3 + r(x)$.

Note that it differs from the MacLaurin expansion $x - 0.1666x^3 + \delta(x)$ which fits best near the origin. The remainders $r(x)$ and $\delta(x)$ are plotted in Fig.19.3.

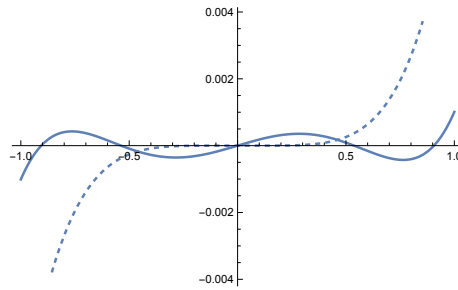


Figure 19.3 The remainders $r(x)$ (full) and $\delta(x)$ (dashed).

19.6 Complete orthonormal systems

Theorem 19.6.1. Let $\{u_k\}_{k=1}^\infty$ be a countable set of orthonormal vectors in \mathcal{H} , and $\{c_k\}_{k=1}^\infty$ a complex sequence. Then

$$\sum_{k=1}^\infty c_k u_k \in \mathcal{H} \iff \sum_{k=1}^\infty |c_k|^2 < \infty$$

and, if the series converges to x , it is $c_k = (u_k|x)$.

Proof. The partial sums $x_n = \sum_{k=1}^n c_k u_k$ form a Cauchy sequence if and only if $\sum_{k=1}^n |c_k|^2$ is a Cauchy sequence in \mathbb{C} : this follows from the identity

$$\|x_n - x_m\|^2 = \left\| \sum_{k=m+1}^n c_k u_k \right\|^2 = \sum_{k=m+1}^n |c_k|^2.$$

Then $x_n \rightarrow x$ iff $c_k \in \ell^2(\mathbb{C})$.

Moreover $c_k = (u_k|x_n) \rightarrow (u_k|x)$ by continuity of the inner product, and $\|x\|^2 = \lim_n \|x_n\|^2 = \lim_n \sum_{k=0}^n |c_k|^2 = \sum_{k=0}^\infty |c_k|^2$. □

Definition 19.6.2. An orthonormal set $\{u_a\}_{a \in A}$ of vectors, $(u_a|u_b) = 0$ if $a \neq b$ and $\|u_a\| = 1$, is *complete* if it is not a subset of another orthonormal set.

An equivalent statement is: an orthonormal set $\{u_a\}_{a \in A}$ is complete if

$$\boxed{(u_a|x) = 0 \quad \forall a \in A \Rightarrow x = 0} \quad (19.35)$$

A Hilbert space with a countable orthonormal complete set of vectors is separable, and it is isomorphic to $\ell^2(\mathbb{C})$.

Theorem 19.6.3 (Parseval's identity). *In a separable Hilbert space, if $\{u_k\}_{k=1}^{\infty}$ is an orthonormal complete basis, then:*

$$x = \sum_{k=1}^{\infty} (u_k|x)u_k, \quad \|x\|^2 = \sum_{k=1}^{\infty} |(u_k|x)|^2, \quad \forall x \in \mathcal{H} \quad (19.36)$$

$$(x|y) = \sum_{k=1}^{\infty} (x|u_k)(u_k|y) \quad (19.37)$$

The numbers $(u_k|x)$ are the *Fourier coefficients* of the expansion.

19.7 Bargmann space

The Bargmann space $\mathcal{B}(\mathbb{C})$ is the linear space of entire functions¹⁰ such that

$$\int \frac{dz d\bar{z}}{\pi} e^{-|z|^2} |f(z)|^2 < \infty$$

where $dz d\bar{z} \equiv dx dy$ and $z = x + iy$. It is a Hilbert space with the inner product

$$(f|g) = \int \frac{d\bar{z} dz}{\pi} e^{-|z|^2} \overline{f(z)} g(z) \quad (19.38)$$

The functions $u_k(z) = z^k / \sqrt{k!}$ are orthonormal:

$$\boxed{\int \frac{d\bar{z} dz}{\pi} e^{-|z|^2} \overline{z^n} z^m = n! \delta_{nm}} \quad (19.39)$$

(this is a useful integral, evaluate it with polar coordinates). Since entire functions have power series expansions, the functions u_k form a complete set.

On suitable domains one defines the linear operators

$$(\hat{a}f)(z) = f'(z), \quad (\hat{a}^\dagger f)(z) = zf(z)$$

¹⁰ V. Bargmann, *On a Hilbert space of analytic functions and an associated integral transform*, Comm. Pure Appl. Math. 14 (1961) 187.

with commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$. They are the lowering and raising operators of the basis functions:

$$\hat{a} u_k = \sqrt{k} u_{k-1}, \quad \hat{a}^\dagger u_k = \sqrt{k+1} u_{k+1}$$

The operator $\hat{N} \equiv \hat{a}^\dagger \hat{a} = z \frac{d}{dz}$ has action $\hat{N} u_k = k u_k$.

The eigenstates of the lowering operator $(\hat{a}\phi_\xi)(z) = \xi\phi_\xi(z)$ are named *coherent states*. They exist for any value $\xi \in \mathbb{C}$. In Bargmann's space they are the functions

$$\phi_\xi(z) = e^{\xi z} = \sum_{k=0}^\infty u_k(\xi) u_k(z)$$

An interesting property is the following: for any $f \in \mathcal{B}(\mathbb{C})$

$$f(z) = \sum_k u_k(z)(u_k|f) = \int \frac{d\bar{\xi}d\xi}{\pi} e^{-|\xi|^2} \phi_z(\bar{\xi}) f(\xi) \tag{19.40}$$

The equality shows that $e^{-|\xi|^2 + \bar{\xi}z}$ is a *reproducing kernel*. In other words coherent states are a continuous basis-set of non-orthogonal functions (an *over-complete set*), i.e. any function is a continuous superposition of coherent states

$$f(z) = \int \frac{d\bar{\xi}d\xi}{\pi} e^{-|\xi|^2} f(\xi) e^{\bar{\xi}z}$$

One can select a countable set of ξ values that belong to a two dimensional lattice $\xi = n_1\omega_1 + n_2\omega_2$, and completeness survives if the area of the fundamental cell (parallelogram with sides ω_1 and ω_2) is less than one.

Coherent states are important in quantum mechanics, semiclassical dynamics, quantum optics, path integral formulation of bosons. A standard reference is: A. Perelomov, *Generalized Coherent States and their Applications*, (Springer-Verlag, Berlin 1986).

Exercise 19.7.1. *The set $H_2(\mathbb{D})$ of functions holomorphic on the unit disk $\mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$ and such that $\int_{\mathbb{D}} \frac{d\bar{z}dz}{\pi} |f(z)|^2 < \infty$ is a Hilbert space with inner product*

$$(f, g) = \int_{\mathbb{D}} \frac{d\bar{z}dz}{\pi} \overline{f(z)} g(z)$$

- i) Show that the functions $u_k(z) = \sqrt{k+1} z^k$ are orthonormal.
- ii) Evaluate the norm of $(z - a)^{-1}$, $|a| > 1$.
- iii) Evaluate the series: $\sum_{k=0}^\infty u_k(z) \overline{u_k(z')}$ ($z, z' \in \mathbb{D}$).

Chapter 20

Trigonometric Series

20.1 Fourier Series

The elementary functions $\cos(kx)$ and $\sin(kx)$ are 2π -periodic and respectively even and odd on $[-\pi, \pi]$. Let f be a 2π -periodic real function and ask the question: which is the expansion in harmonics that “best” approximates f ?

We begin with a finite sum:

$$S_N(x) = \frac{1}{2}a_0 + \sum_{k=1}^N a_k \cos(kx) + b_k \sin(kx) \quad (20.1)$$

As in the least squares method, we require minimization of the quadratic error

$$\delta^2 = \int_{-\pi}^{\pi} dx [f(x) - S_N(x)]^2$$

The conditions for the extremum of δ^2 are:

$$\begin{aligned} 0 &= \frac{\partial \delta^2}{\partial a_0} = - \int_{-\pi}^{\pi} dx [f(x) - S_N(x)] \\ 0 &= \frac{\partial \delta^2}{\partial a_k} = -2 \int_{-\pi}^{\pi} dx [f(x) - S_N(x)] \cos(kx) \\ 0 &= \frac{\partial \delta^2}{\partial b_k} = -2 \int_{-\pi}^{\pi} dx [f(x) - S_N(x)] \sin(kx) \end{aligned}$$

Because of the “orthogonality” of the basis functions

$$\int_{-\pi}^{\pi} dx \cos(mx) \sin(nx) = 0, \quad (20.2)$$

$$\int_{-\pi}^{\pi} dx \cos(mx) \cos(nx) = \int_{-\pi}^{\pi} dx \sin(mx) \sin(nx) = \pi \delta_{mn} \quad (20.3)$$

the coefficients are obtained (Euler):

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} dx f(x) \cos(kx), \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} dx f(x) \sin(kx). \quad (20.4)$$

They are well defined for integrable functions and *they do not depend on N*. This feature is a consequence of orthogonality.

Exercise 20.1.1. *Prove the orthogonality relations (20.2) and (20.3).*

The quadratic error at minimum is evaluated¹:

$$\delta^2 = \left[\int_{-\pi}^{\pi} dx f(x)^2 \right] - \pi \left[\frac{a_0^2}{2} + a_1^2 + \dots + b_N^2 \right]$$

Since $\delta^2 \geq 0$ it is clear that the approximation improves by increasing the number of basis functions. If the error saturates to zero, one gets *Parseval's identity*:

$$\boxed{\int_{-\pi}^{\pi} dx f(x)^2 = \frac{\pi}{2} a_0^2 + \pi \sum_{k=1}^{\infty} (a_k^2 + b_k^2)} \quad (20.5)$$

Example 20.1.2. *Consider the function $f(x) = x$ on $(-\pi, \pi]$, repeated periodically (saw-tooth function). Being an odd function, the Fourier coefficients a_n vanish, and $b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} dx x \sin(nx) = 2(-1)^{n+1}/n$. Then:*

$$x = 2 \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\sin(nx)}{n} \quad (20.6)$$

Parseval's identity is: $\int_{-\pi}^{\pi} dx x^2 = 4\pi \sum_{n=1}^{\infty} 1/n^2$, that is: $\zeta(2) = \pi^2/6$ (Euler's solution of the Basel problem).

¹ Because of orthogonality, the Hessian matrix (the matrix of second derivatives) is diagonal with positive constants.

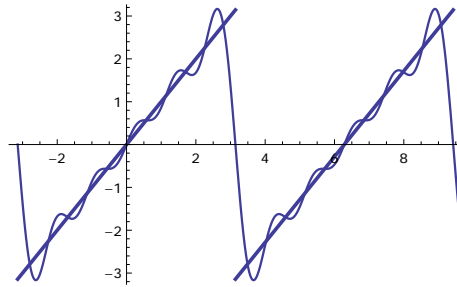


Figure 20.1 The Sawtooth function, and the Fourier approximation S_5

- At $x = \frac{\pi}{2}$ one obtains the sum of the Leibnitz series: $\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \dots$
- At $x = \pi$ the periodic function has two limits: $f(\pi^-) = \pi$ and $f(\pi^+) = -\pi$, while the Fourier series has value 0. The Fourier series, being unable to choose which value to approximate, takes the value in the middle, $S_\infty(\pi) = 0$.

Besides points of discontinuity, which are a zero-measure set, the series provides the same values of the function and the squared error δ^2 is zero.

- Being the function discontinuous, high frequency spiky harmonics are needed to “fill the edges”. Correspondingly, Fourier coefficients decay slow, as $1/n$, and the series has slow convergence.

In the next example the periodic function is continuous, but with discontinuous derivative at $x = \pm\pi$. The Fourier coefficients decay faster, as $1/n^2$.

Example 20.1.3. $f(x) = x^2$ on $[-\pi, \pi)$ (periodic parabolic arc).

Since the function is even on the interval, odd harmonics are absent ($b_n = 0$). The Fourier expansion is

$$x^2 = \frac{\pi^2}{3} + 4 \sum_{n=1}^{\infty} (-1)^n \frac{\cos(nx)}{n^2} \quad (20.7)$$

At $x = \pi$ one reobtains $\zeta(2) = \frac{\pi^2}{6}$. At $x = 0$: $\sum_{n=1}^{\infty} (-1)^n / n^2 = -\frac{\pi^2}{12}$. Parseval's identity $\int_{-\pi}^{\pi} dx x^4 = 2\pi \frac{\pi^4}{9} + 16\pi \sum_{n=1}^{\infty} \frac{1}{n^4}$ gives the useful sum $\zeta(4) = \frac{\pi^4}{90}$.

Exercise 20.1.4. Expand $\log(1 - z)$ in power series for $|z| < 1$. For $z = re^{i\theta}$ obtain:

$$\frac{1}{2} \log(1 + r^2 - 2r \cos \theta) = - \sum_{k=1}^{\infty} \frac{r^k}{k} \cos(k\theta)$$

Exercise 20.1.5. Show that the Fourier series of $\cos(ax)$ on $[-\pi, \pi]$ is:

$$\cos(ax) = \frac{\sin(a\pi)}{\pi a} + \frac{\sin(a\pi)}{\pi} \sum_{k=1}^{\infty} (-1)^k \frac{2a}{a^2 - k^2} \cos(kx), \quad a \notin \mathbb{N}.$$

The value $x = \pi$ gives

$$\cotg(a\pi) = \frac{1}{\pi a} + \frac{1}{\pi} \sum_{k=1}^{\infty} \frac{2a}{a^2 - k^2} \tag{20.8}$$

It is the logarithmic derivative of the famous Euler’s product expansion of the sine (1784), analogous to the factorization of a polynomial in terms of the roots:

$$\sin(\pi z) = \pi z \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2} \right) \tag{20.9}$$

20.1.1 Gibbs phenomenon*

The Fourier series of a function with a finite discontinuity exhibits the *Gibbs phenomenon*, explained by Gibbs in 1899 in a letter to *Nature*. It is an overshooting of the Fourier series caused by the high frequencies needed to emulate the jump, that pile up around the point of discontinuity².

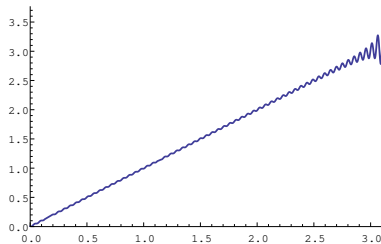


Figure 20.2 The Sawtooth function restricted to $[0, \pi]$ and the Fourier approximation S_{120} , showing the onset of the Gibbs phenomenon near the discontinuity.

If a is a point of discontinuity and Δ_f is the jump of a 2π -periodic function, the partial sum S_N has the jump $\Delta_N = |S_N(a - \pi/N) - S_N(a + \pi/N)|$. Gibbs noted that in the large- N limit the jump Δ_N is not Δ_f :

$$\lim_{N \rightarrow \infty} \frac{\Delta_N}{\Delta_f} = 1.17898\dots$$

² See https://en.wikipedia.org/wiki/Gibbs_phenomenon for some history and details.

Since it is a local effect, it is well illustrated by the periodic sawtooth function of Example 20.1.2. The jump at $a = \pi$ is 2π , while the partial sums give:

$$S_N(\pi - \epsilon) - S_N(\pi + \epsilon) = 4 \sum_{n=1}^N \frac{\sin(n\epsilon)}{n}$$

For $\epsilon \leq \pi/N$ all terms are positive and add up without interfering. At $\epsilon = \pi/N$:

$$\frac{\Delta_N}{\Delta_f} = \frac{2}{\pi} \sum_{k=1}^N \frac{\sin(N\pi/n)}{n} \rightarrow \frac{2}{\pi} \int_0^\pi dt \frac{\sin t}{t} = 1.17898\dots$$

(in the continuum limit $n\pi/N = t$, $dt = \pi/N$). The series overestimates the value of the function by 9%, at each side of the discontinuity.

20.1.2 The Dirichlet kernel

By inserting the integral expressions of the coefficients (20.4) in the finite sum (20.1), one obtains

$$\begin{aligned} S_N(x) &= \int_{-\pi}^{\pi} dy f(y) \left[\frac{1}{2\pi} + \frac{1}{\pi} \sum_{k=1}^N \cos k(x-y) \right] \\ &= \int_{-\pi}^{\pi} dy D_N(x-y) f(y) \end{aligned} \quad (20.10)$$

with *Dirichlet's kernel*

$$D_N(x-y) = \frac{1}{2\pi} \frac{\sin[(N + \frac{1}{2})(x-y)]}{\sin[\frac{1}{2}(x-y)]} \quad (20.11)$$

Properties: $D_N(x + 2\pi) = D_N(x)$, $D_N(-x) = D_N(x)$, $D_N(0) = \frac{1}{\pi}(N + \frac{1}{2})$,

$$\int_{-\pi}^{\pi} dx D_N(x) = \int_{-\pi}^{\pi} \frac{dx}{\pi} \left(\frac{1}{2} + \cos x + \dots + \cos Nx \right) = 1$$

We wish to study the large N limit of the difference $S_N(x) - f(x)$. Given the many applications of Fourier analysis, it is important to clarify under which conditions the difference converges to zero pointwise, uniformly, or almost everywhere.

Exercise 20.1.6. Evaluate Dirichlet's kernel (hint: use the complex representation).

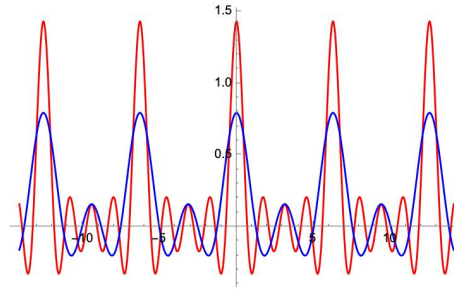


Figure 20.3 The Dirichlet kernel $D_N(x)$ for $N = 2$ (blue), $N = 4$ (red). As N increases it approaches a periodic delta-function.

20.2 Convergence of trigonometric sums

20.2.1 Pointwise convergence

If the function is integrable on a period, the coefficients a_n and b_n of the Fourier series exist. The problem of pointwise convergence of the partial Fourier sum is now addressed for such functions.

Lemma 20.2.1 (Riemann). *If $f \in \mathcal{L}^1(a, b)$ then*

$$\lim_{n \rightarrow \infty} \int_a^b dx f(x) \sin(nx) = 0 \quad (20.12)$$

The same holds for the cosine integral.

Proof. If f' exists and is continuous, a partial integration gives

$$\int_a^b dx f(x) \sin(nx) = -\frac{1}{n} f(x) \cos(nx) \Big|_a^b + \frac{1}{n} \int_a^b dx f'(x) \cos(nx) \quad (20.13)$$

An arbitrary function in $\mathcal{L}^1(a, b)$ can be approximated by functions in $\mathcal{C}^1(a, b)$: for any $\epsilon > 0$ there is a function with continuous derivative such that $\|f - \varphi_\epsilon\|_1 = \int_{[a,b]} dx |f - \varphi_\epsilon| < \epsilon$. Then:

$$\begin{aligned} \left| \int_a^b dx f(x) \sin(nx) \right| &\leq \left| \int_a^b dx [f(x) - \varphi_\epsilon(x)] \sin(nx) \right| + \left| \int_a^b dx \varphi_\epsilon(x) \sin(nx) \right| \\ &\leq \int_a^b dx |f(x) - \varphi_\epsilon(x)| + \left| \int_a^b dx \varphi_\epsilon(x) \sin(nx) \right| \end{aligned}$$

The first term can be made arbitrarily small, the second one decays to zero. □

For periodic functions the lemma suggests a relationship between the degree of regularity of f and the decay of its Fourier coefficients (which dictate how fast the series converges, i.e. how many terms are needed to reproduce the function with small error).

- If f is periodic integrable, then the Fourier coefficients decay as $1/n$.
- If f is periodic continuous with f' integrable, then a_n and b_n decay as $1/n^2$ (the boundary term in (20.13) is zero, the Lemma is applied to f'/n).
- If $f, f', \dots, f^{(k-1)}$ are periodic continuous, and $f^{(k)}$ is integrable, then the coefficients a_n, b_n of f decay at least as $1/n^{k+1}$.

In this example, the coefficients decrease rapidly:

$$\sum_{k=0}^{\infty} \frac{y^k}{k!} \cos(kx) = e^{y \cos x} \cos(y \sin x), \quad \sum_{k=1}^{\infty} \frac{y^k}{k!} \sin(kx) = e^{y \cos x} \sin(y \sin x)$$

Let us go back to the problem of convergence.

$$S_N(x) - f(x) = \int_{-\pi}^{\pi} dy [f(y) - f(x)] D_N(x - y) \quad (20.14)$$

$$= \int_{-\pi}^{\pi} dy [f(y+x) - f(x)] \frac{1}{2\pi} \frac{\sin(N + \frac{1}{2})y}{\sin \frac{1}{2}y} \quad (20.15)$$

There does not exist a theorem for necessary and sufficient conditions for pointwise convergence of the Fourier series. We provide sufficient conditions.

In the integral (20.15) the numerator of D_N produces convergence for large N (the Lemma), but the zero of the denominator has to be neutralized. This is done in the theorem:

Theorem 20.2.2 (Dini³). *Let $f \in \mathcal{L}^1(-\pi, \pi)$ and suppose that at a point x_0 there is $\delta > 0$ such that the Dini condition holds:*

$$\int_{-\delta}^{\delta} dt \left| \frac{f(x_0 + t) - f(x_0)}{t} \right| < \infty \quad (20.16)$$

Then $S_N(x_0) \rightarrow f(x_0)$.

³ Ulisse Dini (1845, 1918) formerly a student in Pisa of Enrico Betti, went to Paris and got acquainted with Charles Hermite and J. L. Francoise Bertrand. He became professor in Pisa, member of the Parliament and senator, and for many years he directed the Scuola Normale. He was the advisor of Luigi Bianchi and Gregorio Ricci-Curbastro (with Betti) and Luigi Fubini. Other students of Betti in Pisa were Cesare Arzelá, Federigo Enriques and Vito Volterra.

Proof.

$$\begin{aligned} S_N(x_0) - f(x_0) &= \int_{-\pi}^{\pi} dt [f(x_0 + t) - f(x_0)] D_N(t) \\ &= \int_{-\pi}^{\pi} dt \left[\frac{f(x_0 + t) - f(x_0)}{t} \frac{t}{2\pi \sin(\frac{1}{2}t)} \right] \sin(N + \frac{1}{2})t \end{aligned}$$

If Dini's condition holds, the term in parenthesis is integrable on $(-\pi, \pi)$. Then, by Riemann's lemma, $|S_N(x_0) - f(x_0)| \rightarrow 0$ as $N \rightarrow \infty$. \square

The Dini condition can be weakened to the existence of the left and right integrals:

$$\int_0^{\delta} dt \left| \frac{f(x_0 + t) - f(x_0^+)}{t} \right|, \quad \int_{-\delta}^0 dt \left| \frac{f(x_0 + t) - f(x_0^-)}{t} \right|.$$

These are sufficient conditions for pointwise convergence of practical use:

Theorem 20.2.3. *If f is a bounded 2π -periodic function with only a finite number of discontinuities where left and right finite limits exist at each discontinuity on $[0, 2\pi]$, and if the derivative exists and the left and right derivatives exist at the discontinuities, then the Fourier series is pointwise convergent to f where f is continuous and takes the middle value $\frac{1}{2}[f(x^+) + f(x^-)]$ at a discontinuity.*

Theorem 20.2.4. *If f is continuous periodic and f' exists except at finitely many points, and f' is piecewise continuous, then: $S_N \rightarrow f$ uniformly on \mathbb{R} ; the Fourier series of f' is obtained by differentiating the series of f term by term.*

Exercise 20.2.5. *Let f be real, 2π -periodic and continuous, with continuous derivative f' , and $\int_{-\pi}^{+\pi} f(x) dx = 0$. Show the Wirtinger inequality:*

$$\int_{-\pi}^{+\pi} |f'(x)|^2 dx \geq \int_{-\pi}^{+\pi} |f(x)|^2 dx$$

When does equality hold?

Miscellanea

1) The following sum can be evaluated for x not an integer multiple of 2π :

$$\sum_{k=1}^n \sin(kx) = \frac{\cos \frac{x}{2} - \cos(N + \frac{1}{2})x}{2 \sin \frac{x}{2}}$$

It implies that $|\sum_{k=1}^n \sin(kx)| < 1/|\sin(x/2)|$ for all n . Then, Abel's lemma 4.3.5 shows that $\sum_k b_k \sin(kx)$ converges for all real x , provided that b_k are definitely a non increasing sequence of positive numbers and $b_k \rightarrow 0$.

For example, the series

$$\sum_{k=2}^{\infty} \frac{\sin(kx)}{\log k}$$

is convergent, but one shows that it is not in $\mathcal{L}^1(-\pi, \pi)$.

2) The Sturm-Hurwitz theorem⁴.

Let f be a real, continuous and 2π -periodic function with Fourier expansion

$$f(x) = \sum_{k=N}^{\infty} [a_k \cos(kx) + b_k \sin(kx)]$$

(all Fourier coefficients a_k, b_k for $k < N$ vanish, and $a_N^2 + b_N^2 \neq 0$), then f has at least $2N$ distinct zeros in $[0, 2\pi)$.

3) The problem of the uniqueness of the Fourier series of a function was proposed by Heine in 1869 to a young Georg Cantor, and became his source of investigation of set theory and transfinite numbers⁵.

4) Trigonometric sums define functions that may be rather extravagant.

Consider the finite sum (it is not a Fourier series because of the modulus) $f_N(x) = \sum_{k=1}^N |\sin(k\pi x)|/k$. The function $f_N(x)$ has a strict local minimum at every rational p/q with $|q| \leq \sqrt{N}$ (*An amusing sequence of functions*, S. Steinerberger, arXiv:1610.04090).

20.3 Fejér sums

The theory developed by Lipót Fejér on trigonometric series allows to prove the “completeness” of the basis of trigonometric functions in the Banach spaces $\mathcal{C}([-\pi, \pi])$ of continuous functions on $[-\pi, \pi]$, and in the spaces $L^1(-\pi, \pi)$ and $L^2(-\pi, \pi)$. It means that any function can be approximated arbitrarily well by a finite combination of trigonometric functions in the topology of the space.

A function that is continuous and 2π -periodic may not have a convergent Fourier series, and therefore may not be reproduced as the limit $N \rightarrow \infty$ of S_N . However, the arithmetic averages of the partial sums (*Fejér sums*) do the job in an excellent way. Consider the

⁴ G. Katriel, From Rolle's theorem to the Sturm-Hurwitz theorem, <https://doi.org/10.48550/arXiv.math/0308159> (2003)

⁵ read the nice paper <http://www.math.caltech.edu/papers/uniqueness.pdf> by A. Kechris.

Fejér sum

$$\sigma_N(x) = \frac{1}{N} [S_0(x) + S_1(x) + \dots + S_{N-1}(x)] = \int_{-\pi}^{\pi} dt f(x+t)\Phi_N(t) \tag{20.17}$$

where $\Phi_N(x)$ is Fejér's kernel:

$$\begin{aligned} \Phi_N(t) &= \frac{1}{N} [D_0(t) + D_1(t) + \dots + D_{N-1}(t)] \\ &= \frac{1}{2\pi} + \frac{1}{\pi} \sum_{k=1}^{N-1} \left(1 - \frac{k}{N}\right) \cos(kt) \\ &= \frac{1}{2\pi N} \frac{\sin^2(Nt/2)}{\sin^2(t/2)} \end{aligned} \tag{20.18}$$

The kernel is a finite sum of trigonometric functions, it is positive and has unit integral on $[-\pi, \pi]$.

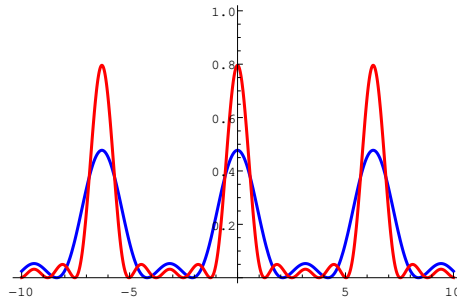


Figure 20.4 The Fejér kernel $\Phi_N(x)$ for $N = 3$ (blue), $N = 5$ (red). As N increases it approaches a periodic delta-function.

The Fejér sums σ_N are the *Cesaro means*⁶ of the Dirichlet sums S_k . The interesting fact about them, is that they behave much better than Dirichlet sums, as the next theorems show.

Theorem 20.3.1 (I Fejér theorem, 1905). *If f is real continuous and 2π -periodic, the sequence of Fejér sums σ_n converges to f uniformly on \mathbb{R} .*

Proof. Since f is real and continuous on $[-\pi, \pi]$ it is bounded, $|f(x)| < M$, and uniformly continuous: $\forall \epsilon \exists \delta : |f(x+t) - f(x)| < \epsilon/2 \forall x, \forall t \text{ s.t. } |t| < \delta$.

⁶ Ernesto Cesaro (1859, 1906) was professor in Naples. He proved that if a sequence a_n converges to a (or diverges) then: the sequence of arithmetic averages $s_n = \frac{1}{n} \sum_{k=1}^n a_k$ and the sequence of geometric averages $p_n = (a_1 \cdots a_n)^{1/n}$ converge to the same limit (or diverge).

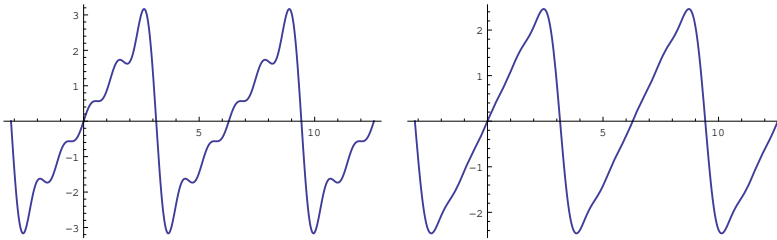


Figure 20.5 The trigonometric approximations S_5 and σ_5 of the Sawtooth function.

Being periodic, f is bounded and uniformly continuous on the whole real line. Let us estimate the difference

$$\sigma_N(x) - f(x) = \int_{-\pi}^{\pi} dy [f(x+y) - f(x)] \Phi_N(y) = J_{<}(x) + J_0(x) + J_{>}(x)$$

where integration is split on three intervals $[-\pi, -\delta] \cup [-\delta, \delta] \cup (\delta, \pi]$.

$$\begin{aligned} |J_0(x)| &\leq \int_{-\delta}^{\delta} dt |f(x+t) - f(x)| \Phi_N(t) < \frac{\epsilon}{2} \int_{-\delta}^{\delta} dt \Phi_N(t) \leq \frac{\epsilon}{2} \\ |J_{>}(x)| &\leq \int_{\delta}^{\pi} dt |f(x+t) - f(x)| \Phi_N(t) < 2M \int_{\delta}^{\pi} dt \Phi_N(t) \\ &\leq \frac{M}{\pi N} \int_{\delta}^{\pi} dt \frac{1}{\sin^2(t/2)} \leq \frac{M}{\pi N} \frac{\pi - \delta}{\sin^2(\delta/2)} \leq \frac{M}{N \sin^2(\delta/2)} \end{aligned}$$

The same estimate is valid for $J_{<}$. Now, given ϵ and δ , left's choose \bar{N} such that $\frac{M}{N} \sin^{-2}(\delta/2) < \epsilon/4$. Then $|\sigma_N(x) - f(x)| < \epsilon$ for all $N > \bar{N}$. \square

The theorem was proven by Fejér in 1905 at the age of 19, and strengthens the theorem by Weierstrass, that states that any continuous and periodic function is uniformly approximated by a sequence of trigonometric polynomials. Fejér has given an explicit expression (the Fejér sums) for such polynomials.

A similar proof can be given for integrable functions:

Theorem 20.3.2 (II Fejér's theorem). *If $f \in \mathcal{L}^1(-\pi, \pi)$, the sequence of Fejér's sums converges to f in $L^1(-\pi, \pi)$.*

Proof. Given f in \mathcal{L}^1 , its Fejér sum $\sigma_N(x) = \int_{-\pi}^{\pi} dy f(x+y) \Phi_N(y)$ is well defined, because Φ_N is a finite sum of trigonometric functions. We show that $\|f - \sigma_N\|_1 = \int_{-\pi}^{\pi} dx |f(x) -$

$\sigma_N(x) \rightarrow 0$ as $N \rightarrow \infty$.

$$\begin{aligned} \|f - \sigma_N\|_1 &= \int_{-\pi}^{\pi} dx \left| \int_{-\pi}^{\pi} dy [f(x+y) - f(x)] \Phi_N(y) \right| \\ &\leq \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy |f(x+y) - f(x)| \Phi_N(y) \end{aligned}$$

The integrals can be exchanged by Fubini's theorem:

$$= \int_{-\pi}^{\pi} dy \Phi_N(y) \int_{-\pi}^{\pi} dx |f(x+y) - f(x)|$$

The integral in y is split on the intervals $[-\pi, -\delta] \cup (-\delta, \delta) \cup [\delta, \pi]$ where δ is by now unspecified but small. Because of the 2π -periodicity of the functions, the first interval is shifted by 2π and added to the third. Then:

$$= \int_{-\delta}^{\delta} + \int_{\delta}^{2\pi-\delta} dy \Phi_N(y) \int_{-\pi}^{\pi} dx |f(x+y) - f(x)|$$

The first integral is:

$$\leq \left[\sup_{|y| < \delta} \int_{-\pi}^{\pi} dx |f(x+y) - f(x)| \right] \int_{-\delta}^{\delta} dy \Phi_N(y) \leq \sup_{|y| < \delta} \int_{-\pi}^{\pi} dx |f(x+y) - f(x)|$$

because Fejér's kernel is normalized; the sup-term can be made smaller than ϵ , for $\delta \leq \delta_\epsilon$. The second integral is:

$$\leq \left[\sup_{\delta_\epsilon < y < 2\pi - \delta_\epsilon} \int_{-\pi}^{\pi} dx |f(x+y) - f(x)| \right] \int_{\delta_\epsilon}^{2\pi - \delta_\epsilon} dy \Phi_N(y) \leq \frac{2\|f\|_1}{N \sin^2(\delta_\epsilon/2)}$$

It is smaller than ϵ provided that N is large enough, once the δ_ϵ of the previous integral is fixed. \square

Corollary 20.3.3. *If $f \in \mathcal{L}^1(-\pi, \pi)$ has all Fourier coefficients $a_n = b_n = 0$, then $f = 0$ a.e.*

Proof. If $a_n = b_n = 0$ for all n , the Dirichlet's sums $S_N(x)$ and Fejér's sums $\sigma_N(x)$ vanish for all N . But II Fejér's theorem shows that $\|f - \sigma_N\|_1 \rightarrow 0$ as $N \rightarrow \infty$. Then $\|f\|_1 = 0 \Rightarrow f = 0$ a.e. \square



Figure 20.6 **Lipót Fejér** (Pécs 1880, Budapest 1959) studied in Budapest and Berlin, as a student of Hermann Schwarz. In Budapest he led a relevant school of analysis, and was thesis advisor of John von Neumann, Paul Erdős, George Pólya, Pál Turán, Marcel Riesz, Gábor Szegő, Michael Fekete, and others.

Figure 20.7 **Andrey N. Kolmogorov** (Tambov 1903, Moscow 1987) is the founder of axiomatic probability theory (1933). Independently with Chapman, he developed the basic equations for stochastic processes. He gave fundamental contributions to the theory of turbulence and of dynamical systems. Among his doctoral students are: Vladimir Arnold, Roland Dobrushin, Eugene Dynkin, Israel Gelfand, Yakov Sinai.

20.3.1 Convergence in the mean

Proposition 20.3.4. *The trigonometric functions*

$$\frac{1}{\sqrt{2\pi}}, \quad \frac{1}{\sqrt{\pi}} \cos(nx), \quad \frac{1}{\sqrt{\pi}} \sin(nx), \quad n = 1, 2, \dots$$

are a complete orthonormal system in $L^2(-\pi, \pi)$.

Proof. If $f \in L^2(-\pi, \pi)$ then $f \in L^1(-\pi, \pi)$ (Schwarz's inequality: $\|f\|_1 = (1\|f\|) \leq \sqrt{2\pi}\|f\|_2$). f orthogonal to all basis elements ($a_n = b_n = 0 \forall n$) implies $f = 0$ a.e. by Corollary 20.3.3. \square

By a change of scale, the Fourier basis in $L^2(a, b)$ is ($n = 1, 2, \dots$):

$$\boxed{\frac{1}{\sqrt{b-a}}, \quad \sqrt{\frac{2}{b-a}} \cos\left(\frac{2\pi nx}{b-a}\right), \quad \sqrt{\frac{2}{b-a}} \sin\left(\frac{2\pi nx}{b-a}\right)} \quad (20.19)$$

What can be said about *pointwise convergence*? Luzin⁷ conjectured (1906) that L^2 convergence implies almost everywhere convergence: $S_N(x) \rightarrow f(x)$ a.e.

The conjecture was proven by Lennart Carleson⁸ in 1966 and extended by Hund to spaces L^p for $p > 1$. The important case $p = 1$ has a different story: in 1923 aging 19, Andrey Kolmogorov provided a Lebesgue integrable function whose sequence of partial sums is a.e. divergent. Two years later he sharpened the result by showing that divergence is everywhere, and became a celebrity.

20.3.2 Complex Fourier basis

The following Fourier basis is sometimes more convenient:

$$u_n(x) = \frac{1}{\sqrt{b-a}} \exp \left[i \frac{2\pi n}{b-a} x \right], \quad n \in \mathbb{Z} \tag{20.20}$$

Since $\{u_n\}_{-\infty}^{+\infty}$ form a complete orthonormal set, any function in $L^2(a, b)$ has the Fourier expansion

$$f = \sum_{n=-\infty}^{\infty} f_n u_n, \quad f_n = (u_n | f) = \int_a^b dx \overline{u_n(x)} f(x) \tag{20.21}$$

where convergence is in L^2 norm (*in the mean*): if $S_N = \sum_{n=-N}^N (u_n | f) u_n$, then $\|S_N - f\|^2 = \int_a^b dx |S_N - f|^2 \rightarrow 0$ as $N \rightarrow \infty$. Moreover:

$$\|f\|_2^2 = \int_a^b dx |f(x)|^2 = \sum_{n=-\infty}^{\infty} |(u_n | f)|^2 \quad (\text{Parseval}) \tag{20.22}$$

Example 20.3.5. $f(x) = (1 - 2a \cos x + a^2)^{-1}$ on $[-\pi, \pi)$ ($a^2 < 1$). The Fourier coefficients can be evaluated by the Residue Theorem in the unit circle ($\zeta = e^{ix}$):

$$\begin{aligned} a_n &= \text{Re} \frac{1}{\pi} \int_{-\pi}^{\pi} dx f(x) e^{inx} = \text{Re} \int_{C(0,1)} \frac{d\zeta}{i\pi\zeta} \frac{\zeta^n}{1 - a\zeta - a/\zeta + a^2} \\ &= -\text{Re} \int_{C(0,1)} \frac{d\zeta}{i\pi a} \frac{\zeta^n}{(\zeta - a)(\zeta - 1/a)} = \frac{2a^n}{1 - a^2} \end{aligned}$$

⁷ Nikolai Luzin and the older Dimitri Egorov were influential mathematicians of Moscow's Mathematical Society during stalinian purges. They were both attacked and censured as reactionaries. Egorov was arrested and died one year after. Luzin, a specialist in real analysis, was processed but rehabilitated. No longer were important papers published on foreign journals. Luzin had important students, like Aleksandr Khinchin, Andrei Kolmogorov, Mickail Lavrentiev, Aleksei Lyapunov, Pavel Uryson.

⁸ L. Carleson, *On the convergence and growth of partial sums of Fourier series*, Acta Math. **116** (1966).

$$\frac{1}{1 - 2a \cos x + a^2} = \frac{1}{1 - a^2} + \frac{2}{1 - a^2} \sum_{n=1}^{\infty} a^n \cos(nx) \quad (20.23)$$

The function is continuous with all its derivatives; the Fourier coefficients decay exponentially, as $e^{-n|\log a|}$.

Note that, with $\cos x = t$, it is $\cos(nx) = T_n(t)$, and the generating function of Chebyshev polynomials is recovered, eq.(11.24).

Exercise 20.3.6. Consider the generating function for Bessel's functions of integer order with z on the unit circle:

$$e^{ix \sin \theta} = \sum_{n=-\infty}^{\infty} e^{in\theta} J_n(x).$$

Prove the properties: $1 = J_0(x)^2 + 2 \sum_{k=1}^{\infty} J_k(x)^2$ (Parseval's identity), and

$$e^{i\mathbf{k} \cdot \mathbf{r}} = J_0(kr) + 2 \sum_{n=1}^{\infty} i^n \cos(n\theta) J_n(kr) \quad (20.24)$$

where θ is the angle formed by the vectors. The formula is useful in scattering theory.

20.4 Fourier series with different basis sets

Consider a function f with period 1. As a periodic function it has a Fourier series expansion on $[0, 1]$, with basis functions $\cos(2k\pi x)$ and $\sin(2k\pi x)$:

$$f(x) = \frac{\alpha_0}{2} + \sum_{k=1}^{\infty} \alpha_k \cos(2k\pi x) + \beta_k \sin(2k\pi x)$$

However, as a function on the interval $[0, 1]$ alone, other trigonometric series are possible. For example, the even/odd extensions of f on $[-1, 1]$,

$$f_e(x) = \begin{cases} f(x) & x \in [0, 1] \\ f(-x) & x \in [-1, 0) \end{cases} \quad f_o(x) = \begin{cases} f(x) & x \in [0, 1] \\ -f(-x) & x \in [-1, 0) \end{cases}$$

can be represented respectively as Fourier series with functions $\cos(k\pi x)$ or $\sin(k\pi x)$. The two series, restricted to the interval $[0, 1]$, give two new trigonometric expansions of f :

$$f(x) = \frac{a_0}{2} + \sum_n a_n \cos(n\pi x) = \sum_n b_n \sin(n\pi x), \quad x \in [0, 1].$$

The functions $\{1, \cos(k\pi x)\}$ and $\{\sin(k\pi x)\}$ form two independent sets of orthogonal functions on $[0, 1]$:

$$\int_0^1 dx \cos(m\pi x) \cos(n\pi x) = \frac{1}{2} \delta_{mn}, \quad \int_0^1 dx \sin(m\pi x) \sin(n\pi x) = \frac{1}{2} \delta_{mn}.$$

Example 20.4.1. Consider the function x on $[0, 1]$. The Fourier expansion has period 1

$$x = \frac{1}{2} - \sum_{k=1}^{\infty} \frac{\sin(2\pi kx)}{\pi k}, \quad 0 < x < 1 \quad (20.25)$$

The expansions on $[-1, 1]$ of the even extension $|x|$ and of the odd extension x , give two new representations of x on $[0, 1]$:

$$x = \frac{1}{2} - 4 \sum_{k=0}^{\infty} \frac{\cos(2k+1)\pi x}{\pi^2(2k+1)^2} \quad x = -2 \sum_{k=1}^{\infty} (-1)^k \frac{\sin(k\pi x)}{\pi k}$$

Outside the interval $[0, 1]$ the three Fourier series describe different periodic functions. Note the faster convergence of the series for $|x|$, which is continuous. For this one, Parseval's identity gives:

$$\sum_{k=0}^{\infty} \frac{1}{(2k+1)^4} = \frac{\pi^4}{96}$$

20.5 From Fourier series to Fourier integrals

Consider the Fourier expansion of a function on the interval $[-\frac{L}{2}, \frac{L}{2}]$:

$$f(x) = \sum_{k=-\infty}^{\infty} \frac{e^{i2\pi kx/L}}{L} f_k, \quad f_k = \int_{-L/2}^{L/2} dy e^{-i2\pi ky/L} f(y)$$

where for convenience the two normalization factors \sqrt{L} are replaced by L in the sum. In view of the limit $L \rightarrow \infty$, introduce the new variable $s = 2\pi k/L$, with spacings $\delta s = 2\pi/L$:

$$f(x) = \sum_s \delta s \frac{e^{isx}}{2\pi} \tilde{f}(s), \quad \tilde{f}(s) = \int_{-L/2}^{L/2} dy e^{-isy} f(y)$$

If f is integrable on \mathbb{R} , the function $\tilde{f}(s)$ exists for $L \rightarrow \infty$. In the same limit, the sum may be replaced by an integral:

$$f(x) = \int_{-\infty}^{\infty} \frac{ds}{2\pi} e^{isx} \int_{-\infty}^{\infty} dy e^{-isy} f(y)$$

According to this formula a function is a continuous superposition of Fourier components, weighted by a function of the continuous index:

$$f(x) = \int_{-\infty}^{\infty} \frac{ds}{\sqrt{2\pi}} e^{isx} (\mathcal{F}f)(s) \quad (20.26)$$

$$(\mathcal{F}f)(s) = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}} e^{-isy} f(y) \quad (20.27)$$

The second line defines the Fourier integral of f (the factors 2π are often distributed differently).

20.6 Applications*

20.6.1 Heat Equation

In his fundamental treatise *Théorie analytique de la chaleur* (1822) Jean Baptiste Fourier discussed the transmission of heat in bodies of various shapes and different boundary conditions. By assuming that the transfer of heat between near regions is proportional to the temperature difference, he obtained the Heat Equation for the temperature field:

$$\frac{1}{D} \frac{\partial T}{\partial t} - \nabla^2 T = 0 \quad (20.28)$$

D is the constant of thermal diffusion.

Fourier solved by trigonometric series the stationary problem of the temperature distribution in a rectangle with sides at different temperatures.

Consider the square $[0, \pi] \times [0, \pi]$ with three sides held at temperature $T = 0$ and one at temperature $T(x, \pi) = x$ (at one corner there is a jump $\Delta T = \pi$). The stationary field $T(x, y)$ solves $T_{xx} + T_{yy} = 0$ with the specified b.c. As Fourier noted, an elementary harmonic solution is $e^{\pm ay} \sin(ax)$. It is zero at $x = 0$ and $x = \pi$ if a is an integer. The linear combination

$$T(x, y) = \sum_{n=1}^{\infty} c_n \sinh(ny) \sin(nx)$$

is a solution and is zero at three sides of the rectangle. The coefficients are determined by the b.c.: $x = \sum_{n=1}^{\infty} c_n \sinh(n\pi) \sin(nx)$. Fourier evaluated the infinite number of unknowns $x_n = c_n \sinh(n\pi)$ through the infinite linear system obtained by taking even derivatives of all order:

$$0 = x_1 \sin x + 2^2 x_2 \sin(2x) + 3^2 x_3 \sin(3x) + \dots$$

$$0 = x_1 \sin x + 2^4 x_2 \sin(2x) + 3^4 x_3 \sin(3x) + \dots$$

...

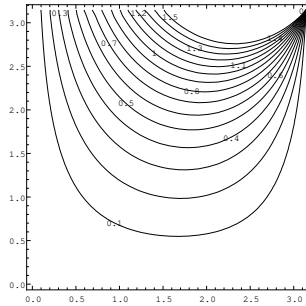


Figure 20.8 Fourier's solution for the temperature distribution in the square.

Instead, we exploit orthogonality: $\int_0^\pi dx x \sin(\ell x) = \sum_n x_n \int_0^\pi dx \sin(\ell x) \sin(nx)$ i.e. $x_\ell = -\frac{2}{\ell}(-1)^\ell$. The solution is:

$$T(x, y) = 2 \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n} \frac{\sinh(ny)}{\sinh(n\pi)} \sin(nx).$$

20.6.2 Temperature profile in the ground

Let us consider the annual or diurnal variation of the thermal profile $T(z, t)$ in the ground, where z is the depth. As heating from the Sun is periodic, we search for time-periodic solutions of (20.28). An elementary one is $T_n(z, t) = \exp(in\omega t)u_n(z)$. The heat equation gives $i \frac{n\omega}{D} u_n = u_n''$. A real solution is

$$T_n(z, t) = e^{-z\sqrt{\frac{n\omega}{2D}}} \cos\left(n\omega(t - t_0) - \sqrt{\frac{n\omega}{2D}}z\right)$$

The general solution is a superposition $\sum_n c_n T_n(z, t)$, with c_n fixed by the initial condition. Given the exponential decrease with depth, we only retain the $n = 1$ term, and choose $t_0 = 0$ so that the temperature T is maximal at the surface at $t = 0$:

$$\frac{T(z, t)}{T_{max}} = e^{-z\sqrt{\frac{\omega}{2D}}} \cos\left(\omega t - \sqrt{\frac{\omega}{2D}}z\right)$$

For the ground the diffusion coefficient is $D \approx 2 \times 10^{-3} \text{ cm}^2/\text{s}$. With period $\tau = 1$ year, $\omega = 2\pi/\tau = 2 \times 10^{-7} \text{ s}^{-1}$, $\sqrt{\omega/2D} \approx 0.7 \times 10^{-2} \text{ cm}^{-1}$. At depth $z = 100 \text{ cm}$ the maximal temperature is a factor $e^{-0.7} \approx 0.5$ smaller than T_{max} , and is reached at $2\pi t/\tau = 0.7$ i.e. after 41 days.

20.6.3 The isoperimetric inequality

The problem of finding the curve of given length enclosing the largest area in the plane is very old (Zenodorus, II BC). The isoperimetric inequality states that the length L of a smooth simple curve enclosing an area A satisfies the general relation⁹

$$\frac{L^2}{A} \geq 4\pi \quad (20.29)$$

with equality holding for the circle (Weierstrass). For a regular polygon:

$$\frac{L^2}{A} = 4\pi \frac{\tan(\pi/n)}{\pi/n}$$

A proof of the inequality based on Fourier series was given in 1902 by Adolf Hurwitz¹⁰. Let $f(z)$ be the holomorphic one-to-one (i.e. univalent) map of the unit disk \mathbb{D} to Ω : $f(z) = a_0 + a_1 z + a_2 z^2 + \dots$, $|z| < 1$. The boundary curve is parametrized by the restriction of $f(z)$ to the circle: $f(e^{i\theta})$.

The area A of Ω and the length L of the boundary are:

$$A = \int_0^1 r dr \int_0^{2\pi} d\theta |f'(re^{i\theta})|^2 \quad (20.30)$$

$$L = \int_0^{2\pi} d\theta |f'(e^{i\theta})| \quad (20.31)$$

The area is evaluated via Plancherel's formula:

$$A = \pi (|a_1|^2 + 2|a_2|^2 + 3|a_3|^2 + \dots) \quad (20.32)$$

It is the sum of the areas of the images of the disk for the single maps $a_k z^k$. Now consider the integral ($f = u + iv$):

$$\int_0^{2\pi} d\theta |f'(e^{i\theta})|^2 = \int_0^{2\pi} d\theta \left[\left(\frac{du}{d\theta} \right)^2 + \left(\frac{dv}{d\theta} \right)^2 \right]$$

Put $\theta = 2\pi s/L$, where L is the length of the boundary and use $ds^2 = du^2 + dv^2$:

$$\int_0^{2\pi} d\theta |f'(e^{i\theta})|^2 = \frac{L}{2\pi} \int_0^L ds \left[\left(\frac{du}{ds} \right)^2 + \left(\frac{dv}{ds} \right)^2 \right] = \frac{L^2}{2\pi}$$

⁹ An ample review is: R. Ossermann, *The isoperimetric inequality*, Bull. Amer. Math. Soc. **84** (6) 1978, pages 1182-1238.

¹⁰ see the historical review by T. I. Porter <https://faculty.fiu.edu/~lhermi/dido/porter1933.pdf>.

Therefore $L^2 = 4\pi^2(|a_1|^2 + 2^2|a_2|^2 + 3^2|a_3|^2 + \dots)$ and the isoperimetric inequality follows:

$$L^2 - 4\pi A = 4\pi^2 \sum_{k=2}^{\infty} (k^2 - k)|a_k|^2 \geq 0$$

Equality occurs if $f(z) = a_0 + a_1 z$, i.e. f maps the unit disk to a disk.

Note that eq.(20.31) is $L = \|f'\|_1$, the norm in $L^1(0, 2\pi)$, but we also found $L^2 = 2\pi \|f'\|_2^2$. In this case the Schwarz inequality $\|g\|_1^2 \leq 2\pi \|g\|_2^2$ is an equality.

An isoperimetric inequality also holds for regions on a sphere of radius R : $L^2/A \geq 4\pi - A/R^2$.

20.6.4 Kepler's equation

The elliptic orbit of a planet with semiaxes $a \geq b$ can be parameterized as $x = a \cos E$, $y = b \sin E$. The eccentric anomaly $0 \leq E \leq 2\pi$ satisfies *Kepler's equation* (17.4), rewritten as $E - M = e \sin E$, where $M = \frac{2\pi}{T} t$ is the mean anomaly (t is the time from the perihelion passage).

A solution was obtained by the astronomer Bessel in 1824 as a Fourier series (some terms were previously obtained by Lagrange, 1770). E is an odd periodic function of M :

$$\begin{aligned} E - M &= \sum_{k=1}^{\infty} B_k \sin(kM) \\ B_k &= \frac{1}{\pi} \int_0^{2\pi} dM (E - M) \sin(kM) = \int_0^{2\pi} dM \left(\frac{dE}{dM} - 1 \right) \frac{\cos kM}{\pi k} \\ &= \frac{2}{k} \int_0^{\pi} \frac{dE}{\pi} \cos(kE - ke \sin E) = \frac{2}{k} J_k(ke) \end{aligned}$$

An integration by parts was made, and $\int_0^{2\pi} dM \cos(kM) = 0$ for $k \geq 1$. The coefficients are Bessel's functions, see eq.(13.5). Then: $E = M + 2J_1(e) \sin M + J_2(2e) \sin(2M) + \frac{2}{3} J_3(3e) \sin(3M) + \dots$

20.6.5 Vibrating string

A thin stretched string is clamped at $x = 0$ and $x = L$. Its deviation from the straight configuration is a function $f(x, t)$ that solves the Wave Equation

$$f_{tt} - c^2 f_{xx} = 0,$$

where c is the speed of wave propagation. The Cauchy problem is specified by initial conditions $f(x, 0) = f_1(x)$ and $f_t(x, 0) = f_2(x)$. Boundary conditions (b.c.) $f(0, t) = 0$ and $f(L, t) = 0$ are imposed at all times.

Multiplication by $\mu_0 f_t$ and integration by parts lead to a conservation law for the total

energy (μ_0 is the linear mass density):

$$E = \frac{\mu_0}{2} \int_0^L dx (f_t^2 + c^2 f_x^2)$$

E is time independent and is fixed by the initial conditions.

The wave equation is first solved for stationary states $f(x, t) = A(t)u(x)$, with solutions $e^{\pm i\omega t}[\alpha e^{ikx} + \beta e^{-ikx}]$, $\omega = kc \geq 0$. The b.c. impose: $\alpha + \beta = 0$ and $\alpha e^{ikL} + \beta e^{-ikL} = 0$, i.e. $\alpha = -\beta$ and $k = \pi n/L$, $n = 0, 1, 2, \dots$ (wave-lengths are quantized). Therefore, the stationary solutions (*normal modes*) are:

$$e^{\pm i\omega_n t} \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, \dots$$

The general solution is a real linear superposition of normal modes

$$f(x, t) = \sum_{n=1}^{\infty} (c_n e^{i\omega_n t} + \bar{c}_n e^{-i\omega_n t}) \sin \frac{n\pi x}{L}, \quad \omega_n = \frac{\pi c}{L} n \quad (20.33)$$

The period of the n^{th} mode is $T_n = \frac{1}{n}(2L/c)$; the longest one is a global period: $f(x, t + T_1) = f(x, t)$. The coefficients c_n are determined by the initial conditions $\sum_n (c_n + \bar{c}_n) \sin(n\pi x/L) = f_1(x)$, $\sum_n i\omega_n (c_n - \bar{c}_n) \sin(n\pi x/L) = f_2(x)$. By means of the orthogonality relation $\int_0^L dx \sin \frac{m\pi x}{L} \sin \frac{n\pi x}{L} = \frac{L}{2} \delta_{mn}$ one evaluates:

$$\operatorname{Re} c_n = \frac{1}{L} \int_0^L dx f_1(x) \sin \frac{n\pi x}{L}, \quad \operatorname{Im} c_n = -\frac{1}{L\omega_n} \int_0^L dx f_2(x) \sin \frac{n\pi x}{L}.$$

The general solution, though describing oscillations of a string of length L , is $2L$ -periodic. The total energy of the solution $f(x, t)$ is extensive (proportional to L) and is the *sum of the energies of the single modes*¹¹:

$$E = L \frac{\mu_0}{2} \sum_{n=1}^{\infty} \omega_n^2 [c_n \bar{c}_n + \bar{c}_n c_n] \quad (20.34)$$

As an example, let us suppose that the string is initially stretched as a triangle, $f_1(x) = \alpha x$ for $0 < x \leq L/2$ and $f_1(x) = \alpha(L - x)$ for $L/2 < x < L$, and left free to vibrate ($f_2 = 0$, no

¹¹ The expression of the energy is ready to undergo "second quantization", which yields an operator for a quantum description of vibrations in terms of elementary quanta called phonons.

initial velocity on the whole length). The coefficients c_n and the solution are evaluated:

$$\begin{aligned} f(x, t) &= \frac{4\alpha L}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n+1)^2} \cos(k_n ct) \sin(k_n x), \quad k_n = n \frac{\pi}{L} \\ &= \frac{2\alpha L}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n+1)^2} [\sin[k_n(x+ct)] + \sin[k_n(x-ct)]] \\ &= \frac{1}{2} [F_1(x+ct) + F_1(x-ct)] \end{aligned}$$

Here, $F_1(x)$ is the $2L$ -periodic function with value $F_1(x) = f_1(x)$ for $0 \leq x \leq L$ and $F_1(x) = -f_1(2L-x)$ for $L \leq x \leq 2L$.

20.6.6 The Euler - Mac Laurin expansion

Dirichlet's kernel $D_N(x-a)$ is 2π -periodic and peaked at the points $a+2\pi n$. If we multiply it by a smooth function and integrate on an interval $[a, b]$, with $b = a+2\pi M$, it is:

$$\int_a^b dx D_N(x-a) f(x) = \int_a^b \frac{dx}{2\pi} f(x) + \sum_{k=1}^N \int_a^b \frac{dx}{\pi} \cos[k(x-a)] f(x)$$

The integral in the left-hand-side is evaluated on sub-intervals $[a, a+\pi)$, $[a+\pi, a+3\pi)$, ... $[b-\pi, b]$. On sub-intervals of width 2π , as N goes to infinity, the kernel becomes a normalized delta function peaked at the center of the interval. On the intervals $[a, a+\pi)$ and $[b-\pi, b]$ only half of the kernel contributes. Therefore the integral is:

$$\sum_{k=0}^M f(a+2\pi k) - \frac{f(b)+f(a)}{2}$$

In the right side we integrate by parts twice and obtain a recursive law:

$$C_k[f] = \int_a^b dx \cos[k(x-a)] f(x) = \frac{1}{k^2} [f'(b) - f'(a)] - \frac{1}{k^2} C_k[f'']$$

For large N :

$$\frac{1}{\pi} \sum_{k=1}^N C_k[f] = \frac{\zeta(2)}{\pi} [f'(b) - f'(a)] - \frac{\zeta(4)}{\pi} [f'''(b) - f'''(a)] + R$$

with remainder $R = \frac{1}{\pi} \sum_k \frac{1}{k^6} C_k[f^{iv}]$. The Euler - Mac Laurin formula gives the corrections to an integral approximating a sum:

$$\sum_{k=0}^M f(a+2\pi k) = \int_a^b \frac{dx}{2\pi} f(x) + \frac{1}{2}[f(b) + f(a)] + \frac{\pi}{6}[f'(b) - f'(a)] - \frac{\pi^3}{90}[f'''(b) - f'''(a)] + R \quad (20.35)$$

20.6.7 Poisson's summation formula

This is a very useful tool in many areas of physics. Given an integrable function $f(t)$ on \mathbb{R} , the sum $F(t) = \sum_{k=-\infty}^{\infty} f(t+kT)$ (if convergent) defines a T -periodic function, which can be expanded in Fourier series. The result is Poisson's summation formula:

$$\sum_{k=-\infty}^{\infty} f(t+kT) = \frac{1}{T} \sum_{\ell=-\infty}^{\infty} \hat{f}_{\ell} e^{i\frac{2\pi}{T}\ell t} \quad (20.36)$$

where

$$\hat{f}_{\ell} = \int_0^T dt F(t) e^{-i\frac{2\pi}{T}\ell t} = \sum_{k=-\infty}^{\infty} \int_{kT}^{(k+1)T} dt f(t) e^{-i\frac{2\pi}{T}\ell t} = \int_{-\infty}^{\infty} dt f(t) e^{-i\frac{2\pi}{T}\ell t}.$$

Example 20.6.1. $f(t) = e^{-at^2}$, $\hat{f}_{\ell} = \sqrt{\frac{\pi}{a}} e^{-\ell^2/4a}$.

$$\sum_{k=-\infty}^{\infty} e^{-a(t+2k\pi)^2} = \frac{1}{2\sqrt{\pi a}} \sum_{\ell=-\infty}^{\infty} e^{-\ell^2/4a + i\ell t} \quad (20.37)$$

In particular, for $t=0$:

$$\sum_{k=-\infty}^{\infty} e^{-4\pi^2 a k^2} = \frac{1}{\sqrt{4\pi a}} \sum_{k=-\infty}^{\infty} e^{-\frac{k^2}{4a}} \quad (20.38)$$

These series arise in the theory of Jacobi's theta functions.

Example 20.6.2. $f(t) = e^{-\omega|t|}$, $\hat{f}_{\ell} = \frac{2\omega}{\omega^2 + k^2}$.

$$\sum_{k=-\infty}^{\infty} e^{-\omega|t+2\pi k|} = \frac{\omega}{\pi} \sum_{\ell=-\infty}^{\infty} \frac{e^{i\ell t}}{\omega^2 + \ell^2} \quad (20.39)$$

For $t = 0$ the l.h.s. is $-1 + 2 \sum_{k=0}^{\infty} e^{-2\pi\omega k} = \coth(\pi\omega)$. Then:

$$\coth(\pi\omega) = \frac{\omega}{\pi} \sum_{\ell=-\infty}^{\infty} \frac{1}{\omega^2 + \ell^2}. \tag{20.40}$$

Example 20.6.3. Poisson's formula is used to extend Riemann's series $\zeta(z)$ on $\text{Re } z > 1$ to a function on $\text{Re } z < 0$ (the strip $0 < \text{Re } z < 1$ is left out).

Let $g(t) = \sum_{k=1}^{\infty} e^{-k^2\pi t}$ and evaluate

$$\int_0^{\infty} dt g(t) t^{z-1} = \sum_{k=1}^{\infty} \int_0^{\infty} dt e^{-k^2\pi t} t^{z-1} = \frac{1}{\pi^z} \zeta(2z) \Gamma(z)$$

Eq.(20.38) shows the symmetry $2g(t) + 1 = (1/\sqrt{t})[2g(1/t) + 1]$ i.e. $g(t) = -1/2 + 1/(2\sqrt{t}) + g(1/t)1/\sqrt{t}$, which is used to evaluate the integral in a different way:

$$\begin{aligned} \frac{1}{\pi^{z/2}} \zeta(z) \Gamma(z/2) &= \int_0^1 dt g(t) t^{z/2-1} + \int_1^{\infty} dt g(t) t^{z/2-1} \\ &= \int_0^1 dt \left[-\frac{1}{2} + \frac{1}{2\sqrt{t}} + \frac{1}{\sqrt{t}} g(1/t) \right] t^{z/2-1} + \int_1^{\infty} dt g(t) t^{z/2-1} \\ &= -\frac{1}{z} - \frac{1}{1-z} + \int_1^{\infty} \frac{dt}{t} (t^{(1-z)/2} + t^{z/2}) g(t) \end{aligned}$$

The r.h.s. is invariant under the replacement $z \rightarrow 1-z$, therefore: $\zeta(z) \Gamma(\frac{z}{2}) = \sqrt{\pi} \zeta(1-z) \Gamma(\frac{1}{2} - \frac{z}{2})$ or

$$\zeta(1-z) = \zeta(z) \frac{2}{(2\pi)^z} \cos(\frac{1}{2}\pi z) \Gamma(z) \tag{20.41}$$

For $z = -2, -4, \dots$ the function $\Gamma(z)$ has poles; however the left-hand side is finite. Then $\zeta(z)$ must be zero at $z = -2, -4, \dots$: these are the "trivial zeros" of Riemann's zeta function. The famous Riemann's hypothesis states that the non-trivial zeros are all located on the line $\text{Re } z = \frac{1}{2}$. The statement is relevant for the study of the distribution of prime numbers¹².

Exercise 20.6.4. Show that $\zeta(-1) = -\frac{1}{12}$, $\zeta(0) = -\frac{1}{2}$ (see exercise 12.3.5).

¹² Riemann's hypothesis is one of the seven problems that were selected by the Clay Mathematics Institute in 2000 (Millennium Prize). The single problem that has been solved so far is Poincaré's conjecture (every simply connected closed 3-manifold is homeomorphic to the 3-sphere) stated in 1904. The winner Grigoriy Perelman declined the one-million \$ prize, and a Fields medal.

20.6.8 Partition function

Consider non-interacting particles in a cubic box with side-length L . The energy levels are $\epsilon_k = \hbar^2 k^2 / 2m$, with $\mathbf{k} = (2\pi/L)\mathbf{n}$, $\mathbf{n} \in \mathbb{Z}^3$. The partition function is:

$$Z = \sum_{\mathbf{k}} e^{-\frac{\epsilon_k}{k_B T}} = \left[\sum_{n=-\infty}^{\infty} \exp\left(-\frac{\lambda^2}{L^2} \pi n^2\right) \right]^3$$

$\lambda = \sqrt{2\pi\hbar^2/mk_B T}$ is the "thermal length" (the de Broglie length of a particle with energy $k_B T$). For $L \gg \lambda$ the terms are a slowly decreasing sequence. The sum can be computed via Poisson's formula (20.38):

$$\sum_{n=-\infty}^{\infty} \exp\left(-\frac{\lambda^2}{L^2} \pi n^2\right) = \frac{L}{\lambda} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{L}{\lambda} \pi n^2\right) = \frac{L}{\lambda} (1 + \text{negligible terms}).$$

It tells us that the standard procedure in statistical mechanics to approximate the sum with an integral (for large L) is legitimate:

$$Z = L^3 \int \frac{d\mathbf{k}}{(2\pi)^3} \exp\left(-\frac{\hbar^2 k^2}{2mk_B T}\right) = \left(\frac{L}{\lambda}\right)^3$$

In general, the extension to 3D of the Poisson sum for a period $2\pi/L$ is:

$$\sum_{\mathbf{k}} f(\mathbf{k}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} f\left(\frac{2\pi}{L} \mathbf{n}\right) = \frac{L^3}{(2\pi)^3} \sum_{\mathbf{m} \in \mathbb{Z}^3} \int_{\mathbb{R}^3} d\mathbf{s} f(\mathbf{s}) e^{iL(\mathbf{m} \cdot \mathbf{s})}$$

If the function $f(\mathbf{k})$ has slow variation on the scale $1/L$, for large L the Fourier terms vanish except the term $\mathbf{m} = 0$:

$$\boxed{\sum_{\mathbf{k}} f(\mathbf{k}) \approx L^3 \int \frac{d\mathbf{k}}{(2\pi)^3} f(\mathbf{k})}$$

20.6.9 Particle in 1D lattice

A particle is bound to a 1d lattice of points $x_k = ka$ where $k \in \mathbb{Z}$ and a is the lattice spacing. The lattice version of the 1d stationary Schrödinger equation is

$$-\frac{\hbar^2}{2m} (\Delta u)_k + V_k u_k = E u_k$$

u_k is the state vector, and the probability for the particle to be in x_k is $|u_k|^2$. The kinetic term contains the one-dimensional discrete Laplacian (see also ex.2.9.7)

$$(\Delta u)_k = \frac{u_{k+1} - 2u_k + u_{k-1}}{a^2}$$

For a smooth function $u(x)$ such that $u(x_k) = u_k$ the continuum limit $a \rightarrow 0$ of Δu is $u''(x)$. The second term V_k is the site-potential.

The equation is rescaled and written in the form

$$\boxed{u_{k+1} + u_{k-1} + v_k u_k = \epsilon u_k} \quad (20.42)$$

with $E = \frac{\hbar^2}{2ma^2}(2 - \epsilon)$ and $V_k = -\frac{\hbar^2}{2ma^2} v_k$. It has the equivalent matrix form:

$$\begin{pmatrix} u_{k+1} \\ u_k \end{pmatrix} = \begin{bmatrix} \epsilon - v_k - 1 & \\ 1 & 0 \end{bmatrix} \begin{pmatrix} u_k \\ u_{k-1} \end{pmatrix}$$

Iteration N times yields the components u_{N+1} , u_N from initial data u_1 , u_0 :

$$\begin{pmatrix} u_{N+1} \\ u_N \end{pmatrix} = T_N(\epsilon) \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}, \quad T_N(\epsilon) = \begin{bmatrix} \epsilon - v_N - 1 & \\ 1 & 0 \end{bmatrix} \dots \begin{bmatrix} \epsilon - v_1 - 1 \\ 1 & 0 \end{bmatrix} \quad (20.43)$$

$T_N(\epsilon)$ is the transfer matrix. Note that $\det T_N(\epsilon) = 1$.

Eq.(20.43) shows that z is an eigenvalue of $T_N(\epsilon)$ if $u_{N+1} = zu_1$ and $u_0 = (1/z)u_N$, i.e. $\{u_1, \dots, u_N\}$ is eigenvector with eigenvalue ϵ of the following matrix with corners:

$$H_N(z) = \begin{pmatrix} v_1 & 1 & & 1/z \\ 1 & v_2 & \ddots & \\ & \ddots & \ddots & 1 \\ z & & 1 & v_N \end{pmatrix}$$

This implies the *duality identity*¹³ among the spectra of the two matrices:

$$\begin{aligned} \det[\epsilon \mathbb{1}_N - H_N(z)] &= z^{-1} \det[T_N(\epsilon) - z \mathbb{1}_2] \\ &= \text{Trace } T_N(\epsilon) - (z + 1/z) \end{aligned} \quad (20.44)$$

¹³ It can be generalized to higher dimensions, L.G.Molinari, *Determinants of block tridiagonal matrices*, Linear Algebra and its Applications **429** (2008) 2221–2226.

Trace $T_N(\epsilon) = \det[\epsilon - H(\pm i)]$ is a real polynomial $p_N(\epsilon)$. If $z = e^{i\phi}$, the matrix $H(e^{i\phi})$ is Hermitian with real eigenvalues $\lambda_k(\phi)$. Eq.(20.44) is

$$\prod_{k=1}^N [\epsilon - \lambda_k(\phi)] = p_N(\epsilon) - 2 \cos(\phi) \tag{20.45}$$

The eigenvalues $\lambda_k(\phi)$ solve $p_N(\epsilon) = 2 \cos(\phi)$. As ϕ changes in $[0, 2\pi]$, the eigenvalues trace N real (non overlapping) bands.

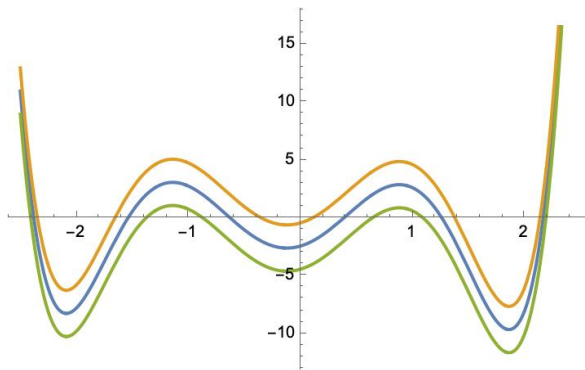


Figure 20.9 $p_6(\epsilon) = \det[\epsilon - H(i)]$ is the blue line. The shift by +2 ($\phi = 0$) is the polynomial $\det[\epsilon - H_6(1)]$ (yellow), the shift by -2 ($\phi = \pi$) is the polynomial $\det[\epsilon - H_6(-1)]$ (green). The intersections with the horizontal axis are the respective eigenvalues. The eigenvalues at intermediate ϕ trace segments among such extrema.

- **The free particle.** If $\nu_k = 0$ the equation (20.42) has solutions $u_k = \exp(\pm ikp)$ with eigenvalue $\epsilon = 2 \cos p$.

With b.c. $u_0 = u_{N+1} = 0$, the N eigenvectors (not normalized) are $u_k^{(\ell)} = \sin(p_\ell k)$ with $p_\ell = \frac{\pi}{N+1} \ell$, $\ell = 1, \dots, N$, and eigenvalues $\epsilon_\ell = 2 \cos p_\ell$. Then $E_\ell = \frac{\hbar^2}{2ma^2} [2 - 2 \cos(\frac{\ell\pi}{N+1})] = \frac{\hbar^2}{2ma^2} 4 \sin^2(\frac{\ell\pi}{N+1})$. For large N and small spacing a such that the length $Na = L$ is finite (continuum limit) we obtain $E_\ell \approx \frac{\hbar^2}{2m} (\frac{2\pi\ell}{L})^2$. They coincide with the spectrum of a free particle $-\frac{\hbar^2}{2m} u''(x) = Eu(x)$ with b.c. $u(0) = u(L) = 0$.

If $N \rightarrow \infty$ but a is finite, the chain is semi-infinite. The eigenvector $\{u_k\} \notin \ell^2(\mathbb{C})$ and the spectrum is the band $-2 \leq \epsilon \leq 2$.

- **The disordered chain.** A vast literature is devoted to the study of (20.42) with independent random numbers ν_k that simulate a disordered potential¹⁴. For such models, in

¹⁴ F. Dyson, *The dynamics of a disordered linear chain*, Phys. Rev. 92 (1953); H. Schmidt, *Disordered one-dimensional crystals*, Phys. Rev. 105 (1957), Crisanti, Paladin, Vulpiani, Products of random matrices, Springer; Cycon, Froese and Simon, Schrödinger operators, Springer; F. Haake, Quantum signatures of chaos, Springer.

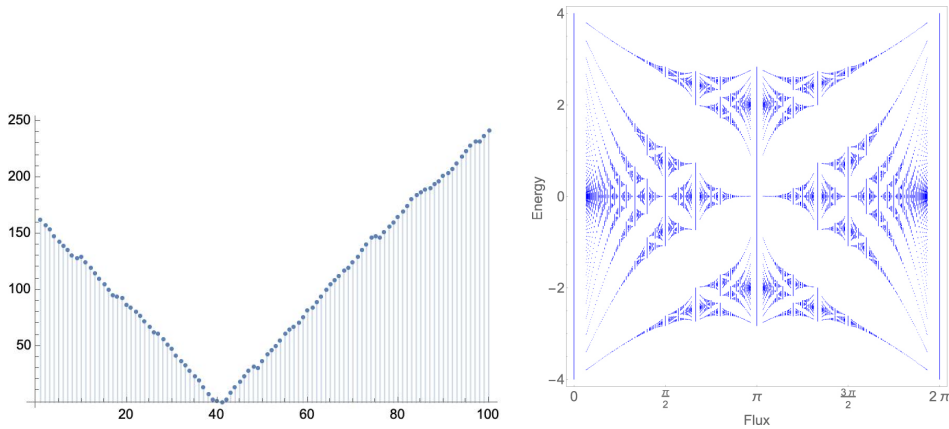


Figure 20.10 Left: The exponential localization of an eigenvector of the 1d Anderson model, with $N=100$ sites and random values v_k in $[-10, 10]$. The occupation probability of site k , $|u_k|^2$ is plotted as $-\log|u_k|^2$. Right: The Hofstadter butterfly ($g = 1$). For a value $2\pi\alpha$, the eigenvalues of (20.46) are in a vertical line. For $\alpha = 0$ or 1 , v_k is constant (free particle). For $\alpha = 1/2$ the bandwidth is $2\sqrt{5}$. (Picture by Y. Hatsuda, H. Katsura and Y. Tachikawa, *New J. Phys.* **18** 103023 (2016), CC BY 3.0, <https://commons.wikimedia.org/w/index.php?curid=71886522>).

$d = 1$, it is known that the eigenvalues of the random transfer matrix $T_N(\epsilon)$ become non-random for large N : $\exp(\pm N\gamma(\epsilon))$. The exponent $\gamma(\epsilon)$ is independent of the sequence $\{v_k\}$ (it is “self-averaging”). This implies that the Hamiltonian of the infinite disordered chain has pure point spectrum with eigenvectors that are exponentially localized around sites of the lattice: $|u_k| \propto e^{-\gamma(\epsilon)|k-k_0|}$ (see Fig.20.10). The exponent is given by the Herbert-Jones-Thouless formula, obtained from (20.45):

$$\gamma(\epsilon) = \int d\epsilon' \rho(\epsilon') \log|\epsilon - \epsilon'|$$

$\rho(\epsilon)$ is the (self-averaging) density of eigenvalues of the random Hamiltonian. For $d = 3$ Philip Anderson (1958) proved that a transition occurs at a critical value of disorder, from extended (i.e. conducting) states (continuum spectrum) to localized states (pure point spectrum). In solid state physics it is named *metal - insulator* transition.

• **Harper model.** Disorder can be deterministic, due to incommensurability of a periodic potential v_k with the lattice. The Harper-Aubry-André model ¹⁵ is

$$u_{k+1} + u_{k-1} + 2g \cos(2\pi k\alpha)u_k = \epsilon u_k \tag{20.46}$$

¹⁵ See the pedagogical paper in <https://doi.org/10.48550/arXiv.1812.06201>

The Fourier expansion $u_k = \sum_{m \in \mathbb{Z}} e^{im(2\pi\alpha k)} \hat{u}_m$ reproduces the equation with inverted coupling:

$$\hat{u}_{k+1} + \hat{u}_{k-1} + \frac{2}{g} \cos(2\pi k\alpha) \hat{u}_k = (\epsilon/g) \hat{u}_k$$

The special case $g = 1$ makes the equation self-dual. It arises in the study of an electron in a square lattice with magnetic flux $2\pi\alpha$ per square cell (Hofstadter, 1976). The spectrum of the infinite tridiagonal Hamiltonian is a Cantor set for any irrational α (Hofstadter's butterfly).

Chapter 21

Bounded Linear Operators

21.1 Linear functionals

The space of linear bounded functionals $\mathcal{B}(\mathcal{H}, \mathbb{C})$ is \mathcal{H}^* , the dual space of \mathcal{H} . The inner product with a fixed vector $(x|\cdot)$ is a linear functional and is bounded by Schwarz's inequality. The following theorem proves that all linear bounded functionals act as inner products.

Theorem 21.1.1 (Riesz's lemma). *For each $F \in \mathcal{H}^*$ there is a unique $x_F \in \mathcal{H}$ such that $Fx = (x_F|x)$ for all $x \in \mathcal{H}$. In addition $\|F\| = \|x_F\|$.*

Proof. If $\text{Ker } F = \mathcal{H}$ then $x_F = 0$. If $\text{Ker } F$ is a proper subspace, then there is a vector y orthogonal to it. Any vector x can be decomposed as $x = (x - y \frac{Fy}{\|y\|^2}) + y \frac{Fy}{\|y\|^2}$, where the first term belongs to $\text{Ker } F$ and the second one is orthogonal to it. The evaluation $(y|x) = Fx \frac{(y|y)}{Fy}$ shows that $Fx = (x_F|x)$ with $x_F = y \frac{\overline{Fy}}{\|y\|^2}$.

The vector x_F is unique: suppose that $Fx = (x_F|x) = (x'_F|x)$ for all x , then $0 = (x_F - x'_F|x)$ i.e. $x_F = x'_F$.

By Schwarz's inequality: $|Fx| = |(x_F|x)| \leq \|x_F\| \|x\|$; equality is attained at $|Fx_F| = \|x_F\|^2$. Therefore: $\|F\| = \sup_x \frac{|Fx|}{\|x\|} = \|x_F\|$. \square

Because of the identification of bounded functionals with vectors, Hilbert spaces are *self-dual*.

Example 21.1.2. *For which $z \in \mathbb{C}$ is the power series $F(z, \mathbf{a}) = \sum_{k=0}^{\infty} a_k z^k$ a bounded functional on $\ell^2(\mathbb{C})$?*

A. *F is a linear bounded functional iff $\{1, z, z^2, \dots\} \in \ell^2$, i.e. $\sum_k |z|^{2k} < \infty$, which is true for $|z| < 1$. Then, by Schwarz's inequality: $|F(z, \mathbf{a})| = |(z^*|\mathbf{a})| \leq \|\mathbf{a}\|_2 / \sqrt{1 - |z|^2}$. The power series is absolutely convergent and holomorphic for all \mathbf{a} if $|z| < 1$.*

Exercise 21.1.3. Consider the functional $F(z, \mathbf{a}) = \sum_{n=1}^{\infty} a_n n^{-z}$ where $z \in \mathbb{C}$ and $\{a_n\} \in \ell^2(\mathbb{C})$. For which z is the functional bounded?

21.2 The adjoint of a bounded operator

The linear bounded operators with domain \mathcal{H} and range in \mathcal{H} form the Banach space $\mathcal{B}(\mathcal{H})$. The set is closed for the involutive action of adjunction:

Theorem 21.2.1. For any operator $\hat{A} \in \mathcal{B}(\mathcal{H})$ there is an operator $\hat{A}^\dagger \in \mathcal{B}(\mathcal{H})$ (the adjoint of \hat{A}) such that:

$$(x|\hat{A}y) = (\hat{A}^\dagger x|y) \quad \forall x, y \in \mathcal{H} \tag{21.1}$$

and $\|\hat{A}^\dagger\| = \|\hat{A}\|$.

Proof. Fix $x \in \mathcal{H}$, the map $y \rightarrow (x|\hat{A}y)$ is a linear bounded functional: $|(x|\hat{A}y)| \leq (\|\hat{A}\|\|x\|)\|y\|$ for all y . Then, by Riesz' theorem, there is a unique vector $v_{A,x}$ such that $(x|\hat{A}y) = (v_{A,x}|y)$ for all y . The correspondence $x \rightarrow v_{A,x}$ defines the adjoint operator: $\hat{A}^\dagger x = v_{A,x}$. It is linear:
 $(\hat{A}^\dagger x + \lambda \hat{A}^\dagger x'|y) = (\hat{A}^\dagger x|y) + \bar{\lambda}(\hat{A}^\dagger x'|y) = (x|\hat{A}y) + \bar{\lambda}(x'|\hat{A}y) = (x + \lambda x'|\hat{A}y) = (\hat{A}^\dagger(x + \lambda x')|y)$.
 Equality of norms follows from Schwarz's inequality and boundedness of \hat{A} : $|(\hat{A}^\dagger x|y)| = |(x|\hat{A}y)| \leq \|x\| \|\hat{A}\| \|y\|$, if $y = \hat{A}^\dagger x$ then $\|\hat{A}^\dagger x\| \leq \|x\| \|\hat{A}\|$ i.e. \hat{A}^\dagger is bounded and $\|\hat{A}^\dagger\| \leq \|\hat{A}\|$.
 The proof of equality is left to the reader. \square

Exercise 21.2.2. Show that:

$$(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger \quad (\lambda \hat{A})^\dagger = \bar{\lambda} \hat{A}^\dagger \tag{21.2}$$

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger \quad (\hat{A}^\dagger)^\dagger = \hat{A} \tag{21.3}$$

$$\hat{A}_n \rightarrow \hat{A} \Rightarrow \hat{A}_n^\dagger \rightarrow \hat{A}^\dagger \tag{21.4}$$

Proposition 21.2.3. Let $\hat{A} \in \mathcal{B}(\mathcal{H})$, then $\text{Ker } \hat{A}$ is closed and

$$\mathcal{H} = \text{Ker } \hat{A} \oplus \overline{\text{Ran } \hat{A}^\dagger} = \text{Ker } \hat{A}^\dagger \oplus \overline{\text{Ran } \hat{A}} \tag{21.5}$$

Proof. Suppose that x_n is a sequence in $\text{Ker } \hat{A}$, and $x_n \rightarrow x$. Then $\|\hat{A}x_n - \hat{A}x\| \leq \|\hat{A}\|\|x_n - x\| \rightarrow 0$ i.e. $\hat{A}x = \lim_n \hat{A}x_n = 0$ i.e. $x \in \text{Ker } \hat{A}$.

Since $\text{Ker } \hat{A}$ is a closed linear subspace, it is $\mathcal{H} = \text{Ker } \hat{A} \oplus (\text{Ker } \hat{A})^\perp$.

$$\begin{aligned} (\text{Ran } \hat{A}^\dagger)^\perp &= \{x : (x|y) = 0 \ \forall y \in \text{Ran } \hat{A}^\dagger\} \\ &= \{x : (x|A^\dagger x') = 0 \ \forall x' \in \mathcal{H}\} \\ &= \{x : (\hat{A}x|x') = 0 \ \forall x' \in \mathcal{H}\} \\ &= \{x : \hat{A}x = 0\} = \text{Ker } \hat{A} \end{aligned}$$

Therefore $(\text{Ker } \hat{A})^\perp = \overline{\text{Ran } \hat{A}^\dagger}$. The second equality results after exchanging the operators. \square

This statement is of practical utility. Consider the equation $\hat{A}x = y$; a solution x exists in \mathcal{H} if y belongs to the range of \hat{A} . If the range is a closed set the solution exists if y is orthogonal to all vectors that solve $\hat{A}^\dagger x' = 0$. In infinite dimensional space the range of a bounded operator need not be a closed subspace.

Exercise 21.2.4. Show that if $\hat{A} \in \mathcal{B}(\mathcal{H})$ is invertible with bounded inverse, then also \hat{A}^\dagger is invertible with bounded inverse, and $(\hat{A}^\dagger)^{-1} = (\hat{A}^{-1})^\dagger$.

If the equation $\hat{A}x = \lambda x$ has a nonzero solution $x \in \mathcal{H}$, then λ and x are respectively an eigenvalue and an eigenvector of \hat{A} , and $|\lambda| \leq \|A\|$.

Definition 21.2.5. An operator $\hat{A} \in \mathcal{B}(\mathcal{H})$ is **self-adjoint** if $\hat{A} = \hat{A}^\dagger$:

$$(\hat{A}x|y) = (x|\hat{A}y), \quad \forall x, y \in \mathcal{H}$$

Theorem 21.2.6. The eigenvalues of a self-adjoint operator in $\mathcal{B}(\mathcal{H})$ are real, and the eigenvectors corresponding to different eigenvalues are orthogonal.

Proof. Let x and x' be eigenvectors corresponding to eigenvalues $\lambda \neq \lambda'$. From $(\hat{A}x|x) = (x|\hat{A}x)$ one obtains $\bar{\lambda} = \lambda$. From $(\hat{A}x|x') = (x|\hat{A}x')$ one obtains $(\lambda - \lambda')(x|x') = 0$ i.e. $x \perp x'$ if $\lambda \neq \lambda'$. \square

Exercise 21.2.7. \hat{A} is normal if $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}$. Show that eigenvectors corresponding to different eigenvalues of a normal operator are orthogonal.

Exercise 21.2.8.

1) Let $\hat{A} \in \mathcal{B}(\mathcal{H})$; show that $\|\hat{A}^\dagger \hat{A}\| = \|\hat{A}\|^2$.

2) If \hat{A} and \hat{B} are bounded and self-adjoint then $\|\hat{A}\hat{B}\| = \|\hat{B}\hat{A}\|$.

Exercise 21.2.9. Show that for a bounded self-adjoint operator:

$$Q_A \equiv \sup_{x \neq 0} \frac{(x|\hat{A}x)}{\|x\|^2} = \|\hat{A}\| \tag{21.6}$$

Proof. Start with $4\text{Re}(y|\hat{A}x) = ((x+y)|\hat{A}(x+y)) - ((x-y)|\hat{A}(x-y))$, $4|\text{Re}(y|\hat{A}x)| \leq Q_A(\|x+y\|^2 + \|x-y\|^2) = 2Q_A(\|x\|^2 + \|y\|^2)$. Now choose $\|x\| = 1$ and $y = \hat{A}x/\|\hat{A}x\|$, and it is almost done.

Exercise 21.2.10. Suppose that $\hat{A} \in \mathcal{B}(\mathcal{H})$, and \mathcal{H} is complex. Prove that:

- 1) if $(x|\hat{A}x) = 0$ for all x then $\hat{A} = 0$;
- 2) if $(x|\hat{A}x)$ is real for all x , then $\hat{A} = \hat{A}^\dagger$.
(if \mathcal{H} is real, condition 1 implies $\hat{A} = -\hat{A}^\dagger$).

Exercise 21.2.11. In $L^2(\mathbb{R})$ consider the linear operator \hat{D}_h , $h \in \mathbb{R}/\{0\}$, $(\hat{D}_h f)(x) = \frac{1}{2h}[f(x+h) - f(x-h)]$.

Is \hat{D}_h bounded? invertible? Write the adjoints of \hat{D}_h and \hat{D}_h^2 .

The *Invariant space conjecture* was posed by John Von Neumann and independently by Arne Beurling, in 1935. It states that for every bounded linear operator \hat{A} on a complex separable infinite-dimensional Hilbert space, there is a proper closed subspace M that is mapped into itself¹.

21.2.1 Integral operators

The classification of linear integral equations bears the names of Vito Volterra (1860-1940) and Ivar Fredholm (1866-1927). An integral equation is the natural transposition to the continuum of the discrete equation $f_i = g_i + \sum_j k_{ij} f_j$.

Consider the inhomogeneous equation

$$f(x) = g(x) + \lambda \int_{\Omega} dy k(x, y) f(y),$$

where λ is a parameter, k is the *kernel* of the integral operator, g is assigned and f is the unknown function. In operator form it is $f = g + \lambda \hat{K} f$,

$$(\hat{K} f)(x) = \int_{\Omega} dy k(x, y) f(y) \tag{21.7}$$

¹ They proved the conjecture for compact operators. For a general proof see Charles Neville (2023), <https://doi.org/10.48550/arXiv.2307.08176>.

A solution exists if g belongs to the range of $1 - \lambda \hat{K}$.

Let $\Omega = [0, 1]$ for definiteness. If $k \in \mathcal{L}^2(Q)$ (Q is the unit square) then \hat{K} is a bounded operator on $L^2(0, 1)$: by Fubini's theorem the function $y \rightarrow |k(x, y)|$ is measurable and belongs to $\mathcal{L}^2(0, 1)$; by Schwarz's inequality $|(\hat{K}f)(x)| \leq \|k(x, \cdot)\| \|f\|_2$. Squaring and integration in x gives:

$$\|\hat{K}f\|_2 \leq \|k\| \|f\|_2$$

where $\|k\|^2 = \int_Q dx dy |k(x, y)|^2$. The adjoint operator is now evaluated²:

$$\begin{aligned} (h|\hat{K}f) &= \int_0^1 dx \overline{h(x)} \left[\int_0^1 dy k(x, y) f(y) \right] \\ &= \int_0^1 dy \left[\int_0^1 dx \overline{k(x, y) h(x)} \right] f(y) = (\hat{K}^\dagger h|f) \\ (\hat{K}^\dagger h)(x) &= \int_0^1 dy \overline{k(y, x) h(y)} \end{aligned} \tag{21.8}$$

The integral operator is self-adjoint if $k(x, y) = \overline{k(y, x)}$.

A solution of $(I - \lambda \hat{K})f = g$ exists if $g \in \text{Ran}(I - \lambda \hat{K})$ i.e. $g \perp \text{Ker}(I - \lambda \hat{K}^\dagger)$. This means that g must be orthogonal to the eigenvectors $\bar{\lambda} \hat{K}^\dagger u = u$.

In particular, if $|\lambda| \|K\| < 1$, it is $\text{Ker}(I - \bar{\lambda} \hat{K}^\dagger) = \{0\}$ and $\text{Ker}(I - \lambda \hat{K}) = \{0\}$, and $(I - \lambda \hat{K})^{-1}$ exists with domain \mathcal{H} . The operator can be expanded in a geometric series that converges for any g :

$$f = g + \lambda \hat{K}g + \lambda^2 \hat{K}^2 g + \dots$$

The powers of the operator are integral operators with kernels $k_1(x, y) = k(x, y)$, $k_{n+1}(x, y) = \int_0^1 du k(x, u) k_n(u, y)$.

Example 21.2.12. Consider the integral equation, with $g \in \mathcal{L}^2(0, 1)$:

$$f(x) = g(x) + \int_0^x f(y) dy, \quad x \in [0, 1]$$

² the steps are justified by Fubini's theorem for the exchange of order of integration: let $f(x, y)$ be measurable on $M \times N$, then $\int_M dm (\int_N dm |f|) < \infty$ iff $\int_N dm (\int_M dm |f|) < \infty$ and, if they are finite it is:

$$\int_M dm \left(\int_N dm f \right) = \int_N dm \left(\int_M dm f \right)$$

It corresponds to the Cauchy problem $f' = f + g'$ with $f(0) = g(0)$. The kernel $k(x, y) = \theta(x - y)$ has L^2 norm $1/\sqrt{2}$, therefore the iterative solution of the integral equation converges, with kernels $k_{n+1}(x, y) = \theta(x - y)(x - y)^n/n!$. The convergent Neumann series gives

$$f(x) = g(x) + \int_0^x dy e^{x-y} g(y)$$

Example 21.2.13. In $L^2(0, 2\pi)$ (real functions) consider the equation

$$f = \lambda \hat{K} f + g, \quad (\hat{K} f)(x) = \int_0^{2\pi} dy \sin(x+y) f(y), \quad \lambda \in \mathbb{R}$$

It is $(\hat{K} f)(x) = f_1 \sin x + f_2 \cos x$, where $f_1 = \int dx \cos(x) f(x)$ and $f_2 = \int dx \sin(x) f(x)$. The operator \hat{K} is rank 2 and self-adjoint. The problem is then two-dimensional and the solution, if existent, has the form:

$$f(x) = \lambda(f_1 \sin x + f_2 \cos x) + g(x)$$

By taking the inner products with $\cos x$ and $\sin x$ we get:

$$\begin{bmatrix} 1 & -\lambda\pi \\ -\lambda\pi & 1 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix}$$

where $g_1 = (\cos|g)$ and $g_2 = (\sin|g)$. The solution exists for any g and is unique if $1 - \lambda^2\pi^2 \neq 0$.

- If $\lambda \neq \pm \frac{1}{\pi}$, matrix inversion gives f_1 and f_2 , and:

$$f(x) = g(x) + \lambda \int_0^{2\pi} dy \frac{\sin(x+y) + \lambda\pi \cos(x-y)}{1 - \lambda^2\pi^2} g(y)$$

- If $\lambda = \frac{1}{\pi}$, a solution exists if $g \in \text{Ran}(I - \frac{1}{\pi}\hat{K})$ i.e. $g \perp \text{Ker}(I - \frac{1}{\pi}\hat{K})$ ($\hat{K} = \hat{K}^\dagger$). The functions $\hat{K}u = \pi u$, up to a pre-factor, are: $u(x) = \sin x + \cos x$. Then: $\int_0^{2\pi} dx (\sin x + \cos x) g(x) = g_1 + g_2 = 0$. The solution is

$$f(x) = \frac{f_1}{\pi} \sin x + \frac{f_1 - g_1}{\pi} \cos x + g(x)$$

where f_1 is an arbitrary constant.

- If $\lambda = -\frac{1}{\pi}$ the case is treated similarly.

Exercise 21.2.14.

1) Show that $\hat{T} \in \mathcal{B}(L^2(\mathbb{R}))$, is self-adjoint, and $\|\hat{T}\| \leq \sqrt{\pi}$. Is it invertible?

$$(\hat{T}f)(x) = \int_{-\infty}^{\infty} dy \frac{f(y)}{x^2 + y^2 + 1}$$

2) Estimate the norm of the operator \hat{T} on $L^2[0, 1]$:

$$(\hat{T}f)(x) = \int_0^1 dy \frac{f(y)}{\sqrt[4]{|x-y|}}, \quad x \in [0, 1]$$

21.3 Orthogonal projections

Given a closed subspace M and a vector x , the projection theorem states that $x = p + w$, where $p \in M$ and $w \in M^\perp$, and the decomposition is unique. This permits to introduce the orthogonal projection operator on M , $\hat{P}: x \rightarrow p$, and prove the following properties:

Proposition 21.3.1. \hat{P} is linear, $\|\hat{P}\| = 1$, $\hat{P}^\dagger = \hat{P}$, $\hat{P}^2 = \hat{P}$.

Proof. If $x = p + w$ and $x' = p' + w'$, then $x + \lambda x' = (p + \lambda p') + (w + \lambda w')$, where $p + \lambda p' \in M$ and $w + \lambda w' \in M^\perp$. As the decomposition is unique, necessarily it is $P(x + \lambda x') = p + \lambda p' = \hat{P}x + \lambda \hat{P}x'$.

. Boundedness: $\|x\|^2 = \|\hat{P}x + w\|^2 = \|\hat{P}x\|^2 + \|w\|^2 \geq \|\hat{P}x\|^2$ then $\|\hat{P}x\| \leq \|x\|$. Equality holds for $x \in M$. Then $\hat{P} \in \mathcal{B}(\mathcal{H})$ and $\|\hat{P}\| = 1$.

. Self-adjointness: $(x - \hat{P}x | y - \hat{P}y) = (x - \hat{P}x | y)$ (because $x - \hat{P}x \in M^\perp$), for analogous reason $(x - \hat{P}x | y - \hat{P}y) = (x | y - \hat{P}y)$; then $(\hat{P}x | y) = (x | \hat{P}y)$.

. Idempotency: $\hat{P}^2 x = \hat{P}p = p = \hat{P}x$, then $\hat{P}^2 = \hat{P}$. □

It is convenient to reverse the approach and define orthogonal projection operators through the afore properties:

Definition 21.3.2. $\hat{P} \in \mathcal{B}(\mathcal{H})$ is an orthogonal projector if $\hat{P}^2 = \hat{P}$, $\hat{P}^\dagger = \hat{P}$.

1) The subspace of projection is $M = \text{Ran} \hat{P}$.

2) $1 - \hat{P}$ is an orthogonal projector if \hat{P} is. Since $(1 - \hat{P})(\hat{P}y) = 0$, it is

$\text{Ker}(1 - \hat{P}) = M$. Therefore M is closed.

3) Let $y = x - \hat{P}x$, then $\hat{P}y = 0$ and $(y | \hat{P}x) = 0 \forall x$, i.e. $\text{Ker} \hat{P} = M^\perp$.

4) Since $M \oplus M^\perp = \mathcal{H}$, a projector has only the eigenvalues 1 and 0, with eigenspaces M and M^\perp .

Example 21.3.3.

1) In $L^2(\mathbb{R})$ the multiplication operator $f \rightarrow \chi_{[a,b]}f$, where $\chi_{[a,b]}$ is the characteristic function of an interval $[a, b]$, is an orthogonal projector. The invariant subspace M is given by

functions that vanish a.e. for $x \notin [a, b]$.

2) The operators $(P_{\pm}f)(x) = \frac{1}{2}[f(x) \pm f(-x)]$ are orthogonal projectors on the orthogonal subspaces of (a.e.) even and odd functions.

3) If $\{u_k\}_{k=1}^N$ are orthonormal vectors, $\hat{P}x = \sum_{k=1}^N (u_k|x)u_k$ is the orthogonal projection on the linear subspace spanned by the vectors u_k . This is true also for $N = \infty$. For a complete orthonormal set $\hat{P} = 1$ (identity operator).

Exercise 21.3.4. Let \hat{P} and \hat{P}' be projectors on subspaces M and M' , then:

1) $\hat{P} + \hat{P}'$ is a projector iff $M \perp M'$. In this case $\hat{P} + \hat{P}' = \hat{P}_{M \oplus M'}$.

2) $\hat{P}\hat{P}'$ is a projector iff \hat{P} and \hat{P}' commute. In this case $\hat{P}\hat{P}' = \hat{P}_{M \cap M'}$.

Exercise 21.3.5. Show that the projection operator on the linear subspace spanned by the linearly independent vectors $x_1 \dots x_n$ is $\hat{P}y = \sum_{ij} x_i [G^{-1}]_{ij} (x_j|y)$, where $G_{ij} = (x_i|x_j)$ is Gram's matrix.

Exercise 21.3.6. Let $(\hat{D}_N f)(x) = \int_0^{2\pi} dy D_N(x-y) f(y)$, where $D_N(x)$ is the Dirichlet kernel (20.11), and $f \in L^2(0, 2\pi)$. Show that \hat{D}_N is a projector, and identify the subspace.

21.4 Unitary operators

Definition 21.4.1. A linear operator \hat{U} with domain \mathcal{H} and range in \mathcal{H} is an **isometry** if $\|\hat{U}x\| = \|x\|$ for all x . If also $\text{Ran } \hat{U} = \mathcal{H}$ the operator is **unitary**, that we now consider.

1) The conservation of the norm implies that $\text{Ker } \hat{U} = \{0\}$ i.e. \hat{U}^{-1} exists and, by the polarization identities, conservation of the inner product

$$\boxed{(\hat{U}x|\hat{U}y) = (x|y) \quad \forall x, y} \tag{21.9}$$

2) A unitary operator is bounded with norm $\|\hat{U}\| = 1$.

3) $(x|y) = (\hat{U}x|\hat{U}y) = (\hat{U}^\dagger \hat{U}x|y) \forall x, y$, then $\hat{U}^\dagger \hat{U}x = x$ for all x i.e.

$$\boxed{\hat{U}^\dagger \hat{U} = I} \tag{21.10}$$

i.e. $\hat{U}^\dagger = \hat{U}^{-1}$. \hat{U}^{-1} is a unitary operator: $\|x\| = \|\hat{U}(\hat{U}^\dagger x)\| = \|\hat{U}^\dagger x\|$ for all x .

4) If λ is an eigenvalue of \hat{U} , then $|\lambda| = 1$. Eigenvectors with different eigenvalues are orthogonal.

5) The product of unitary operators is unitary.

Exercise 21.4.2. If \hat{U} and \hat{V} are unitary then $\|\hat{U}\hat{A}\hat{V}\| = \|\hat{A}\| \forall \hat{A} \in \mathcal{B}(\mathcal{H})$.

Exercise 21.4.3. If $\{u_k\}_{k=1}^\infty$ is a complete orthonormal system and $\{q_k\}_{k=1}^\infty$ are numbers in $[0, 2\pi]$, show that $\hat{U}x = \sum_{k=1}^\infty e^{iq_k}(u_k|x)u_k$ exists for all x and defines a unitary operator.

Exercise 21.4.4. Let $\hat{H} \in \mathcal{B}(\mathcal{H})$ be self-adjoint. Show that the Cayley transform of \hat{H} , $(1 - i\hat{H})(1 + i\hat{H})^{-1}$, is well defined and is a unitary operator. What is the Cayley transform of a projector?

Exercise 21.4.5. \hat{P} is a projector; evaluate $e^{i\theta\hat{P}}$ and $(z - \hat{P})^{-1}$ ($z \neq 0, 1$).

21.5 Hilbert-Schmidt operators*

The Banach algebra $\mathcal{B}(\mathcal{H})$ of linear bounded operators on \mathcal{H} contains an important subset that is a Hilbert space.

Let $\{u_i\}_{i=1}^\infty$ be a complete orthonormal set of vectors in \mathcal{H} (it is countable for separable Hilbert spaces, and we restrict to this case). A bounded operator \hat{A} is Hilbert-Schmidt (HS) if the following sum is finite:

$$\sum_{j=1}^{\infty} \|\hat{A}u_j\|^2 < \infty \quad (21.11)$$

Proposition 21.5.1. *The finite value of the sum does not depend on the basis.*

Proof. For a basis set $\{u'_j\}$ it is (Parseval identity):

$$\|\hat{A}u_j\|^2 = \sum_k |(u'_k|\hat{A}u_j)|^2 = \sum_k |(u_j|\hat{A}^\dagger u'_k)|^2$$

The sum is absolutely convergent. A further sum on j is also absolutely convergent by hypothesis. The sums may be exchanged:

$$\sum_j \|\hat{A}u_j\|^2 = \sum_k \sum_j |(u_j|\hat{A}^\dagger u'_k)|^2 = \sum_k \|\hat{A}^\dagger u'_k\|^2$$

If $u'_j = u_j$ it is $\sum_j \|\hat{A}u_j\|^2 = \sum_k \|\hat{A}^\dagger u_k\|^2$. For the same equality: $\sum_j \|\hat{A}^\dagger u_j\|^2 = \sum_k \|\hat{A}u'_k\|^2 = \sum_k \|\hat{A}u_k\|^2$ i.e. $\sum_j \|\hat{A}u_j\|^2 = \sum_j \|\hat{A}u'_j\|^2$. \square

Remark 21.5.2. $\sum_{j=1}^\infty \|\hat{A}u_j\|^2 = \sum_{j=1}^\infty (\hat{A}u_j|\hat{A}u_j) = \sum_{j=1}^\infty (u_j|(\hat{A}^\dagger \hat{A})u_j)$.

The last (basis-independent) sum is the trace of the operator $\hat{A}^\dagger \hat{A}$: $\text{tr}(\hat{A}^\dagger \hat{A})$.

Proposition 21.5.3. $\text{HS}(\mathcal{H})$ is a normed space, with HS-norm

$$\|\hat{A}\|_2 = \sqrt{\text{tr}(\hat{A}^\dagger \hat{A})} \tag{21.12}$$

The triangle inequality follows from $\|(\hat{A} + \hat{B})u_j\|^2 \leq 2\|\hat{A}u_j\|^2 + 2\|\hat{B}u_j\|^2$.

Exercise 21.5.4. Show that

- 1) if \hat{A} is HS and \hat{B} is bounded, then $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ are HS;
- 2) $\|\hat{A}\| \leq \|\hat{A}\|_2$ (then, if $\hat{A}_n \rightarrow \hat{A}$ in HS, it is $\hat{A}_n \rightarrow \hat{A}$ in $\mathcal{B}(\mathcal{H})$).

Theorem 21.5.5. The linear space $\text{HS}(\mathcal{H})$ of Hilbert-Schmidt operators is a Hilbert space with inner product:

$$(\hat{A}|\hat{B})_{\text{HS}} = \text{tr}(\hat{A}^\dagger \hat{B}) = \sum_{j=1}^{\infty} (\hat{A}u_j|\hat{B}u_j). \tag{21.13}$$

Proof. The definition is well-posed: $|(\hat{A}u_j|\hat{B}u_j)| \leq \|\hat{A}u_j\| \|\hat{B}u_j\| \leq \frac{1}{2}\|\hat{A}u_j\|^2 + \frac{1}{2}\|\hat{B}u_j\|^2$. For HS operators the sums on the basis u_j are finite and

$$|(\hat{A}|\hat{B})_{\text{HS}}| \leq \frac{1}{2}(\|\hat{A}\|_2^2 + \|\hat{B}\|_2^2)$$

It is easily shown that (21.13) is an inner product, with HS norm (21.12).

To prove completeness, consider a Cauchy sequence \hat{A}_n :

$$\forall \epsilon > 0 \quad \exists N_\epsilon \text{ such that } \|\hat{A}_n - \hat{A}_m\|_2 \leq \epsilon^2, \quad \forall n, m > N_\epsilon$$

The inequality $\|\hat{A}\| \leq \|\hat{A}\|_2$ implies that \hat{A}_n is Cauchy in $\mathcal{B}(\mathcal{H})$: then $\hat{A}_n \rightarrow \hat{A}$ in the sup-norm, where \hat{A} is linear and bounded.

The Cauchy condition in hypothesis implies, for all $N, n, m > N_\epsilon$

$$\sum_{j=1}^N \|(\hat{A}_n - \hat{A}_m)u_j\|^2 < \epsilon^2$$

Since $\hat{A}_m u_j \rightarrow \hat{A} u_j$, it is $\sum_{j=1}^N \|(\hat{A}_n - \hat{A})u_j\|^2 < \epsilon^2$ for all $N, n > N_\epsilon$ (continuity of the norm). Then $\hat{A}_n - \hat{A} \in \text{HS}$ i.e. $\hat{A} \in \text{HS}$. □

Exercise 21.5.6.

- 1) If \hat{U} is unitary, show that $\text{U}\hat{A} = \hat{U}^\dagger \hat{A} \hat{U}$ is a unitary operator on $\text{HS}(\mathcal{H})$.

2) With \hat{B} and \hat{C} bounded, consider the following operators on HS:

$$\begin{aligned} D_{\hat{B}}\hat{A} &= [\hat{A}, \hat{B}] && \text{Derivative} \\ \hat{A} \circ \hat{C} &= \frac{1}{2}(\hat{A}\hat{C} + \hat{C}\hat{A}) && \text{Jordan product} \end{aligned}$$

Prove the properties (they justify names derivative and product):

$$[D_{\hat{B}}, D_{\hat{C}}] = D_{[\hat{C}, \hat{B}]}, \quad D_{\hat{B}}(\hat{A} \circ \hat{C}) = \hat{A} \circ D_{\hat{B}}\hat{C} + \hat{C} \circ D_{\hat{B}}\hat{A}, \quad (21.14)$$

$$(\hat{A}_1 | D_{\hat{B}} \hat{A}_2)_{\text{HS}} = (D_{\hat{B}^\dagger} \hat{A}_1 | \hat{A}_2)_{\text{HS}} \quad (\hat{A}_1 | \hat{B} \circ \hat{A}_2)_{\text{HS}} = (\hat{B}^\dagger \circ \hat{A}_1 | \hat{A}_2)_{\text{HS}} \quad (21.15)$$

$$(\hat{A} \circ \hat{B}) \circ \hat{C} - \hat{A} \circ (\hat{B} \circ \hat{C}) = \frac{1}{4}[\hat{B}, [\hat{A}, \hat{C}]] \quad (21.16)$$

21.6 Notes on spectral theory*

The section collects some results on the spectrum of bounded operators.

While the point spectrum is familiar (the eigenvalues of finite square matrices), the continuous spectrum appears in infinite dimensions, and is here introduced through the important example of the position operator.

The spectrum of a bounded linear operator is the set $\sigma(\hat{A}) = \sigma_p \cup \sigma_c \cup \sigma_r$ in \mathbb{C} , whose terms are now explained.

21.6.1 Point spectrum (the eigenvalues)

$z \in \sigma_p(\hat{A})$ if z is an eigenvalue: the equation $\hat{A}u = zu$ has solution $u \in \mathcal{H}$. Equivalent statements are: $\text{Ker}(z - \hat{A}) \neq \{0\}$ or $(z - \hat{A})^{-1}$ does not exist.

- If $\hat{A} = \hat{A}^\dagger$, then $\sigma_p(\hat{A}) \subseteq \mathbb{R}$ (thrm.21.2.6)

Example 21.6.1. If H is a Hermitian $n \times n$ matrix with eigenvalues λ_j , and $\Lambda = \max_j |\lambda_j|$, then $\|H\| = \Lambda$.

Proof. It is $H = \sum_j \lambda_j P_j$ and $1 = \sum_j P_j$, where P_j is the orthogonal projection on the subspace of eigenvectors with eigenvalue λ_j . Then $\|Hx\|^2 = \sum_j |\lambda_j|^2 \|P_j x\|^2 \leq \Lambda^2 \sum_j \|P_j x\|^2 = \Lambda^2 \|x\|^2$. Then $\|H\| \leq \Lambda$. Equality is achieved for x in the subspace of eigenvalue with maximal modulus. \square

21.6.2 Continuous spectrum (approximate eigenvalues)

The position operator

On $L^2[0, L]$, the “position” operator multiplies a function f by the function $x(t) = t$:

$$\hat{Q}f = xf, \quad \text{i.e.} \quad (\hat{Q}f)(t) = tf(t)$$

The operator is bounded, $\|\hat{Q}f\| \leq L\|f\|$, and is self-adjoint:

$$(g|\hat{Q}f) = \int_0^L dt \overline{g(t)} t f(t) = \int_0^L dt t \overline{g(t)} f(t) = (\hat{Q}g|f).$$

The eigenvalue equation $\hat{Q}f = \lambda f$ has no solution in $L^2[0, L]$: $(t - \lambda)f(t) = 0$ a.e. $t \in [0, L]$ implies $f = 0$ a.e. Absence of eigenvalues means that $\sigma_p(\hat{Q}) = \emptyset$.

We may ask if there are “approximate eigenfunctions” (also named Weyl sequence) $\|u_n\| = 1$, such that

$$\|\hat{Q}u_n - \lambda u_n\| \rightarrow 0$$

The answer is yes: given λ consider the normalized functions $u_\eta = \frac{1}{\sqrt{2\eta}} \chi_{[\lambda-\eta, \lambda+\eta]}$ and evaluate

$$\|\hat{Q}u_\eta - \lambda u_\eta\|^2 = \int_0^L dt (t - \lambda)^2 u_\eta(t)^2 = \frac{\eta^2}{3} \rightarrow 0$$

Note that the limit $\eta \rightarrow 0$ of u_η does not exist in Hilbert space (the functions do not form a Cauchy sequence). We say that λ is a generalized eigenvalue and, for vanishing η , u_η is a generalized eigenfunction. The set of such eigenvalues is the continuous spectrum. In this case $\sigma_c(\hat{Q}) = [0, L]$.

(Envisage a family $u_n \in L^2[0, L]$ such that $\lim_{n \rightarrow \infty} \|Qu_n\|_2 = L$. Then conclude that $\|Q\| = L$).

The position operator on \mathbb{R} is unbounded, and is discussed in 23.3.12.

$z \in \sigma_c(\hat{A})$ if z is a generalized eigenvalue:

$$z \notin \sigma_p(\hat{A}) \text{ and } \exists \{u_n\}, \|u_n\| = 1, \text{ such that } \lim_{n \rightarrow \infty} \|\hat{A}u_n - zu_n\| = 0.$$

1) $\{u_n\}$ is not a Cauchy sequence: $u_n \rightarrow u$ and continuity of \hat{A} would imply that u is an eigenvector and $z \in \sigma_p(\hat{A})$.

2) If $z \in \sigma_c(\hat{A})$ the resolvent $(z - \hat{A})^{-1}$ exists, but is not bounded.

Proof. Suppose that it does (then the domain is \mathcal{H} and it is bounded):

$$1 = |(u_n|(z - \hat{A})^{-1}(z - \hat{A})u_n)| \leq \|(z - \hat{A})^{-1}\| \|zu_n - \hat{A}u_n\|$$

since for $n \rightarrow \infty$ the last factor is zero, the other factor cannot be finite. □

3) If $z \in \sigma_c(\hat{A})$ then $\bar{z} \in \sigma_c(\hat{A}^\dagger)$ and $\{0\} = \text{Ker}(\bar{z} - \hat{A}^\dagger) = \text{Ran}(z - \hat{A})^\perp$ i.e. $\mathcal{H} = \mathcal{D}(z - \hat{A})^{-1}$. Therefore, either $\mathcal{D}(z - \hat{A})^{-1} = \mathcal{H}$ (but the resolvent is not bounded) or $\mathcal{D}(z - \hat{A})^{-1}$ is a dense in \mathcal{H} .

4) Since $|(u_n|(\hat{A} - z)u_n)| \leq \|\hat{A}u_n - zu_n\| \rightarrow 0$, it is $z = \lim_{n \rightarrow \infty} (u_n|\hat{A}u_n)$.

• If $\hat{A} = \hat{A}^\dagger$, then $\sigma_c(\hat{A}) \subseteq \mathbb{R}$, and $|z| \leq \|\hat{A}\|$.

21.6.3 Residual spectrum

The third set is the residual spectrum $\sigma_r(\hat{A})$: the set of values z such that the resolvent $(z - \hat{A})^{-1}$ exists but the domain is not dense in \mathcal{H} .

• If $\hat{A} = \hat{A}^\dagger$ then $\sigma_r(\hat{A}) = \emptyset$.

Proof: existence of the resolvent implies $\{0\} = \text{Ker}(z - \hat{A}) = \text{Ran}(z - \hat{A})^\perp$ i.e. $\text{Ran}(z - \hat{A})$ is dense in \mathcal{H} . □

21.6.4 Resolvent set

$\rho(\hat{A}) = \mathbb{C} / \sigma(\hat{A})$ is the resolvent set: it contains the values z such that the resolvent operator $(z - \hat{A})^{-1}$ exists and belongs to $\mathcal{B}(\mathcal{H})$.

1) The resolvent set is open (proof omitted).

2) $\hat{R}(z)$ is an analytic function of $z \in \rho(\hat{A})$ i.e. it admits norm-convergent power expansions $R(z) = \sum_k \hat{R}_k(z - z_0)^k$ with operator coefficients on any disk in the resolvent set.

Example 21.6.2. On the space of square-summable sequences $\ell^2(\mathbb{C})$ consider the linear operator

$$(\hat{T}\mathbf{u})_k = u_{k+1} - u_k, \quad k = 0, 1, 2, \dots$$

It is bounded: $\|\hat{T}\mathbf{u}\|^2 = \sum_{k=1}^\infty |u_{k+1} - u_k|^2 \leq 4\|\mathbf{u}\|^2$: then $\|\hat{T}\| \leq 2$.

The eigenvalue equation $\hat{T}\mathbf{u} = z\mathbf{u}$ is $u_{k+1} = (z + 1)u_k$, which is solved: $u_k = (z + 1)^k u_0$. We distinguish three cases:

• *The eigenvector belongs to ℓ^2 if $\sum_{k=0}^\infty |z + 1|^{2k} < \infty$, i.e. $|z + 1| < 1$. The point spectrum is the set of proper eigenvalues in the open unit disk centred in $z = -1$: $\sigma_p(\hat{T}) = \{|z + 1| < 1\}$. The operator $(z - \hat{T})$ is not invertible.*

Since there is a sequence of proper eigenvalues with limit point -2 , the sup-norm is $\|\hat{T}\| = 2$.

• *The boundary eigenvalues are $z = -1 + e^{i\theta}$, $\theta \in [0, 2\pi]$, with eigenvectors $u_k = u_0 e^{ik\theta}$ that are not ℓ^2 . However, each eigenvalue admits the approximate eigenvectors in ℓ^2 : $u_{\epsilon,k} = e^{ik\theta - \epsilon k}$. It is $\|\hat{T}u_\epsilon - (-1 + e^{i\theta})u_\epsilon\|^2 = \sum_{k=0}^\infty |u_{\epsilon,k+1} - e^{i\theta}u_{\epsilon,k}|^2 = \sum_{k=0}^\infty e^{-2\epsilon k} |e^{-\epsilon} - 1|^2 =$*

$|e^{-\epsilon} - 1| \|u_\epsilon\|^2$. Then $\sigma_C(\hat{T}) = \{z : |z + 1| = 1\}$ is the continuous spectrum. The resolvent operator $(z - \hat{T})^{-1}$ exists (but is unbounded).

• The complementary set is the resolvent set $\rho(\hat{T}) = \{z : |z + 1| > 1\}$. It is an open set. For such values, the eigenvectors $u_k = (z + 1)^k u_0$ are not ℓ^2 and cannot be modified to approximate eigenvectors. The resolvent operator $(z - \hat{T})^{-1}$ exists (and is bounded).

21.6.5 Spectrum of bounded self-adjoint operators

For a bounded self-adjoint operator \hat{A} the spectrum is a real closed set in the interval $[-\|\hat{A}\|, \|\hat{A}\|]$, with empty residual subset. The eigenvectors span the Hilbert subspace \mathcal{H}_p , with orthogonal complement \mathcal{H}_c : $\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_c$. Each subspace is invariant for the action of the self-adjoint operator.

i) if $\lambda_k \in \sigma_p$ and $\lambda \in \sigma_c$, then $(u_k | u_n^\lambda) \rightarrow 0$ for $n \rightarrow \infty$.

Proof: $|\lambda_k - \lambda| |(u_k | u_n^\lambda)| = |(\hat{A} - \lambda) u_k | u_n^\lambda| = |(u_k | (\hat{A} - \lambda) u_n^\lambda)| \leq \|(\hat{A} - \lambda) u_n^\lambda\| \rightarrow 0$.

It follows that the generalized eigenvectors can be taken in \mathcal{H}_c .

ii) if $\lambda \neq \mu \in \sigma_c$ then, $(u_n^\lambda | u_m^\mu) \rightarrow 0$.

Proof: $(\hat{A} - \lambda) u_n^\lambda | u_m^\mu = (u_n^\lambda | (\hat{A} - \mu) u_m^\mu) + (\lambda - \mu) (u_n^\lambda | u_m^\mu)$. Then $|(\lambda - \mu) (u_n^\lambda | u_m^\mu)| \leq \|(\hat{A} - \lambda) u_n^\lambda\| + \|(\hat{A} - \mu) u_m^\mu\| \rightarrow 0$ for $m, n \rightarrow \infty$.

Let us conclude by quoting the spectral theorem. More is found in Sect.23.4.

Theorem 21.6.3 (The spectral theorem³). *If \hat{A} is bounded and self-adjoint, $x \in \mathcal{H}$, and $\mathcal{C}(\sigma)$ is the set of continuous real functions f on $\sigma(\hat{A})$ then, by the Riesz-Markov-Kakutani theorem, for every positive linear functional $f \rightarrow (x | f(\hat{A})x)$ there exists a measure $\mu_x(\lambda)$ on $\sigma(\hat{A})$ such that*

$$(x | f(\hat{A})x) = \int_{\sigma} f(\lambda) d\mu_x(\lambda)$$

In general the measure decomposes into $\mu_x = \mu_{pp} + \mu_{ac} + \mu_{sc}$, the pure point, the absolutely continuous, and the singular continuous measures. The first one is concentrated on points (the eigenvalues), the absolutely continuous is defined by the existence of a Lebesgue integrable function such that $d\mu_{ac}(\lambda) = m_x(\lambda) d\lambda$. The singular continuous is supported on Cantor-like sets and is a rare occurrence (an example is the Hofstadter butterfly in fig.20.10).

One may wonder what is the relation between the a.c. measure and the generalized eigenvectors⁴. Certain operators have their answer in the space of distributions.

³ from Reed and Simon, Functional Analysis, Academic Press.

⁴ A (difficult) answer is provided by M. Christ, A. Kiselev and Y. Last, Approximate eigenvectors and spectral theory (2000), https://www.researchgate.net/publication/2585555_Approximate_Eigenvectors_and_Spectral_Theory

Example 21.6.4. The following operator on $L^2[-1, 1]$

$$(\hat{T}f)(t) = \begin{cases} tf(t) & \text{if } 0 \leq t \leq 1 \\ 0 & \text{if } -1 \leq t < 0 \end{cases}$$

is bounded and self-adjoint. The eigenvalue equation $\hat{T}f = \lambda f$ has solution $\lambda = 0$ for any function f which is (a.e.) zero for $t > 0$. The values $0 < \lambda \leq 1$ do not allow for a proper eigenfunction and belong to the continuum spectrum with generalized eigenfunctions. Therefore $\sigma(\hat{T}) = \{0\} \cup (0, 1]$. The orthogonal eigenspaces are $M_0 = \{f | f(t) = 0 \ t > 0\}$ and $M_{(0,1]} = \{f | f(t) = 0 \ t < 0\}$, $M_0 \oplus M_{(0,1]} = L^2[-1, 1]$.

21.7 The (unbounded) derivative operator

In $L^2[a, b]$ the operator $\hat{P}f = -if'$ requires that f' exists and is also square-integrable. \hat{P} is an important unbounded operator. The domain is restricted, and the spectrum is pure point but with no upper bound.

To properly define it, we introduce a useful set: a function f is *absolutely continuous* on $[a, b]$ (f is AC $[a, b]$) if there is an integrable function h such that:

$$f(x) = f(a) + \int_a^x dx' h(x'), \quad x \in (a, b).$$

The functions AC $[a, b]$ are continuous and differentiable: $f' = h$ a.e. and form a linear subset in $\mathcal{L}^p(a, b)$ for all $p \geq 1$. If h is a continuous function, by the theorem of the mean: $f'(x) = h(x)$.

The “linear momentum” operator⁵

$$(\hat{P}f)(x) = -if'(x) \tag{21.17}$$

acts on functions AC $[a, b]$ such that $f' \in \mathcal{L}^2[a, b]$.

If f_1 and f_2 are such functions, integration by parts gives:

$$(f_1 | \hat{P}f_2) = -i \int_a^b dx \overline{f_1(x)} f_2'(x) = -i \overline{f_1} f_2 \Big|_a^b + (\hat{P}f_1 | f_2).$$

The operator is symmetric provided that the boundary terms cancel. This is achieved if the domain is restricted by appropriate boundary conditions (b.c.). These are important choices:

- $f(b) = f(a) = 0$ (Dirichlet b.c.)
- $f(b) = \pm f(a)$ (periodic/antiperiodic b.c.)

⁵ physicists introduce Planck's constant, $\hat{P}f = -i\hbar f'$.

- $f(b) = e^{i\theta} f(a)$ (Bloch b.c. with $\theta \in \mathbb{R}$).

They produce three different definitions of \hat{P} (same action but different domains where it is symmetric).

With periodic b.c. the operator \hat{P} has a complete orthonormal set of eigenfunctions $\hat{P}u_k = 2\pi/(b-a)ku_k$, $k \in \mathbb{Z}$, given by the Fourier basis (20.20).

Chapter 22

Unitary Groups

If the Hilbert space is the mathematical stage for quantum mechanics, continuous symmetries are main actors in the play, and correspond to unitary operators¹. Of special importance are the groups that depend continuously on one parameter, like rotations around a given axis, or translations along a given direction. They correspond to special families of unitary operators. The following theorem is very important and useful (it is stated without proof²).

22.1 Stone's theorem

Definition 22.1.1. A family of unitary operators $\{\hat{U}_s, s \in \mathbb{R}\}$, is a **strongly continuous one-parameter unitary group** if:

$$\hat{U}_s \hat{U}_{s'} = \hat{U}_{s+s'}$$
$$\lim_{s \rightarrow 0} \|\hat{U}_s x - x\| = 0 \quad \forall x \in \mathcal{H}.$$

It is clear that the group is Abelian, $\hat{U}_0 = I$ and $\hat{U}_s^{-1} = \hat{U}_{-s}$. For such groups, the following fundamental theorem holds

Theorem 22.1.2 (Stone's theorem). *Let \hat{U}_s be a strongly continuous one-parameter unitary group on a Hilbert space. There is a self-adjoint operator \hat{H} such that*

$$\hat{U}_s = e^{-is\hat{H}} \tag{22.1}$$

¹ Discrete symmetries may correspond also to anti-unitary (i.e. antilinear and norm conserving) operators. An example is time-reversal.

² see for example: K. Schmüdgen, *Unbounded Self-adjoint Operators on Hilbert Space*, Springer 2012.

\hat{H} is the **generator** of the group, with domain

$$\mathcal{D}(\hat{H}) = \{x \in \mathcal{H} \text{ such that } \lim_{s \rightarrow 0} \frac{\hat{U}_s x - x}{-is} \text{ exists}\},$$

and $\hat{H}x$ is precisely the above limit.

In this example we consider a bounded self-adjoint operator and generate a unitary group.

Example 22.1.3. If $\hat{H} \in \mathcal{B}(\mathcal{H})$ and $\hat{H} = \hat{H}^\dagger$, then $\hat{U}_t = e^{-it\hat{H}}$, $t \in \mathbb{R}$, are unitary operators and form a one-parameter strongly continuous group.

Proof. The sequence $\hat{U}_n(t) = \sum_{k=0}^n (-it\hat{H})^k / k!$ converges in $\mathcal{B}(\mathcal{H})$ for all t .

- It is $\hat{U}_n(t)^\dagger = \hat{U}_n(-t)$; the adjunction is a continuous map, then $\hat{U}_t^\dagger = \hat{U}_{-t}$.
- The operators form a 1-parameter group: $\hat{U}_t \hat{U}_s = \hat{U}_{t+s}$.
- \hat{U}_t is isometric: $(\hat{U}_t x | \hat{U}_t y) = (\hat{U}_t^\dagger \hat{U}_t x | y) = (x | y)$.
- Given $y \in \mathcal{H} \exists x$ s.t. $\hat{U}_t x = y$? It is $\hat{U}_{-t} y$. Then $\text{Ran } \hat{U}_t = \mathcal{H}$ (\hat{U}_t is unitary).
- Strong continuity: $\|\hat{U}_n(t)x - x\| \leq \sum_{k=1}^n \frac{|t|^k}{k!} \|\hat{H}\|^k \|x\| \leq (e^{|t|\|\hat{H}\|} - 1)\|x\| \forall n$. Continuity of the norm replaces $\hat{U}_n x$ with $\hat{U}x$. The limit $t \rightarrow 0$ gives 0. □

22.2 Weyl operators*

Two important families of unitary operators on $L^2(\mathbb{R}^3)$ are: *translations by vectors* $\mathbf{a} \in \mathbb{R}^3$:

$$(\hat{U}_{\mathbf{a}} f)(\mathbf{x}) = f(\mathbf{x} - \mathbf{a}), \quad \hat{U}_{\mathbf{a}} \hat{U}_{\mathbf{a}'} = \hat{U}_{\mathbf{a}+\mathbf{a}'} \tag{22.2}$$

multiplication by a phase factor with vector $\mathbf{p} \in \mathbb{R}^n$:

$$(\hat{V}_{\mathbf{p}} f)(\mathbf{x}) = e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}} f(\mathbf{x}), \quad \hat{V}_{\mathbf{p}} \hat{V}_{\mathbf{p}'} = \hat{V}_{\mathbf{p}+\mathbf{p}'} \tag{22.3}$$

Planck's constant \hbar is here introduced to give \mathbf{x} , \mathbf{a} the physical dimension of length, and \mathbf{p} the dimension of momentum.

The translations along a fixed direction $\hat{U}_{\mathbf{a}n}$, $a \in \mathbb{R}$, and phase multiplications $\hat{V}_{\mathbf{p}n}$, $p \in \mathbb{R}$, are strongly continuous one-parameter unitary groups³. Stone's theorem implies the existence of self-adjoint generators.

³ The set $\mathcal{C}_c(X)$ of continuous functions with compact support in X is dense in $L^p(X)$, $p \geq 1$. Therefore, given $f \in \mathcal{L}^2(\mathbb{R}^3)$ and $\epsilon > 0$ there is $g \in \mathcal{C}_c(\mathbb{R})$ such that $\|f - g\|_2 < \epsilon$.
 $\|\hat{U}_{\mathbf{a}} f - f\|_2 = \|(\hat{U}_{\mathbf{a}}(f - g) - (f - g) + (\hat{U}_{\mathbf{a}} g - g))\|_2 \leq \|(\hat{U}_{\mathbf{a}}(f - g))\|_2 + \|f - g\|_2 + \|(\hat{U}_{\mathbf{a}} g - g)\|_2 \leq 2\epsilon + \|\hat{U}_{\mathbf{a}} g - g\|_2$.
 The last term, squared, is: $\int |g(\mathbf{x} - \mathbf{a}) - g(\mathbf{x})|^2 d\mathbf{x} \rightarrow 0$ as $\mathbf{a} \rightarrow 0$ because of continuity and the integral is on a finite-measure set.

On the dense set $\mathcal{S}(\mathbb{R}^3)$ (\mathcal{C}^∞ rapidly decreasing functions) a Taylor expansion gives:

$$(\hat{U}_{\mathbf{a}\mathbf{n}}\varphi)(\mathbf{x}) = f(\mathbf{x} - \mathbf{a}\mathbf{n}) = \varphi(\mathbf{x}) + (-\mathbf{a}\mathbf{n}\cdot\nabla)\varphi(\mathbf{x}) + \frac{1}{2!}(-\mathbf{a}\mathbf{n}\cdot\nabla)^2\varphi(\mathbf{x}) + \dots$$

Therefore, the generator of translations with direction \mathbf{n} is the self-adjoint operator $\mathbf{n}\cdot\hat{\mathbf{P}}$ whose restriction to $\mathcal{S}(\mathbb{R}^3)$ is $-i\hbar\mathbf{n}\cdot\nabla$. Then:

$$\hat{U}_{\mathbf{a}} = \exp\left[-\frac{i}{\hbar}\mathbf{a}\cdot\hat{\mathbf{P}}\right], \quad \hat{P}_k\varphi = -i\hbar\frac{\partial\varphi}{\partial x_k}$$

\hat{P}_k is the generator of translations along the direction k . Momentum operators are self-adjoint on a dense domain in $L^2(\mathbb{R}^3)$ and act as derivatives on the subset $\mathcal{S}(\mathbb{R}^3)$. The property $\hat{U}_{\mathbf{a}}\hat{U}_{\mathbf{a}'} = \hat{U}_{\mathbf{a}'}\hat{U}_{\mathbf{a}}$ for all vectors \mathbf{a} and \mathbf{a}' implies the commutation relation $[\hat{P}_i, \hat{P}_j] = 0$.

The generator of the one-parameter group $(\hat{V}_{p\mathbf{n}}f)(\mathbf{x}) = \exp(-\frac{i}{\hbar}p\mathbf{n}\cdot\mathbf{x})f(\mathbf{x})$ is the (unbounded) self-adjoint operator $\mathbf{n}\cdot\hat{\mathbf{Q}}$, and

$$\hat{V}_{\mathbf{p}} = \exp\left[-\frac{i}{\hbar}\mathbf{p}\cdot\hat{\mathbf{Q}}\right], \quad (\hat{Q}_i f)(\mathbf{x}) = x_i f(\mathbf{x}).$$

The operators \hat{Q}_i are self-adjoint and commute on a dense domain in $L^2(\mathbb{R}^3)$. The generators \hat{Q}_i and \hat{P}_i $i = 1, 2, 3$ form *Heisenberg's algebra*:

$$[\hat{Q}_i, \hat{Q}_j] = 0, \quad [\hat{P}_i, \hat{P}_j] = 0, \quad [\hat{Q}_i, \hat{P}_j] = i\hbar\delta_{ij}$$

The first two commutation relations correspond to the fact that the unitary groups are Abelian. The mixed commutator, proportional to the identity operator, reflects a simple relation among the groups (Weyl's commutation relation):

$$\hat{V}_{\mathbf{p}}\hat{U}_{\mathbf{a}} = e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{a}}\hat{U}_{\mathbf{a}}\hat{V}_{\mathbf{p}} \tag{22.4}$$

Proof. $(\hat{V}_{\mathbf{p}}\hat{U}_{\mathbf{a}}f)(\mathbf{x}) = e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}(\hat{U}_{\mathbf{a}}f)(\mathbf{x}) = e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}f(\mathbf{x} - \mathbf{a}) = e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{a}}(\hat{V}_{\mathbf{p}}f)(\mathbf{x} - \mathbf{a})$
 $= e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{a}}(\hat{U}_{\mathbf{a}}\hat{V}_{\mathbf{p}}f)(\mathbf{x}).$ □

Exercise 22.2.1. Show that the translation operator $(\hat{U}_a f)(x) = f(x - a)$ does not have eigenvectors in $L^2(\mathbb{R})$. (Hint: a periodic function cannot be integrable).

22.3 Dilations and Virial property*

On $L^2(\mathbb{R})$ the operators

$$(\hat{D}_\lambda f)(x) = e^{-\lambda/2}f(e^{-\lambda}x), \quad \lambda \in \mathbb{R} \tag{22.5}$$

are a strongly continuous one-parameter unitary group. Expansions in small λ on functions in the dense subspace $\mathcal{S}(\mathbb{R})$ (see chapter on Schwartz space) give the generator

$$\hat{D}_\lambda = \exp(-i\lambda\hat{D}), \quad \hat{D} = \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})$$

Show that

$$\hat{D}_\lambda^\dagger \hat{Q} \hat{D}_\lambda = e^\lambda \hat{Q}, \quad \hat{D}_\lambda^\dagger \hat{P} \hat{D}_\lambda = e^{-\lambda} \hat{P}$$

Scale transformations are related to the *Virial property*. This is illustrated for the anharmonic oscillator,

$$\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{1}{2} k^2 \hat{Q}^2 + b \hat{Q}^4, \quad b > 0$$

If $\hat{H}\psi = E\psi$ with $\|\psi\| = 1$, then $E = \frac{1}{2m} \langle \hat{P}^2 \rangle + \frac{1}{2} k^2 \langle \hat{Q}^2 \rangle + b \langle \hat{Q}^4 \rangle$, where $E = \langle \hat{H} \rangle = (\psi | \hat{H} \psi)$ etc. are average values. The action of a scale transformation is: $\langle \hat{D}_\lambda^\dagger \hat{H} \hat{D}_\lambda \rangle = e^{-2\lambda} \frac{1}{2m} \langle \hat{P}^2 \rangle + e^{2\lambda} \frac{1}{2} k^2 \langle \hat{Q}^2 \rangle + b e^{4\lambda} \langle \hat{Q}^4 \rangle$. The linear expansion in λ is:

$$-\frac{1}{m} \langle \hat{P}^2 \rangle + k^2 \langle \hat{Q}^2 \rangle + 4b \langle \hat{Q}^4 \rangle = i(\psi | [\hat{D}, \hat{H}] \psi) = 0$$

The right hand side is zero for an eigenvector. An identity is obtained among the averaged terms that contribute to the total energy.

If $b = 0$, one gets the equality of kinetic and potential energy of the harmonic oscillator, $\langle \frac{1}{2m} \hat{P}^2 \rangle = \langle \frac{1}{2} k^2 \hat{Q}^2 \rangle$, that is used e.g. in the theory of specific heats.

22.4 Space rotations, SO(3)

Space rotations act on vectors in \mathbb{R}^3 as 3×3 real matrices R that preserve lengths, $RR^t = I_3$, and orientation, $\det R = 1$. They form the group $SO(3)$. Being unitary, rows or columns of R are orthogonal and normalized, and the eigenvalues are on the unit circle. They solve the real cubic equation $\det(zI_3 - R) = 0$, that necessarily has a real zero equal to one.

The unit eigenvalue corresponds to the real invariant eigenvector: $R\mathbf{n} = \mathbf{n}$.

The other pair of eigenvalues may be $1, 1$ or $-1, -1$ (then R is the identity matrix or a diagonal matrix describing two reflections) or $e^{\pm i\varphi}$ with eigenvectors $\mathbf{u} \pm i\mathbf{v}$ making with \mathbf{n} an orthogonal set in \mathbb{C}^3 . This implies that $\mathbf{n}, \mathbf{u}, \mathbf{v}$ are orthogonal in \mathbb{R}^3 . The eigenvalue equation $R(\mathbf{u} \pm i\mathbf{v}) = e^{\pm i\varphi}(\mathbf{u} \pm i\mathbf{v})$ i.e.

$$R\mathbf{u} = \mathbf{u} \cos \varphi - \mathbf{v} \sin \varphi$$

$$R\mathbf{v} = \mathbf{u} \sin \varphi + \mathbf{v} \cos \varphi$$

shows that the action of R on the two vectors is to rotate them in the plane perpendicular to \mathbf{n} . For the rotation to be anticlockwise, the orientation $\mathbf{n} = \mathbf{v} \times \mathbf{u}$ is chosen. The trace of the matrix gives easy access to the angle of rotation:

$$\text{tr}R = 1 + 2 \cos \varphi$$

Every vector \mathbf{x} can be expanded in the orthonormal basis: $\mathbf{x} = x_n \mathbf{n} + x_u \mathbf{u} + x_v \mathbf{v}$ where $x_n = \mathbf{x} \cdot \mathbf{n}$ etc. The action of R is:

$$\begin{aligned} R\mathbf{x} &= x_n \mathbf{n} + x_u (\mathbf{u} \cos \varphi - \mathbf{v} \sin \varphi) + x_v (\mathbf{u} \sin \varphi + \mathbf{v} \cos \varphi) \\ &= x_n \mathbf{n} + (x_u \mathbf{u} + x_v \mathbf{v}) \cos \varphi + (x_v \mathbf{u} - x_u \mathbf{v}) \sin \varphi \\ &= x_n \mathbf{n} + (\mathbf{x} - x_n \mathbf{n}) \cos \varphi + \mathbf{n} \times \mathbf{x} \sin \varphi \\ &= \mathbf{x} \cos \varphi + (1 - \cos \varphi) (\mathbf{n} \cdot \mathbf{x}) \mathbf{n} + \mathbf{n} \times \mathbf{x} \sin \varphi \end{aligned}$$

Exercise 22.4.1. Write the rotation as a matrix on the column vector $(x, y, z)^t$.

The invariant unit vector \mathbf{n} identifies the rotation axis. This vector and the rotation angle φ measured anticlockwise, are a parametrization of $\text{SO}(3)$. The expansion for an infinitesimal angle provides the neighbourhood of the identity matrix, which is very instructive

$$R\mathbf{x} = \mathbf{x} + \mathbf{n} \times \mathbf{x} \delta\varphi + \dots = (I_3 + \delta\varphi \mathbf{n} \cdot \mathbf{A} + \dots) \mathbf{x}$$

$$A_1 = \begin{bmatrix} 00 & 0 \\ 00 & -1 \\ 01 & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 01 \\ 0 & 00 \\ -100 \end{bmatrix}, \quad A_3 = \begin{bmatrix} 0 & -10 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (22.6)$$

The rotations with same invariant vector form a commutative subgroup:

$$R(\mathbf{n}\varphi_1)R(\mathbf{n}\varphi_2) = R(\mathbf{n}(\varphi_1 + \varphi_2)) \quad (22.7)$$

If one angle is infinitesimal: $R(\mathbf{n}\varphi)(I_3 + \delta\varphi \mathbf{n} \cdot \mathbf{A} + \dots) = R(\mathbf{n}(\varphi + \delta\varphi))$. Since the factors can be exchanged, the matrices $R(\mathbf{n}\varphi)$ commute with $\mathbf{n} \cdot \mathbf{A}$ (then, they have the same eigenvectors). Moreover, in the limit $\delta\varphi$ to zero:

$$\frac{d}{d\varphi} R(\mathbf{n}\varphi) = (\mathbf{n} \cdot \mathbf{A}) R(\mathbf{n}\varphi) \quad (22.8)$$

with the initial condition $R(0) = I_3$. Since factors commute, the solution is

$$R(\mathbf{n}\varphi) = e^{\varphi \mathbf{n}\cdot\mathbf{A}} \tag{22.9}$$

The matrix $\mathbf{n}\cdot\mathbf{A}$ is the *generator* of rotations along the direction \mathbf{n} . The three matrices A_i are the generators of rotations around the three coordinate directions, and are a *basis* for antisymmetric matrices.

Real antisymmetric matrices form a linear space that is closed under the operation $A, A' \rightarrow [A, A']$. The commutator is a Lie product⁴, and the linear space with Lie product is the *Lie algebra* $so(3)$ of the $SO(3)$ group. Because A_i are a basis, the Lie product of two basis matrices is expanded in the basis:

$$[A_i, A_j] = \epsilon_{ijk} A_k \tag{22.10}$$

The coefficients⁵ ϵ_{ijk} are the *structure constants* of $so(3)$ and characterize the rotation group.

The **Cayley-Hamilton theorem** states that a $n \times n$ matrix is a zero of its characteristic polynomial: if $\det(z - M) = z^n - a_1 z^{n-1} + \dots + (-1)^n a_n$ then:

$$M^n - a_1 M^{n-1} + \dots + (-1)^n \det M = 0$$

The statement shows that M^n is a linear combination of M^{n-1}, \dots, M, I . But then also M^{n+1} and higher powers are combinations of powers less than n . In particular, there are coefficients e_k such that $\exp(M) = e_1 M^{n-1} + \dots + e_n I$.

For a rotation matrix R :

$$e^{\varphi(\mathbf{n}\cdot\mathbf{A})} = \alpha I_3 + \beta(\mathbf{n}\cdot\mathbf{A}) + \gamma(\mathbf{n}\cdot\mathbf{A})^2$$

The coefficients are found by acting the matrix identity on the three eigenvectors of R , that are also eigenvectors of $\mathbf{n}\cdot\mathbf{A}$ with eigenvalues $0, \pm i$:

$$1 = \alpha, \quad e^{\pm i\varphi} = \alpha \pm i\beta - \gamma$$

The general expression of a rotation matrix is re-obtained:

$$R(\mathbf{n}\varphi) = I_3 + \sin \varphi(\mathbf{n}\cdot\mathbf{A}) + (1 - \cos \varphi)(\mathbf{n}\cdot\mathbf{A})^2 \tag{22.11}$$

⁴ In a linear space X , a Lie product is a bilinear map $* : X \times X \rightarrow X$ such that $x * x = 0, x * y = -y * x, (x * y) * z + (y * z) * x + (z * x) * y = 0$ (Jacobi property).

⁵ $\epsilon_{123} = 1$ and cyclic, $\epsilon_{213} = -1$ and cyclic, zero otherwise. Recall that the vector product of two vectors is $(\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk} a_j b_k$, the determinant of a 3×3 matrix is $\det M = \epsilon_{ijk} M_{1i} M_{2j} M_{3k}$. A useful sum is $\epsilon_{ijk} \epsilon_{rsk} = \delta_{ir} \delta_{js} - \delta_{is} \delta_{jr}$ (repeated indices are summed).

The exponential form (22.9) shows that a rotation matrix is univocally identified by a vector $\mathbf{n}\varphi$ in the ball of radius π . The center is the unit of the group. A diameter corresponds to the subgroup of rotations with same rotation axis; the two opposite points $\pm\mathbf{n}\pi$ at the surface give the same rotation and must be identified. The diameter is actually a circle. Therefore, the manifold of parameters is a sphere with opposite points at the surface being identified. The identification makes the manifold doubly connected: two rotations (two points A, B in the sphere) may be connected by two inequivalent paths (one path cannot be continuously deformed into the other). A choice is: the chord AB; the other choice is the path that joins A to a surface point $C = C'$ (antipode) and continues to B.

Example 22.4.2. Find the angle and the invariant vector of the rotation

$$R = e^A, \quad A = \begin{bmatrix} 0 & 3 & 1 \\ -30 & -5 & \\ -15 & 0 & \end{bmatrix}.$$

$A = -A^t$ is normal⁶ and has the same eigenvectors of R . If z is an eigenvalue of A , then e^z is an eigenvalue of R . The invariant vector solves $A\mathbf{n} = 0$:

$$\begin{bmatrix} 0 & 3 & 1 \\ -30 & -5 & \\ -15 & 0 & \end{bmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} = 0 \Rightarrow \mathbf{n} = \pm \frac{1}{\sqrt{35}} \begin{pmatrix} 5 \\ 1 \\ -3 \end{pmatrix} \quad (22.12)$$

The eigenvalues of A solve $0 = \det(zI_3 - A) = z^3 + 35z$. They are $0, \pm i\sqrt{35}$. The angle of rotation is therefore $\sqrt{35}$ (mod. 2π).

Since the rotation angle is positive if anticlockwise with respect to the direction of \mathbf{n} , we must decide the sign of \mathbf{n} . This can be done by checking the infinitesimal rotation of a conveniently chosen vector: a rotation with same axis but infinitesimal angle is $I_3 + \frac{\epsilon}{\sqrt{35}}A + \dots$. The vector $\mathbf{v} = (0, 0, 1)^t$ transforms to $\mathbf{v} + \delta\mathbf{v}$ where

$$\delta\mathbf{v} = \frac{\epsilon}{\sqrt{35}} \begin{pmatrix} 1 \\ -5 \\ 0 \end{pmatrix} = \epsilon \mathbf{n} \times \mathbf{v}$$

provided that \mathbf{n} is chosen with the upper sign in (22.12).

⁶ A square matrix is normal if it commutes with the adjoint. The eigenvectors of a normal matrix are orthogonal.

22.4.1 SU(2)

More fundamental than SO(3) for the theory of rotations is the group SU(2) of unitary 2×2 complex matrices, $U^\dagger U = I$ with $\det U = 1$:

$$U = \begin{bmatrix} z & w \\ -\bar{w} & \bar{z} \end{bmatrix}, \quad |z|^2 + |w|^2 = 1 \quad (22.13)$$

The parameters span the surface of the unit sphere in \mathbb{R}^4 , which is simply connected. With $\operatorname{Re} z = \cos(\varphi/2)$ and $\operatorname{Im}^2 z + |w|^2 = \sin^2(\varphi/2)$, another parametrization of SU(2) is obtained:

$$U(\mathbf{n}\varphi) = \cos \frac{\varphi}{2} - i \mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{\varphi}{2} \quad (22.14)$$

σ_i are the Pauli matrices (16.1) and \mathbf{n} is a unit vector. It is simple to check that the expression corresponds to the exponential representation:

$$U(\mathbf{n}\varphi) = e^{-\frac{i}{2}\varphi \mathbf{n} \cdot \boldsymbol{\sigma}} \quad (22.15)$$

The generators $\sigma_i/2$ are a basis for traceless Hermitian 2×2 matrices, which is the Lie algebra $su(2)$ of SU(2), with Lie product $H, H' \rightarrow -i[H, H']$. The structure constants are the same of $so(3)$:

$$-i \left[\frac{\sigma_i}{2}, \frac{\sigma_j}{2} \right] = \epsilon_{ijk} \frac{\sigma_k}{2} \quad (22.16)$$

The exponential function maps the Lie algebra to the Lie group:

$$\exp : su(2) \rightarrow SU(2).$$

Despite the diversity of SO(3) and SU(2), their exponential representations are formally identical: only a replacement of the basis matrices changes one into another, the structure constants being the same.

For SU(2) the parameter space is the ball in \mathbb{R}^3 of radius 2π . In this case, all “surface” points correspond to the single matrix of inversion: $U(\pm \mathbf{n}2\pi) = -1$. Each diameter of the ball is a 1-parameter subgroup with end-points (matrices) $\pm \mathbf{n}2\pi$ in common with all diameters. The parametrization (22.13) of SU(2) matrices as points of the surface of the unit sphere in \mathbb{R}^4 ($|z|^2 + |w|^2 = 1$) manifestly shows that the manifold is *simply connected*: this makes SU(2) more fundamental (covering group) than SO(3).

Exercise 22.4.3. Show that $U^\dagger \boldsymbol{\sigma} U = R\boldsymbol{\sigma}$, $R \in SO(3)$. Therefore $\pm U$ correspond to the same R matrix.

22.4.2 Representations

In physics, space rotations are a subgroup of the Galilei and of the Lorentz groups of symmetries of physical laws in Newtonian or relativistic physics.

An observer O is specified by an orthonormal frame \mathbf{e}_k , which can be identified as rigid rulers for measuring positions, at right angles, with origin where O resides. A rotated observer O' is another orthonormal frame \mathbf{e}'_k with same origin and orientation. A point P has coordinates x'_k linked by a rotation matrix to the coordinates measured by O : $x'_k = R_{kj}x_j$.

Suppose that O and O' measure in every point some quantity (a field). In the simplest case the quantity is a number (a scalar) that is a property of the point. O and O' measure two scalar fields f and f' , and the values of the two fields at the same physical point P (of coordinates x and x') must be the same: $f(x) = f'(x')$ i.e.

$$\boxed{f'(x) = f(R^{-1}x)} \quad (22.17)$$

If they measure a vector field (for example a force field), they measure a physical arrow at each point. Since they use rotated frames, the components of the arrow at a point are different: $\sum_k V_k(x)\mathbf{e}_k = \sum_k V'_k(x')\mathbf{e}'_k$ i.e.

$$\boxed{V'_k(x) = R_{kj}V_j(R^{-1}x)} \quad (22.18)$$

The two laws describe the transformation of a scalar field and a vector field under rotations. A spinor 1/2 field is a two component complex field that transforms with a $SU(2)$ rotation:

$$\boxed{\psi'_a(x) = U(R)_{ab}\psi_b(R^{-1}x)} \quad (22.19)$$

If the (scalar, spinor, vector or whatever) fields F and F' measured by O and O' are thought of as points in the *same* functional space, the rotation of coordinates R induces a map $U_R : F \rightarrow F'$. Since fields can be linearly combined, the map is asked to be linear. Moreover, if two rotations R and R' are done in the order, the observer O'' is linked to O by $x'' = R'Rx$, and thus $F'' = U_{R'R}F$ i.e. maps form a **linear representation** of the rotation group:

$$\boxed{U_{R'R} = U_{R'}U_R} \quad (22.20)$$

Let us consider some relevant cases.

- Think of a **scalar field** f as a “point” in the function space $L^2(\mathbb{R}^3)$.

A rotation induces the linear map $f' = \hat{U}_R f$ defined by $(\hat{U}_R f)(x) = f(R^{-1}x)$. The operators \hat{U}_R are unitary because Lebesgue’s measure is rotation invariant, then $\hat{U}_{R^{-1}} = \hat{U}_R^\dagger$.

The commutative subgroup of rotations $R(\mathbf{n}\varphi)$ with fixed direction \mathbf{n} corresponds to a commutative unitary subgroup $\hat{U}_{\mathbf{n}}(\varphi)\hat{U}_{\mathbf{n}}(\varphi') = \hat{U}_{\mathbf{n}}(\varphi + \varphi')$ (a strongly continuous one-parameter group). By Stone's theorem there is a self-adjoint (unbounded) generator such that $\hat{U}_{\mathbf{n}}(\varphi) = e^{-\frac{i}{\hbar}\varphi\hat{L}(\mathbf{n})}$. The self-adjoint operator $\hat{L}(\mathbf{n})$ is the generator of the one parameter group, and is conveniently found by considering the action of an infinitesimal rotation on the set of analytic functions:

$$\begin{aligned} (\hat{U}_{\mathbf{n}}(\delta\varphi)f)(\mathbf{x}) &= f(\mathbf{x} - \delta\varphi \mathbf{n} \times \mathbf{x} + \dots) \\ &= f(\mathbf{x}) - \delta\varphi (\mathbf{n} \times \mathbf{x})_k \frac{\partial f}{\partial x_k}(\mathbf{x}) + \dots \\ &= f(\mathbf{x}) - \frac{i}{\hbar} \delta\varphi (\mathbf{n} \cdot \mathbf{L}f)(\mathbf{x}) + \dots \end{aligned}$$

The generator is found to be $\hat{L}(\mathbf{n}) = \mathbf{n} \cdot \mathbf{L}$, the projection along \mathbf{n} of the *orbital angular momentum*

$$\boxed{\mathbf{L} = \mathbf{Q} \times \mathbf{P}} \quad (22.21)$$

The three operators \hat{L}_x , \hat{L}_y and \hat{L}_z satisfy the Lie algebra

$$\boxed{\frac{1}{i\hbar} [\hat{L}_i, \hat{L}_j] = \epsilon_{ijk} \hat{L}_k} \quad (22.22)$$

and generate the unitary subgroups representing rotations around the three coordinate axis.

- For a 1/2 **spinor field** ψ_a ($a = 1, 2$), the expansion near unity of (22.19) gives

$$\begin{aligned} [U_{\mathbf{n}}(\delta\varphi)\psi]_a(\mathbf{x}) &= \left[I - i\delta\varphi \mathbf{n} \cdot \frac{\boldsymbol{\sigma}}{2} + \dots \right]_{ab} \left(I - \frac{i}{\hbar} \delta\varphi \mathbf{n} \cdot \mathbf{L} + \dots \right) \psi_b(\mathbf{x}) \\ &= \psi_a(\mathbf{x}) - \frac{i}{\hbar} \delta\varphi (\mathbf{n} \cdot \mathbf{J})_{ab} \psi_b(\mathbf{x}) + \dots \end{aligned}$$

The generator is the projection along \mathbf{n} of the total angular momentum, which is the vector sum of *spin* and *orbital* angular momentum operators, acting independently on spin variables (components a, b) and on position variables:

$$\boxed{\mathbf{J} = \mathbf{S} + \mathbf{L}} \quad (22.23)$$

where $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ are the spin operators (matrices) for spin 1/2 particles.
Also in this case the algebra is that of angular momentum (rotation group):

$$\boxed{\frac{1}{i\hbar} [\hat{J}_i, \hat{J}_j] = \epsilon_{ijk} \hat{J}_k.} \quad (22.24)$$

Chapter 23

Unbounded Linear Operators*

The theory of bounded linear operators is elegant and provides general results despite the particular definitions. However, many linear operators of interest in quantum mechanics, such as differential operators, are unbounded. Quantum observables are associated to self-adjoint operators, and the mathematical problem arises to construct the self-adjoint extension from an initial definition.

The theory is difficult and specialized. Here some useful concepts are sketched, as the graph, the adjoint, the resolvent and the spectrum of an operator.

23.1 The graph of an operator

The graph of a real function f is the set of points (x, y) in \mathbb{R}^2 , where $x \in \mathcal{D}(f)$ and $y = f(x)$. A very useful tool is the *graph of a linear operator*, introduced by Von Neumann. It is the set in $\mathcal{H}^2 = \mathcal{H} \times \mathcal{H}$

$$\mathcal{G}(\hat{A}) = \{(x, y) : x \in \mathcal{D}(\hat{A}), y = \hat{A}x\} \quad (23.1)$$

\mathcal{H}^2 , with elements $X = (x, y)$, is a linear space with the rules $\lambda X = (\lambda x, \lambda y)$ and $X + X' = (x + x', y + y')$. It is a Hilbert space with inner product

$$(X|X') = (x|x') + (y|y').$$

The norm is $\|X\|^2 = \|x\|^2 + \|y\|^2$. Completeness is readily proven: if X_n is a Cauchy sequence, $\|X_n - X_m\|^2 = \|x_n - x_m\|^2 + \|y_n - y_m\|^2 < \epsilon$ for all $n, m > N_\epsilon$, then x_n and y_n are both Cauchy sequences, and converge in \mathcal{H} to x and y . The pair $X = (x, y)$ is the limit of X_n in \mathcal{H}^2 : $\|X_n - X\|^2 = \|x_n - x\|^2 + \|y_n - y\|^2 \rightarrow 0$.

The graph of a linear operator is a linear subspace in \mathcal{H}^2 . Conversely, a linear subspace \mathcal{S} is the graph of a linear operator if $(x, y) \in \mathcal{S}$ and $(x, y') \in \mathcal{S}$ imply $y = y'$ (the assignment $x \rightarrow y$ is unique). This is equivalent to: $(0, y) \in \mathcal{S} \Rightarrow y = 0$.

If the inverse of the operator \hat{A} exists, its graph is

$$\mathcal{G}(\hat{A}^{-1}) = \{(y, x) : (x, y) \in \mathcal{G}(\hat{A})\} \tag{23.2}$$

Definition 23.1.1. A linear operator \hat{A}' is an *extension* of a linear operator \hat{A} if $\mathcal{G}(\hat{A}) \subset \mathcal{G}(\hat{A}')$ (in other words: $\mathcal{D}(\hat{A}) \subset \mathcal{D}(\hat{A}')$ and $\hat{A}' = \hat{A}$ on $\mathcal{D}(\hat{A})$).

23.2 Closed operators

A graph is a closed set if every Cauchy sequence X_n in the graph converges to a point X in the graph (a Cauchy sequence X_n is convergent because \mathcal{H}^2 is complete; the point is that the limit X must be in the graph).

Definition 23.2.1. A linear operator \hat{A} is **closed** if its graph is a closed set.

This definition is an example of how useful the concept of graph is. Without it, the definition is: \hat{A} is closed if $\forall x_n$ in $\mathcal{D}(\hat{A})$ such that $x_n \rightarrow x$ and $\hat{A}x_n \rightarrow y \Rightarrow x \in \mathcal{D}(\hat{A})$ and $y = \hat{A}x$.

Remark 23.2.2.

1) “ \hat{A} is closed” does not mean that $\mathcal{D}(\hat{A})$ is closed nor that \hat{A} is continuous: it only means that $\mathcal{D}(\hat{A})$ contains the limit points of convergent sequences such that also the sequence $\hat{A}x_n$ converges, and converges to the image of the limit point (the graph is very useful to visualize this).

2) If \hat{A} is closed, $\text{Ker } \hat{A}$ is a closed subspace.

3) The inverse of a closed linear operator is closed.

If the graph $\mathcal{G}(\hat{A})$ of a linear operator is not closed, the set can be always extended to its closure $\overline{\mathcal{G}(\hat{A})}$ by adding the frontier. The closure is still a linear subspace¹ and it is the smallest closed extension of the set. However, it might not be a graph of a linear operator, as it may fail to have the property $(0, y) \in \overline{\mathcal{G}(\hat{A})} \Rightarrow y = 0$.

Definition 23.2.3. If $\overline{\mathcal{G}(\hat{A})}$ is the graph of a linear operator $\overline{\hat{A}}$, the operator $\overline{\hat{A}}$ is the *closure* of \hat{A} , and it is the minimal closed extension of \hat{A} . It is $\mathcal{G}(\overline{\hat{A}}) = \overline{\mathcal{G}(\hat{A})}$.

¹ If two limit points X and X' belong to the frontier there are two sequences X_n and X'_n convergent to them. $X + \lambda X'$ belongs to the closure because it is the limit of $X_n + \lambda X'_n$ that belongs to the graph, a linear space.

Proposition 23.2.4. *If $\overline{\mathcal{G}(\hat{A})}$ is not a graph of a linear operator, then \hat{A} has no closed extensions.*

Proof. If $\overline{\mathcal{G}(\hat{A})}$ is not a graph, it contains a point $(0, y)$ with $y \neq 0$. Suppose that \hat{A} has a closed extension \hat{A}^c ; then $\overline{\mathcal{G}(\hat{A})}$ is necessarily a proper subset of $\mathcal{G}(\hat{A}^c)$. But if $(0, y) \in \mathcal{G}(\hat{A}^c)$, the set cannot be the graph of an operator. \square

The property of being a closed operator will be a prerequisite for the introduction of the spectrum. The following theorem due to Banach is important:

Theorem 23.2.5 (closed graph theorem). *Let \hat{A} be a linear operator with a closed domain. Then \hat{A} is continuous if and only if \hat{A} is closed.*

Proof. If \hat{A} is continuous and $x_n \rightarrow x$ is a convergent sequence in $\mathcal{D}(\hat{A})$, then $x \in \mathcal{D}(\hat{A})$ (by hypothesis) and $\hat{A}x_n \rightarrow \hat{A}x$. This means that $\mathcal{G}(\hat{A})$ is closed, i.e. the operator is closed. Suppose that \hat{A} is closed, with a closed domain. Then for any convergent sequence x_n in $\mathcal{D}(\hat{A})$ such that $\hat{A}x_n$ is also convergent (to y), it is $x_n \rightarrow x \in \mathcal{D}(\hat{A})$ and $y = \hat{A}x$. Since the graph is closed, it is $y = \hat{A}x_n$, i.e. \hat{A} is continuous. \square

By the general theorem 18.3.5, if \hat{A} has a closed domain, \hat{A} is continuous if and only if \hat{A} is bounded.

23.3 The adjoint operator

Let us enquire about the existence of the adjoint operator. According to the definition given for bounded operators, the adjoint operator should map $x \in \mathcal{D}(\hat{A}^\dagger)$ to an element x' such that $(x'|y) = (x|\hat{A}y)$ for all $y \in \mathcal{D}(\hat{A})$. The vector x' corresponding to x must be unique; suppose that there are two such vectors, then $(x' - x''|y) = 0$ for all $y \in \mathcal{D}(\hat{A})$, i.e. $x' - x'' \in \mathcal{D}(\hat{A})^\perp$. Since we need $x' = x''$, it must be $\{0\} = \mathcal{D}(\hat{A})^\perp$ i.e. $\mathcal{H} = \mathcal{D}(\hat{A})^{\perp\perp} = \overline{\mathcal{D}(\hat{A})}$ i.e. \hat{A} must be *densely defined*.

Proposition 23.3.1. *If \hat{A} is a densely defined linear operator, then the adjoint \hat{A}^\dagger exists, it is a linear operator, and the domain is the maximal set*

$$\begin{aligned} \mathcal{D}(\hat{A}^\dagger) &= \{x \in \mathcal{H} : \forall y \in \mathcal{D}(\hat{A}) \exists x' \text{ s.t. } (x'|y) = (x|\hat{A}y)\}, \\ \hat{A}^\dagger x &= x'. \end{aligned}$$

This is the relation between \hat{A} and its adjoint:

$$\boxed{(\hat{A}^\dagger x|y) = (x|\hat{A}y), \quad \forall x \in \mathcal{D}(\hat{A}^\dagger), \forall y \in \mathcal{D}(\hat{A})} \quad (23.3)$$

The requirement that the domain of the adjoint is maximal, implies the following statement:

Proposition 23.3.2. *Let \hat{A} be densely defined. If \hat{A}' is an extension of \hat{A} , then the adjoint of \hat{A} is an extension of the adjoint of \hat{A}' :*

$$\hat{A} \subseteq \hat{A}' \Rightarrow \hat{A}'^\dagger \subseteq \hat{A}^\dagger \quad (23.4)$$

The graphs of \hat{A} and \hat{A}'^\dagger are closely related. Let us introduce the involution $V(x, y) = (y, -x)$. It has the properties: $(VX|X') = (X|VX')$, $V(\mathcal{S}^\perp) = (V\mathcal{S})^\perp$, $V^2X = -X$, $V^2\mathcal{S} = \mathcal{S}$ (\mathcal{S} is a linear subspace).

Proposition 23.3.3 (Graph of the adjoint operator).

$$\mathcal{G}(\hat{A}^\dagger) = (V\mathcal{G}(\hat{A}))^\perp \quad (23.5)$$

Proof. If $(x, x') \in \mathcal{G}(\hat{A}^\dagger)$ then $x \in \mathcal{D}(\hat{A}^\dagger)$ and, for all $y \in \mathcal{D}(\hat{A})$,

$$(x|\hat{A}y) = (x'|y) \Leftrightarrow (x|\hat{A}y) + (x'|-y) = 0 \Leftrightarrow ((\hat{A}y, -y)|(x, x')) = 0$$

in the inner product of \mathcal{H}^2 . Then: $X \in \mathcal{G}(\hat{A}^\dagger) \Leftrightarrow (VX'|X) = 0, \forall X' \in \mathcal{G}(\hat{A})$. This gives $(X'|VX) = 0$ i.e. $V\mathcal{G}(\hat{A}^\dagger) = \mathcal{G}(\hat{A})^\perp$ i.e. $\mathcal{G}(\hat{A}^\dagger) = V(\mathcal{G}(\hat{A})^\perp)$ and the statement is obtained. \square

This characterization of the graph of the adjoint has an important corollary. Since $V\mathcal{G}(\hat{A})$ is a linear subspace (not necessarily the graph of a linear operator), its orthogonal complement $\mathcal{G}(\hat{A}^\dagger)$ is closed, and so is the operator:

Corollary 23.3.4. *The adjoint of a linear operator is a closed operator.*

Proposition 23.3.5. *If \hat{A} is densely defined, then $\text{Ker } \hat{A}^\dagger = (\text{Ran } \hat{A})^\perp$*

Proof. $(\text{Ran } \hat{A})^\perp = \{x \in \mathcal{H} : (x|\hat{A}x') = 0, \forall x' \in \mathcal{D}(\hat{A})\} = \{x \in \mathcal{H} : (\hat{A}^\dagger x|x') = 0, \forall x' \in \mathcal{D}(\hat{A})\}$. Since \hat{A} is densely defined the set is $\{x \in \mathcal{H} : \hat{A}^\dagger x = 0\} = \text{Ker } \hat{A}^\dagger$. \square

Suppose that also \hat{A}^\dagger is densely defined: then $\hat{A}^{\dagger\dagger}$ exists and is closed (because it is the adjoint of \hat{A}^\dagger). We show that it is the closure of \hat{A} :

Proposition 23.3.6. $\hat{A}^{\dagger\dagger} = \overline{\hat{A}}$.

Proof. $\mathcal{G}(\hat{A}^{\dagger\dagger}) = V(\mathcal{G}(\hat{A}^\dagger))^\perp = (\mathcal{G}(\hat{A}))^{\perp\perp} = \overline{\mathcal{G}(\hat{A})} = \mathcal{G}(\overline{\hat{A}})$. \square

Corollary 23.3.7. $\hat{A}^{\dagger\dagger\dagger} = (\hat{A}^\dagger)^{\dagger\dagger} = \overline{\hat{A}^\dagger} = \hat{A}^\dagger$ because \hat{A}^\dagger is closed.

23.3.1 Self-adjointness

In applications one often encounters operators that are densely defined and symmetric. The issue is then to establish their self-adjoint extensions (self-adjointness is a requirement for an operator to represent an observable in quantum mechanics).

Definition 23.3.8. A densely defined linear operator \hat{A} is **symmetric** if

$$(\hat{A}x|y) = (x|\hat{A}y), \quad \forall x, y \in \mathcal{D}(\hat{A}) \quad (23.6)$$

The definition is equivalent to the statement $\hat{A} \subseteq \hat{A}^\dagger$: \hat{A}^\dagger is a closed extension of the symmetric operator \hat{A} . However, the smallest closed extension of \hat{A} (if it exists) is $\overline{\hat{A}} = \hat{A}^{\dagger\dagger}$. Then, in general (the last inclusion holds for a symmetric operator), $\hat{A} \subseteq \overline{\hat{A}} = \hat{A}^{\dagger\dagger} \subseteq \hat{A}^\dagger$.

Exercise 23.3.9. Show that the eigenvalues of a symmetric operator are real, and the eigenvectors with different eigenvalues are orthogonal.

Definition 23.3.10. A densely defined operator \hat{A} is **self-adjoint** if $\hat{A} = \hat{A}^\dagger$.

- 1) If \hat{A} is self-adjoint then it is closed, and $\hat{A} = \overline{\hat{A}} = \hat{A}^{\dagger\dagger} = \hat{A}^\dagger$.
- 2) If \hat{A} is symmetric and \hat{A}' is a self-adjoint extension of it, then $\hat{A} \subset \hat{A}' = \hat{A}'^\dagger \subseteq \hat{A}^\dagger$. Therefore the self-adjoint extension of \hat{A} , if it exists, is “between” \hat{A} and \hat{A}^\dagger .
- 3) If \hat{A} is self-adjoint it is $\text{Ker } \hat{A} = (\text{Ran } \hat{A})^\perp$, i.e.

$$\boxed{\mathcal{H} = \text{Ker } \hat{A} \oplus \overline{\text{Ran } \hat{A}}} \quad (23.7)$$

An intermediate situation is $\hat{A} \subset \hat{A}^\dagger$ and $\overline{\hat{A}} = \overline{\hat{A}^\dagger} = \hat{A}^\dagger$ (because the adjoint is closed). This occurs frequently in practice, and deserves a definition:

Definition 23.3.11. A densely defined operator is **essentially self-adjoint** if \hat{A} is symmetric and $\overline{\hat{A}}$ is self-adjoint.

If \hat{A} is essentially self-adjoint: $\hat{A} \subset \overline{\hat{A}} = \hat{A}^{\dagger\dagger} = \hat{A}^\dagger$. The closure is the unique self-adjoint extension of \hat{A} (suppose that \hat{B} is another self-adjoint extension and $\overline{\hat{A}} \subset \hat{B}$; then $\hat{B} = \hat{B}^\dagger \subset \overline{\hat{A}}$, which is impossible).

Example 23.3.12. The position operator $(\hat{Q}_0 f)(x) = xf(x)$ is well defined on the domain $\mathcal{S}(\mathbb{R})$ of \mathcal{C}^∞ functions of rapid decay (next chapter), which is a linear space dense in $L^2(\mathbb{R})$. The domain is invariant under the action of \hat{Q}_0 , and \hat{Q}_0 is symmetric on it:

$$(\hat{Q}_0 \varphi | \psi) = (\varphi | \hat{Q}_0 \psi), \quad \forall \varphi, \psi \in \mathcal{S}$$

The domain of \hat{Q}_0^\dagger is the set of functions $f \in L^2(\mathbb{R})$ such that there is $g \in L^2$ such that $(g|\varphi) = (f|\hat{Q}_0\varphi) \forall \varphi \in \mathcal{S}(\mathbb{R})$. This is:

$$\int_{\mathbb{R}} \overline{(g - xf)} \varphi dx = 0, \quad \forall \varphi \in \mathcal{S}(\mathbb{R}).$$

Since \mathcal{S} is dense in L^2 , this means $g = xf$ a.e., i.e.

$$\mathcal{D}(\hat{Q}_0^\dagger) = \{f \in L^2(\mathbb{R}) \text{ s.t. } \int_{\mathbb{R}} |xf|^2 dx < \infty\}, \quad \hat{Q}_0^\dagger f = xf$$

This domain contains \mathcal{S} . What about $\hat{Q}_0^{\dagger\dagger}$? The iteration of the above construction shows that the domain is unchanged and $\hat{Q}_0^\dagger = \hat{Q}_0^{\dagger\dagger}$. Therefore \hat{Q}_0 is essentially self-adjoint, and the operator $\hat{Q} = \hat{Q}_0^\dagger$ is the self-adjoint extension of \hat{Q}_0 .

23.4 Remarks on spectral theory

The resolvent set $\rho(A)$ of a $n \times n$ matrix A are the complex numbers z such that $z - A$ is invertible ($\text{Ker}(z - A) = \{0\}$, i.e. $Au = zu$ only has the trivial solution $u = 0$). The matrix $(z - A)^{-1}$ is called the resolvent of A at z .

The set $\sigma(A) = \mathbb{C} / \rho(A)$ is the spectrum. For finite matrices it only consists of the eigenvalues, for which $Au = zu$ has a non-trivial solution.

In Hilbert space, if \hat{A} is a closed linear operator and if $z - \hat{A}$ is invertible, the resolvent at z , $\hat{R}(z) = (z - \hat{A})^{-1}$, is closed, with domain $\text{Ran}(z - \hat{A})$.

If the domain coincides with \mathcal{H} , $\hat{R}(z)$ is bounded by the *closed graph theorem* 23.2.5, and z belongs to the *resolvent set* $\rho(\hat{A})$:

$$z \in \rho(\hat{A}) \iff \hat{R}(z) \in \mathcal{B}(\mathcal{H})$$

1) $\hat{R}(z)$ is an analytic function of $z \in \rho(\hat{A})$, i.e. it admits a norm-convergent power expansion on any disk in the resolvent set: $\hat{R}(z) = \sum_{n=0}^{\infty} \hat{C}_n (z - z_0)^n$.

2) For $z_1, z_2 \in \rho(\hat{A})$ the “resolvent identity” holds:

$$\hat{R}(z_1)\hat{R}(z_2) = -\frac{\hat{R}(z_2) - \hat{R}(z_1)}{z_2 - z_1} \quad (23.8)$$

The set $\mathbb{C}/\rho(\hat{A}) = \sigma(\hat{A})$ is the **spectrum** of \hat{A} . It may be decomposed into the *pure*, the *continuous* and the *residual* spectrum: $\sigma(\hat{A}) = \sigma_p(\hat{A}) \cup \sigma_c(\hat{A}) \cup \sigma_r(\hat{A})$.

$$\sigma_p(\hat{A}) = \{z : \exists(z - \hat{A})^{-1}\}, \quad (23.9)$$

$$\sigma_c(\hat{A}) = \{z : \exists(z - \hat{A})^{-1} \overline{\text{Ran}(z - \hat{A})} = \mathcal{H}\}, \quad (23.10)$$

$$\sigma_r(\hat{A}) = \{z : \exists(z - \hat{A})^{-1}, \overline{\text{Ran}(z - \hat{A})} \neq \mathcal{H}\}. \quad (23.11)$$

$z \in \sigma_p$ means that $\hat{A}u = zu$ has solution in $\mathcal{D}(\hat{A})$. σ_p is the set of eigenvalues and, in a separable Hilbert space, it is at most countable

$z \notin \sigma_p(\hat{A})$ means that $(z - \hat{A})^{-1}$ exists, with three disjoint possibilities: the resolvent has domain \mathcal{H} (and is necessarily bounded, $z \in \rho(\hat{A})$), the domain is dense in \mathcal{H} ($z \in \sigma_c$), the closure of the domain is a subset of \mathcal{H} ($z \in \sigma_r$).

23.4.1 Spectral decomposition of self-adjoint operators

For self-adjoint operators the eigenvalues are real, and the residual spectrum is empty. Now it is proven that $\sigma_c(\hat{A}) \subseteq \mathbb{R}$.

Proof. Suppose that $\lambda = \lambda_1 + i\lambda_2 \in \sigma_c(\hat{A})$ with $\lambda_2 \neq 0$. Then $(\lambda - \hat{A})^{-1}$ exists with domain $\text{Ran}(\lambda - \hat{A})$ dense in \mathcal{H} . We obtain the inequality

$$\|(\lambda - \hat{A})x\|^2 = \dots = \|(\lambda_1 - \hat{A})x\|^2 + |\lambda_2|^2 \|x\|^2 > |\lambda_2|^2 \|x\|^2$$

for all $x \in \mathcal{D}(\hat{A})$. This implies that $(\lambda - \hat{A})^{-1}$ is bounded on a dense domain, and extends to an operator in $\mathcal{B}(\mathcal{H})$. But then λ would be in $\rho(\hat{A})$. \square

The spectrum of a $n \times n$ Hermitian matrix is pure point with eigenvalues λ_k . Distinct eigenvalues correspond to orthogonal eigenvectors. The eigenvectors with same eigenvalue λ_k span an eigenspace with projector P_k . The projectors commute and are a "resolution of the identity": $\sum_k P_k = 1$. The spectral decomposition of the matrix H is:

$$H = \sum_{\lambda_k \in \sigma_p} \lambda_k P_k$$

For self-adjoint operators in Hilbert spaces the projectors associated to a non-empty σ_p span in general a subspace \mathcal{H}_p of the Hilbert space. To have a resolution of the identity one needs to consider the full spectrum.

The following inputs are given with no proof, and are illustrated by the example of the position operator.

Definition 23.4.1. A **resolution of the identity** (or **spectral family**) is a family of projection operators $\{\hat{E}_t, t \in \mathbb{R}\}$ such that:

$$\hat{E}_t \hat{E}_s = \hat{E}_{\min(t,s)} \tag{23.12}$$

$$\lim_{t \rightarrow s^+} \|\hat{E}_t x - \hat{E}_s x\| \rightarrow 0, \quad \forall x \in \mathcal{H} \tag{23.13}$$

$$\lim_{t \rightarrow -\infty} \hat{E}_t x = 0, \quad \lim_{t \rightarrow +\infty} \hat{E}_t x = x, \quad \forall x \in \mathcal{H} \tag{23.14}$$

Remarks:

- 1) Property (23.12) implies $\hat{E}_t \hat{E}_s = \hat{E}_s \hat{E}_t$.
- 2) The support of the spectral family is the closure of the set of t -values such that $\hat{E}_t \neq 0$ and $\hat{E}_t \neq 1$. The closed subspaces $\mathcal{M}_t = \text{Ran } \hat{E}_t$ have the properties:

$$\mathcal{M}_s \subseteq \mathcal{M}_t \text{ if } s \leq t, \quad \mathcal{M}_s = \bigcap_{t>s} \mathcal{M}_t, \quad \bigcap_{t \in \mathbb{R}} \mathcal{M}_t = \{0\}, \quad \overline{\bigcup_{t \in \mathbb{R}} \mathcal{M}_t} = \mathcal{H}$$

- 3) For $t \geq s$, define the projector $\hat{E}_{(s,t]} = \hat{E}_t - \hat{E}_s$. Property (23.13) says that $\|\hat{E}_{(t,t+\delta]} x\| \rightarrow 0$, as $\delta \rightarrow 0^+$.

$$\mu_x(s, t) = (x | \hat{E}_{(s,t]} x) = \|\hat{E}_{(s,t]} x\|^2$$

is a positive measure, and $\mu_x(-\infty, s) \leq \mu_x(-\infty, t) \leq \mu_x(\mathbb{R}) = \|x\|^2$.

The complex measures $\mu_{xy}(s, t) = (x | \hat{E}_{(s,t]} y)$ are combinations of positive measures with vectors $x \pm y, x \pm iy$ (via the polarization formula).

Example 23.4.2. In $L^2(\mathbb{R})$ the projection operators $(\hat{E}_t f)(x) = \chi_{(-\infty,t]}(x) f(x), t \in \mathbb{R}$ are a spectral family.

Property (23.12) follows from $\chi_{(-\infty,t]} \chi_{(-\infty,s]} = \chi_{(-\infty,u]}$ where $u = \min(s, t)$. Property (23.13):

$$\|\hat{E}_t f - \hat{E}_s f\|^2 = \int |(\chi_{(-\infty,t]} - \chi_{(-\infty,s]}) f|^2 dx = \int_s^t |f|^2 dx \rightarrow 0 \quad t \rightarrow s^+$$

Properties (23.14) are obvious.

The spectral measure is $\mu_{f,g}(-\infty, t) = \int_{-\infty}^t \overline{f} g dx$. It is a continuous function of t and is a.e. differentiable:

$$d\mu_{f,g}(t) = (f | d\hat{E}_t g) = \overline{f(t)} g(t) dt$$

If F is a bounded real continuous function, and \hat{Q} is the position operator:

$$(f|F(\hat{Q})g) = \int_{\mathbb{R}} \overline{f(t)} F(t) g(t) dt = \int_{\mathbb{R}} F(t) d\mu_{fg}(t)$$

In the weak sense, the spectral theorem for multiplication operators is

$$F(\hat{Q}) = \int_{\mathbb{R}} F(t) d\hat{E}_t$$

The general statement is found Reed and Simon, Functional Analysis Vol 1, Academic Press:

Theorem 23.4.3 (The spectral theorem). *If \hat{A} is self-adjoint, there is a unique spectral family \hat{E}_t such that*

$$\mathcal{D}(\hat{A}) = \left\{ x \in \mathcal{H} : \int_{\sigma(\hat{A})} t^2 (x|d\hat{E}_t x) < \infty \right\} \quad \hat{A}x = \int_{\sigma(\hat{A})} t d\hat{E}_t x.$$

More about the operators \hat{Q} and \hat{P} is in the chapter on distributions and Fourier II. I conclude by recalling a beautiful characterization of the continuous spectrum of a Hamiltonian operator $\hat{H} = \frac{1}{2m}\hat{P}^2 + \hat{V}$, with a short range potential (RAGE theorem - Ruelle, Amrein, Enss, Georgescu). Omitting technicalities, a normalized vector belongs to \mathcal{H}_c if the time average of the probability to be confined in a ball of radius r vanishes:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int_{|\mathbf{x}| < r} d\mathbf{x} |\psi(\mathbf{x}, t)|^2 = 0$$

In quantum mechanics the continuous energy spectrum is associated to scattering states; states whose evolution remains localized belong to \mathcal{H}_p .

Chapter 24

Schwartz Space and Fourier Transform

24.1 Introduction

As Laurent Schwartz recalls, his intuition of distributions came one night in 1944, just after the liberation of France. The two volumes *Théorie des distributions* were published in 1950, and the same year he received the “Fields medal” with Atle Selberg¹.

Similar work on *generalized functions* was done by the Russian mathematicians Israel M. Gel’fand and his collaborator E. Shilov. Other contributors to the ideas were S. Bochner, J. Leray, K. Friedrichs and S. Sobolev.

Distributions are a powerful tool for the study of differential equations. They do not stand alone, but require a set of well-behaved *test functions* φ that decay fast to zero, with some notion of convergence. The linear sequentially continuous functionals are the *distributions*. They include integral functionals $\varphi \rightarrow \int dx f(x)\varphi(x)$ where f belongs to a large set because of the good properties of φ . Some operations on test functions may be extended to such general(ized) functions, always to be understood in the weak sense, i.e. action on test functions.

Schwartz introduced two sets of test functions: the space $\mathcal{D}(\mathbb{R}^n)$ of \mathcal{C}^∞ functions with compact support in \mathbb{R}^n , and the larger Schwartz space $\mathcal{S}(\mathbb{R}^n)$ of rapidly decreasing \mathcal{C}^∞ functions. The dual spaces are respectively the space of distributions $\mathcal{D}'(\mathbb{R}^n)$ and the smaller space of tempered distributions $\mathcal{S}'(\mathbb{R}^n)$.

Because of their relevance in physics, we privilege the study of the Schwartz space (in

¹ The Fields golden medal is assigned every four years by the International Mathematical Union to mathematicians not older than 40. It was established by the Canadian professor J. C. Fields. The Italians in the Fields list are Enrico Bombieri (1947) and Alessio Figalli (2018).



Figure 24.1 Laurent Schwartz (Paris 1915, Paris 2002) was nephew of Jacques Hadamard; his wife Marie-Helene Levy was daughter of probabilist Paul Levy. Because of their Jewish origins, during the second world war they worked at the university of Strasbourg with different names. After the war he taught in Grenoble and Nancy and, from 1958 to 1980, at the École Polytechnique. He was politically engaged and was suspended for two years for his opposition to the Algerian war. In 1951 he earned the Fields medal for the theory of distributions. Among his students are Jacques-Louis Lyon, Alexander Grothendieck, Francois Bruhat.

Figure 24.2 Israel Gelfand (Odessa 1913, New Brunswick 2009). At the age of 16 Gelfand already attended lectures at Moscow State University, and when he was 19 he was admitted directly to the graduate school. He completed a doctorate on abstract functions and linear operators in 1935 under Kolmogorov. He started a famous weekly Mathematics Seminar, and devoted much effort to education of young mathematicians. In 1990 he moved to USA. He won three Orders of Lenin and the first Wolf prize in mathematics (1978), with Siegel, for his important contributions to functional analysis and the theory of representations of groups.

$n = 1$) and its dual. There are other motivations: \mathcal{S} is left invariant by the important multiplication and derivation operators, and the Fourier transform is a bijection on it².

² Bibliography: Reed and Simon *Functional Analysis*, Academic Press; Blanchard and Bruning, *Mathematical Methods in Physics*, Birkhauser (2003).

24.2 The Schwartz space

Definition 24.2.1. The Schwartz space $\mathcal{S}(\mathbb{R})$ of *rapidly decreasing* functions is the set of \mathcal{C}^∞ functions $\varphi : \mathbb{R} \rightarrow \mathbb{C}$ such that for all $m, n \in \mathbb{N}$:

$$\|\varphi\|_{m,n} = \sup_{x \in \mathbb{R}} |x^m (D^n \varphi)(x)| < \infty \quad (24.1)$$

Here $D = d/dx$. The functions and their derivatives fall off at infinity more quickly than the inverse of any polynomial. By the obvious properties:

$$1) \|\lambda \varphi\|_{m,n} = |\lambda| \|\varphi\|_{m,n},$$

$$2) \|\varphi_1 + \varphi_2\|_{m,n} \leq \|\varphi_1\|_{m,n} + \|\varphi_2\|_{m,n},$$

the Schwartz space is a linear space, and $\|\cdot\|_{m,n}$ is a family of *seminorms* for it (actually each one is a norm on \mathcal{S}).

Note the inclusions:

$\mathcal{S}(\mathbb{R}) \subset \mathcal{C}(\mathbb{R})$ (Banach space of bounded continuous functions with sup norm):

$$\|\varphi\|_\infty = \sup_{x \in \mathbb{R}} |\varphi(x)| = \|\varphi\|_{0,0} < \infty$$

$\mathcal{S}(\mathbb{R}) \subset \mathcal{L}^1(\mathbb{R})$. The following trick is frequently used:

$$\|\varphi\|_1 = \int_{\mathbb{R}} dx |\varphi(x)| \leq \sup_x |(1+x^2)\varphi(x)| \int_{\mathbb{R}} \frac{dx}{1+x^2} \leq (\|\varphi\|_{0,0} + \|\varphi\|_{2,0})\pi$$

$\mathcal{S}(\mathbb{R}) \subset \mathcal{L}^p(\mathbb{R})$:

$$\|\varphi\|_p^p = \int_{\mathbb{R}} dx |\varphi|^p = \int_{\mathbb{R}} dx |\varphi|^{p-1} |\varphi| \leq \dots \leq \|\varphi\|_{0,0}^{p-1} \|\varphi\|_1.$$

The space contains the Hermite functions:

$$h_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{1}{2}x^2} H_n(x). \quad (24.2)$$

It will be shown that \mathcal{S} is dense in L^2 (and others). It is a “paradise” that hosts operators that would be otherwise not easy to define.

24.2.1 Seminorms and convergence

Definition 24.2.2. A sequence of functions φ_r converges to φ in $\mathcal{S}(\mathbb{R})$ if:

$$\|\varphi_r - \varphi\|_{m,n} \rightarrow 0, \quad \forall m, n.$$

Convergence in $\mathcal{S}(\mathbb{R})$ is very restrictive, as this example illustrates: the sequence $\varphi_r(x) = \frac{1}{2r} e^{-(rx)^2}$ is uniformly convergent to zero ($\|\varphi_r\|_{0,0} \rightarrow 0$), but it does not converge to zero for all seminorms: $\|\varphi_r\|_{0,1} = \sup_x |xr e^{-(rx)^2}| = \sup_y |y e^{-y^2}| = 1/\sqrt{2e}$.

Definition 24.2.3. A sequence φ_r in $\mathcal{S}(\mathbb{R})$ is a Cauchy sequence if it is Cauchy for every seminorm, i.e.

$$\forall \epsilon, m, n \exists N_{\epsilon, m, n} \text{ such that } \|\varphi_r - \varphi_s\|_{m, n} < \epsilon \quad \forall r, s > N_{\epsilon, m, n}.$$

Theorem 24.2.4. $\mathcal{S}(\mathbb{R})$ is complete in the seminorm topology³ (every Cauchy sequence is seminorm-convergent).

Exercise 24.2.5.

- 1) Show that $\|\cdot\|_{0,2}$ is a norm in $\mathcal{S}(\mathbb{R})$.
- 2) Show that convergence in $\mathcal{S}(\mathbb{R})$ implies L^2 convergence.

Proposition 24.2.6. The linear operators $(\hat{Q}_0\varphi)(x) = x\varphi(x)$ and $(\hat{P}_0\varphi)(x) = -i\varphi'(x)$ on $\mathcal{S}(\mathbb{R})$ are continuous in the seminorm topology.

Proof. The identity $D^n(x\varphi) = xD^n\varphi + nD^{n-1}\varphi$ implies $\|Q_0\varphi\|_{m, n} = \sup_x |x^m D^n(x\varphi)| \leq \|\varphi\|_{m+1, n} + n\|\varphi\|_{m, n-1}$. Similarly: $\|P_0\varphi\|_{m, n} = \sup_x |x^m D^n\varphi'| = \|\varphi\|_{m, n+1}$. If $\varphi_k \rightarrow 0$ then $Q_0\varphi_k \rightarrow 0$ and $P_0\varphi_k \rightarrow 0$. □

24.3 The Fourier Transform in $\mathcal{S}(\mathbb{R})$

Definition 24.3.1. The Fourier transform and antitransform of a function in $\mathcal{S}(\mathbb{R})$ are:

$$(\mathcal{F}\varphi)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \varphi(x) \tag{24.3}$$

$$(\mathcal{F}^{-1}\varphi)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{ikx} \varphi(x) \tag{24.4}$$

The notation anticipates that $\mathcal{F}\mathcal{F}^{-1} = 1$: this will be a main result to prove. The transforms are related by $(\mathcal{F}^{-1}\varphi)(k) = (\mathcal{F}\varphi)(-k)$ and are well defined, as $\mathcal{S}(\mathbb{R}) \subset \mathcal{L}^1(\mathbb{R})$.

Theorem 24.3.2. \mathcal{F} and \mathcal{F}^{-1} are continuous maps of $\mathcal{S}(\mathbb{R})$ to itself.

Proof. The function $\mathcal{F}\varphi$ is \mathcal{C}^∞ , as derivatives can be exchanged with the integral:

$$\frac{d^n}{dk^n} (\mathcal{F}\varphi)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} (-ix)^n \varphi(x) e^{-ikx}$$

³ such spaces are named *Frechét spaces*. For a proof see Reed-Simon, *Functional Analysis*, Academic Press

We must show that all seminorms of $\mathcal{F}\varphi$ are finite:

$$\begin{aligned} k^m \frac{d^n}{dk^n} (\mathcal{F}\varphi)(k) &= \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} (-ix)^n \varphi(x) \left(-i \frac{d}{dx}\right)^m e^{-ikx} \\ &= \dots = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \left(i \frac{d}{dx}\right)^m [(-ix)^n \varphi(x)] \end{aligned}$$

Multiply and divide by $1+x^2$ and note that $D^m(x^n\varphi) = \sum_{p=0}^m c_p x^{n-p} D^{m-p}\varphi$ ($c_p = 0$ if $n-p < 0$). The precise values have no relevance here). Then:

$$\|\mathcal{F}\varphi\|_{m,n} \leq \sum_{p=0}^m |c_p| (\|\varphi\|_{n-p,m-p} + \|\varphi\|_{n-p+2,m-p}) \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} \frac{1}{1+x^2} < \infty$$

The bound also implies that the Fourier transform is continuous (a sequence \mathcal{S} -convergent to zero is mapped to a sequence \mathcal{S} -convergent to zero). The same conclusions hold for \mathcal{F}^{-1} . \square

Theorem 24.3.3 (Inversion theorem).

$$\varphi(x) = \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{ikx} (\mathcal{F}\varphi)(k) \quad (24.5)$$

Proof. The double integral is meaningful because $\mathcal{F}\varphi \in \mathcal{S}(\mathbb{R})$:

$$I(x) = \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{ikx} \int_{\mathbb{R}} \frac{dy}{\sqrt{2\pi}} e^{-iky} \varphi(y)$$

To circumvent the difficulty that the integrals cannot be exchanged, let us replace the function $(\mathcal{F}\varphi)(k)$ with $e^{-\epsilon k^2} (\mathcal{F}\varphi)(k) \in \mathcal{S}(\mathbb{R})$. The product function is in $\mathcal{S}(\mathbb{R})$ and converges to $\mathcal{F}\varphi$ as $\epsilon \rightarrow 0$ pointwise and in the seminorm topology. Since \mathcal{F}^{-1} is continuous: $I(x) = \lim_{\epsilon \rightarrow 0} I_\epsilon(x)$ and

$$\begin{aligned} I_\epsilon(x) &= \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{ikx} e^{-\epsilon k^2} \int_{\mathbb{R}} \frac{dy}{\sqrt{2\pi}} e^{-iky} \varphi(y) \\ &= \int_{\mathbb{R}} dy \varphi(y) \frac{1}{\sqrt{4\epsilon\pi}} e^{-(x-y)^2/4\epsilon} \end{aligned}$$

The function φ multiplies a Gaussian (the Heat kernel) whose integral is one. Then:

$$I_\epsilon(x) - \varphi(x) = \int_{\mathbb{R}} dy [\varphi(x+y) - \varphi(x)] \frac{e^{-y^2/4\epsilon}}{\sqrt{4\epsilon\pi}}$$

Take the modulus and use Lagrange's theorem:

$$\begin{aligned}
 |I_\epsilon(x) - \varphi(x)| &\leq \int_{\mathbb{R}} dy |\varphi(x+y) - \varphi(x)| \frac{e^{-y^2/4\epsilon}}{\sqrt{4\epsilon\pi}} \\
 &\leq \sup_{\xi} |\varphi'(\xi)| \int_{\mathbb{R}} dy |y| \frac{e^{-y^2/4\epsilon}}{\sqrt{4\epsilon\pi}} = 2\sqrt{\frac{\epsilon}{\pi}} \|\varphi\|_{0,1}
 \end{aligned}$$

For $\epsilon \rightarrow 0$ the limit is zero, for all x . □

Corollary 24.3.4. $(\mathcal{F}^2\varphi)(x) = \varphi(-x)$; $\mathcal{F}^3 = \mathcal{F}^{-1}$, $\mathcal{F}^4 = 1$.

Proof. $(\mathcal{F}^2\varphi)(x) = (\mathcal{F}^{-1}\mathcal{F}\varphi)(-x) = \varphi(-x)$; $(\mathcal{F}^3\varphi)(x) = (\mathcal{F}^2\mathcal{F}\varphi)(x) = (\mathcal{F}\varphi)(-x)$. □

Proposition 24.3.5. *The Hermite functions (24.2) are eigenfunctions of the Fourier transform:*

$$\boxed{(\mathcal{F} h_n)(k) = (-i)^n h_n(k)} \tag{24.6}$$

Proof. The generating function of the Hermite functions is obtained from the generator (11.17) of Hermite polynomials:

$$\frac{1}{\sqrt[4]{\pi}} e^{-t^2+2tx-\frac{1}{2}x^2} = \sum_{n=0}^{\infty} \frac{(t\sqrt{2})^n}{\sqrt{n!}} h_n(x) \tag{24.7}$$

By acting with \mathcal{F} (integrate the variable x):

$$\frac{1}{\sqrt[4]{\pi}} \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-t^2+2tx-\frac{1}{2}x^2} e^{-ikx} = \sum_{n=0}^{\infty} \frac{(t\sqrt{2})^n}{\sqrt{n!}} (\mathcal{F} h_n)(k)$$

The integral of the left hand side is again a generator of Hermite functions:

$$\frac{1}{\sqrt[4]{\pi}} e^{t^2-2ikt-\frac{1}{2}k^2} = \sum_{n=0}^{\infty} \frac{(-it\sqrt{2})^n}{\sqrt{n!}} h_n(k)$$

The equality of coefficients of powers t^n of the two series gives the result. □

Proposition 24.3.6. *With the inner product of $L^2(\mathbb{R})$, $\forall \varphi, \psi \in \mathcal{S}(\mathbb{R})$:*

$$(\varphi|\mathcal{F}\psi) = (\mathcal{F}^{-1}\varphi|\psi) \tag{24.8}$$

$$(\mathcal{F}\psi|\mathcal{F}\varphi) = (\psi|\varphi) \tag{24.9}$$

In particular $\|\mathcal{F}\psi\|_2 = \|\psi\|_2$.

Proof.

$$\begin{aligned} \int_{\mathbb{R}} dk \overline{\varphi(k)} (\mathcal{F}\psi)(k) &= \int_{\mathbb{R}} dk \overline{\varphi(k)} \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \psi(x) \\ &= \int_{\mathbb{R}} dx \psi(x) \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} \overline{\varphi(k)} e^{-ikx} = \int_{\mathbb{R}} dx \psi(x) \overline{(\mathcal{F}^{-1}\varphi)(k)} \end{aligned}$$

The other relations follow. □

Example 24.3.7 (Fourier transform of $x^n e^{-a^2 x^2}$).

$$\int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} x^n e^{-a^2 x^2} e^{-ikx} = i^n \frac{\partial^n}{\partial k^n} \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-a^2 x^2 - ikx} = \frac{i^n}{a\sqrt{2}} \frac{\partial^n}{\partial k^n} e^{-\frac{k^2}{4a^2}}$$

Use Rodrigues formula (11.21) to evaluate the derivatives:

$$\int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} x^n e^{-a^2 x^2} e^{-ikx} = \frac{1}{(2ia)^n} \frac{1}{a\sqrt{2}} e^{-\frac{k^2}{4a^2}} H_n\left(\frac{k}{2a}\right) \quad (24.10)$$

Example 24.3.8 (continuation). The “unitarity” (24.9) of the Fourier transform and the result (24.10) give the integral identity:

$$\int_{\mathbb{R}} dx e^{-(a^2+b^2)x^2} x^{n+p} = \frac{2i^{n-p}}{(2a)^{n+1}(2b)^{p+1}} \int_{\mathbb{R}} dk e^{-k^2 \frac{a^2+b^2}{4a^2b^2}} H_n\left(\frac{k}{2a}\right) H_p\left(\frac{k}{2b}\right)$$

Note that $n+p$ must be even (or the result is zero). The left hand side is evaluated with $x^2 = t$ and gives a Gamma function⁴. The final formula is

$$\int_{\mathbb{R}} dk e^{-k^2 \frac{a^2+b^2}{4a^2b^2}} H_n\left(\frac{k}{2a}\right) H_p\left(\frac{k}{2b}\right) = \frac{(-1)^{\frac{n+p}{2}} (2a)^{n+1} (2b)^{p+1}}{2 (a^2+b^2)^{\frac{n+p+1}{2}}} \Gamma\left(\frac{n+p+1}{2}\right)$$

Proposition 24.3.9.

$$\hat{Q}_0 \mathcal{F} = \mathcal{F} \hat{P}_0, \quad \hat{P}_0 \mathcal{F} = -\mathcal{F} \hat{Q}_0, \quad (24.11)$$

⁴ A useful source of tabulated integrals is Gradshteyn - Ryzhik, *Tables of Integrals, Products and Series*, Academic Press.

Proof. In the formula below, integrate by parts; boundary terms cancel because φ is of rapid decrease:

$$\begin{aligned} (\hat{Q}_0 \mathcal{F} \varphi)(k) &= k(\mathcal{F} \varphi)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} \varphi(x) i \frac{d}{dx} e^{-ikx} \\ &= \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} (-i) \frac{d}{dx} \varphi(x) = (\mathcal{F} \hat{P}_0 \varphi)(k) \end{aligned}$$

The other equality is proven similarly. □

Exercise 24.3.10. Show that $\hat{P}_0^2 + \hat{Q}_0^2$ and \mathcal{F} commute.

24.4 Convolution product

Definition 24.4.1. The **convolution product** of two functions in $\mathcal{S}(\mathbb{R})$ is

$$\boxed{(\psi * \varphi)(x) = \int_{\mathbb{R}} dy \psi(x-y) \varphi(y)} \quad (24.12)$$

Theorem 24.4.2. $\psi * \varphi \in \mathcal{S}(\mathbb{R})$. The map $\psi \rightarrow \psi * \varphi$ is linear and continuous,

$$\boxed{\mathcal{F}(\psi * \varphi) = \sqrt{2\pi} (\mathcal{F} \psi)(\mathcal{F} \varphi) \quad , \quad (\mathcal{F} \psi) * (\mathcal{F} \varphi) = \sqrt{2\pi} \mathcal{F}(\psi \varphi)} \quad (24.13)$$

The convolution product is commutative, associative and distributive.

Proof. The convolution of two functions in \mathcal{S} is in \mathcal{S} :

$$\begin{aligned} |x^m D^n (\psi * \varphi)(x)| &= \left| \int_{\mathbb{R}} dy x^m D_x^n \psi(x-y) \varphi(y) \right| \\ &\leq \sum_{k=0}^m \binom{m}{k} \int_{\mathbb{R}} dy |x-y|^{m-k} D_x^n \psi(x-y) |y^k \varphi(y)| \\ &\leq \sum_{k=0}^m \binom{m}{k} \sup_z |z^{m-k} D_z^n \psi(z)| \int_{\mathbb{R}} dy |y^k \varphi(y)| \end{aligned}$$

Let us introduce factors $(1+y^2)$ in the integral and take the sup:

$$\|\psi * \varphi\|_{m,n} \leq \pi \sum_{k=0}^m \binom{m}{k} \|\psi\|_{m-k,n} (\|\varphi\|_{0,0} + \|\varphi\|_{2,0})$$

Then $\psi * \varphi$ is in $\mathcal{S}(\mathbb{R})$. Moreover, if $\varphi_r \rightarrow 0$ it follows that $\psi * \varphi_r \rightarrow 0$ (continuity). Now the Fourier transform:

$$\begin{aligned}\mathcal{F}(\psi * \varphi)(k) &= \int \frac{dx}{\sqrt{2\pi}} e^{-ikx} \int dy \psi(x-y)\phi(y) \\ &= \int dy \phi(y) e^{-iky} \int \frac{dx}{\sqrt{2\pi}} e^{-ik(x-y)} \psi(x-y) \\ &= \sqrt{2\pi} (\mathcal{F}\varphi)(k) (\mathcal{F}\psi)(k)\end{aligned}$$

The other relation follows: replace ψ, φ by $\mathcal{F}\psi, \mathcal{F}\varphi$; then $\mathcal{F}(\mathcal{F}\psi * \mathcal{F}\varphi)(x) = \sqrt{2\pi}\psi(-x)\varphi(-x)$. Apply $\mathcal{F}^{-1} = \mathcal{F}^3$ and obtain $\mathcal{F}\psi * \mathcal{F}\varphi = \sqrt{2\pi}\mathcal{F}(\psi\varphi)$.

The identity $\mathcal{F}[(\varphi_1 * \varphi_2) * \varphi_3] = \sqrt{2\pi}\mathcal{F}(\varphi_1 * \varphi_2)\mathcal{F}(\varphi_3) = 2\pi\mathcal{F}(\varphi_1)\mathcal{F}(\varphi_2)\mathcal{F}(\varphi_3)$ shows that the product is associative. \square

24.4.1 The Heat Equation

In one space dimension the heat (or diffusion) equation is

$$\boxed{\left(\frac{1}{D} \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right) u(x, t) = 0} \quad (24.14)$$

The *Heat Kernel* is the function of time $t > 0$ and space coordinate x :

$$K_t(x-y) = \frac{1}{\sqrt{4Dt\pi}} \exp\left[-\frac{(x-y)^2}{4Dt}\right] \quad (24.15)$$

As a function of x it is peaked in y , with height decreasing in time; its space integral is one at all times t . The heat kernel solves the heat equation with initial condition $K_0(x-y) = \delta(x-y)$. It describes the diffusive spread in time of a quantity (temperature, pollutant density, ...) that is initially delta-localized in $x = y$. The width of the Gaussian grows with the square root law $\approx \sqrt{Dt}$.

Since the Heat equation is linear, the linear superposition of heat kernels weighted by a function $\varphi(y)$ is also a solution; it is the convolution:

$$u(x, t) = (K_t * \varphi)(x) = \int_{\mathbb{R}} dy K_t(x-y)\varphi(y) \quad (24.16)$$

It solves the Heat equation with the initial condition $u(x, 0) = \varphi(x)$.

The same result is obtained with the aid of Fourier integral. Put

$$u(x, t) = \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{ikx} \tilde{u}(k, t)$$

in the Heat equation, and obtain the first order equation

$$\frac{1}{D} \frac{d}{dt} \tilde{u}(k, t) + k^2 \tilde{u}(k, t) = 0 \Rightarrow \tilde{u}(k, t) = C(k) e^{-Dtk^2}$$

The initial condition imposes $C(k) = \tilde{u}(k, 0) = \tilde{\varphi}(k)$. The solution in x -space is then obtained:

$$u(x, t) = \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{ikx - k^2 Dt} \tilde{\varphi}(k)$$

This is the Fourier antitransform of the product of two Fourier transforms: $\tilde{\varphi}(k)$ and $e^{-k^2 Dt}$. Then it coincides (up to numerical factor) with the convolution product (24.16) of the Heat kernel and the initial condition, i.e. (24.16).

24.4.2 Laplace equation in the strip*

Consider the Laplace equation $u_{xx} + u_{yy} = 0$ in the strip $-\infty < x < \infty, 0 \leq y \leq 1$ with boundary conditions (b.c.) $u(x, 0) = u_0(x), u(x, 1) = u_1(x)$.

For simplicity, let $u_0, u_1 \in \mathcal{S}(\mathbb{R})$. In the Fourier representation

$$u(x, y) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} \tilde{u}(k, y) \tag{24.17}$$

Laplace's equation gives: $-k^2 \tilde{u} + \tilde{u}_{yy} = 0$, i.e. $\tilde{u}(k, y) = A_k \exp(ky) + B_k \exp(-ky)$. The functions A_k and B_k are determined by the b.c. at $y = 0$ and $y = 1$: $\tilde{u}_0(k) = A_k + B_k$ and $\tilde{u}_1(k) = A_k e^k + B_k e^{-k}$. Then:

$$\tilde{u}(k, y) = \tilde{u}_0(k) \frac{\sinh[k(1-y)]}{\sinh k} + \tilde{u}_1(k) \frac{\sinh(ky)}{\sinh k}$$

To evaluate (24.17) we exploit the property $\sqrt{2\pi} \mathcal{F}^{-1}(\mathcal{F} f \mathcal{F} g) = f * g$.

Note that

$$\int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} \frac{\sinh(ky)}{\sinh k} = \sqrt{\frac{\pi}{2}} \frac{\sin(\pi y)}{\cosh(\pi x) + \cos(\pi y)} \equiv S_y(x)$$

(see ex.14.3.22) and similarly define $S_{1-y}(x)$. Then $\tilde{u}(k, y) = \tilde{u}_0(k) \tilde{S}_{1-y}(k) + \tilde{u}_1(k) \tilde{S}_y(k)$. The Fourier transform (24.17) becomes the sum of two convolutions. The solution of the

Laplace equation in the strip is obtained:

$$\begin{aligned} u(x, y) &= \frac{1}{\sqrt{2\pi}} [(S_{1-y} * u_0)(x) + (S_y * u_1)(x)] \\ &= \frac{1}{2} \int_{-\infty}^{\infty} dx' \left[\frac{\sin(\pi y) u_0(x')}{\cosh[\pi(x-x')] - \cos(\pi y)} + \frac{\sin(\pi y) u_1(x')}{\cosh[\pi(x-x')] + \cos(\pi y)} \right]. \end{aligned}$$

The b.c. are fulfilled: the function $\frac{1}{2} \frac{\sin(\pi y)}{\cosh[\pi(x-x')] - \cos(\pi y)}$ for $y \rightarrow 0$ tends to $\delta(x-x')$ and for $y \rightarrow 1$ tends to 0. The function with the other sign has a complementary behaviour.

Chapter 25

Tempered Distributions

Depuis l'introduction par Dirac de la fameuse fonction $\delta(x)$, qui serait nulle partout sauf pour $x = 0$ et serait infinie pour $x = 0$ de telle sorte que $\int_{-\infty}^{+\infty} dx \delta(x) = +1$, les formules du calcul symbolique sont devenues plus inacceptables pour la rigueur des mathématiciens. Ecrire que la fonction d'Heaviside $\theta(x)$ égale à 0 pour $x < 0$ et à 1 pour $x \geq 0$ a pour dérivé la fonction de Dirac $\delta(x)$ dont la définition même est mathématiquement contradictoire, et parler de dérivées $\delta'(x)$, $\delta''(x)$... de cette fonction dénuée d'existence réelle, c'est dépasser les limites qui nous sont permises ... (L. Schwartz, "Théorie des Distributions", Hermann & C. Paris, 1950)

25.1 Introduction

A linear continuous functional on $\mathcal{S}(\mathbb{R})$ is a linear map¹:

$$f : \varphi \in \mathcal{S}(\mathbb{R}) \rightarrow \langle f | \varphi \rangle \in \mathbb{C}$$

such that $\langle f | \varphi_k \rangle \rightarrow 0$ for any seminorm-convergent sequence $\varphi_k \rightarrow 0$.

Definition 25.1.1. The space of linear continuous functionals on $\mathcal{S}(\mathbb{R})$ is the space $\mathcal{S}'(\mathbb{R})$ of *tempered distributions*².

It is a linear space with: $\langle f + \lambda g | \varphi \rangle = \langle f | \varphi \rangle + \lambda \langle g | \varphi \rangle$.

A sufficient condition for continuity is boundedness with respect to a seminorm (or sums or products of seminorms). For example, there is a constant C_f and a seminorm

¹ We adopt Dirac's *bra* and *ket* notation to write the action of a tempered distribution on test functions

² A nice and instructive presentation is: I. Richards and H. Youn, *Theory of distributions: a non-technical introduction*, Cambridge University Press (1990).

such that³:

$$| \langle f | \varphi \rangle | \leq C_f \| \varphi \|_{k,m} \quad \forall \varphi \in \mathcal{S}(\mathbb{R}).$$

The **regular distributions** are the integral functionals

$$\langle f | \varphi \rangle = \int_{\mathbb{R}} dx f(x) \varphi(x)$$

Since test functions are “very good”, the integral makes sense also with “bad functions”. We must ensure that the integral exists, and continuity:

- 1) f is locally integrable (i.e. integrable on any compact subset of the line),
- 2) f is algebraically bounded at large x : there are constants $C > 0$, $R > 0$, and an integer $n > 0$ such that $|f(x)| \leq C|x|^n$ for all $|x| > R$.

Then:

$$\begin{aligned} | \langle f | \varphi \rangle | &\leq \int_{-R}^R dx |f(x)| |\varphi(x)| + C \int_{|x|>R} dx |x|^n |\varphi(x)| \\ &\leq \| \varphi \|_{00} \int_{-R}^R dx |f(x)| + C \pi \sup_x [|x|^n (1+x^2) |\varphi(x)|] \\ &\leq K (\| \varphi \|_{00} + \| \varphi \|_{n,0} + \| \varphi \|_{2+n,0}) \end{aligned}$$

where K depends on f but not on the test function.

Regular distributions extend the linear functionals on L^2 : if $f \in \mathcal{L}^2(\mathbb{R})$ then $\langle f | \varphi \rangle = \int_{\mathbb{R}} dx f(x) \varphi(x)$ is a regular distribution on $\mathcal{S}(\mathbb{R})$ (use Schwarz inequality and recall that $\| \varphi \|_2^2$ is bounded by seminorms).

Definition 25.1.2 (convergence in \mathcal{S}').

$$f_n \rightarrow f \quad \text{in } \mathcal{S}'(\mathbb{R}) \quad \text{if} \quad \langle f_n | \varphi \rangle \rightarrow \langle f | \varphi \rangle \quad \forall \varphi \in \mathcal{S}(\mathbb{R}) \quad (25.1)$$

Example 25.1.3. The sequence $f_n(x) = \cos(nx)$ has no limit as a function. However, as a regular distribution it has limit zero: $\langle f_n | \varphi \rangle = \int_{\mathbb{R}} dx \cos(nx) \varphi(x) \rightarrow 0$ as $n \rightarrow \infty$, for all φ (Riemann-Lebesgue theorem), i.e. $f_n \rightarrow 0$ in $\mathcal{S}'(\mathbb{R})$.

³ Recall that a sequence φ_n converges to zero whenever all seminorms vanish. Then boundedness is sufficient for $f\varphi_n$ to vanish as $n \rightarrow \infty$.

25.2 Special distributions

25.2.1 Dirac's delta function

The Dirac's delta at a point $a \in \mathbb{R}$ is the functional

$$\langle \delta_a | \varphi \rangle = \varphi(a) \quad (25.2)$$

Since $|\varphi(a)| \leq \|\varphi\|_{0,0}$, the functional δ_a is continuous. It is customary (and convenient) to write the action of the functional as if it were a regular one, with a generalized function:

$$\langle \delta_a | \varphi \rangle = \int_{\mathbb{R}} dx \delta(x-a) \varphi(x)$$

There are several approximations of Dirac's delta by regular distributions; these two are particularly important and useful:

Proposition 25.2.1 (Lorentzian or Cauchy distribution).

$$\lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{\pi} \frac{1}{(x-a)^2 + \epsilon^2} = \delta(x-a) \quad (25.3)$$

Proof. For any ϵ the function has unit integral, and defines a regular distribution. Let's show that for any test function φ , the action on φ converges to $\varphi(a)$ as $\epsilon \rightarrow 0$. This amounts to the vanishing of

$$I = \int_{\mathbb{R}} dx \frac{\epsilon}{\pi} \frac{\varphi(x) - \varphi(a)}{(x-a)^2 + \epsilon^2}$$

shift the variable by a and take the symmetric part of numerator

$$\begin{aligned} &= \int_{\mathbb{R}} dx \frac{\epsilon}{2\pi} \frac{\varphi(a+x) + \varphi(a-x) - 2\varphi(a)}{x^2 + \epsilon^2} \\ |I| &\leq \frac{\epsilon}{2\pi} \int_{\mathbb{R}} dx \frac{|\varphi(a+x) + \varphi(a-x) - 2\varphi(a)|}{x^2} \end{aligned}$$

The integral is a finite number, as the function is finite in $x = 0$ and decays at least as $|x|^{-2}$ at infinity. Then the limit $\epsilon \rightarrow 0^+$ is zero. \square

Proposition 25.2.2.

$$\lim_{R \rightarrow \infty} \int_{-R}^{+R} \frac{dk}{2\pi} e^{-ik(x-y)} = \delta(x-y) \quad (25.4)$$

Proof. For finite R the action on a test function is:

$$\int_{-\infty}^{+\infty} dx \int_{-R}^R \frac{dk}{2\pi} e^{-ik(x-y)} \varphi(x) = \int_{-R}^{+R} \frac{dk}{\sqrt{2\pi}} e^{iky} (\mathcal{F}\varphi)(k)$$

In the limit $R \rightarrow \infty$ we recover the inverse Fourier transform, i.e. $\varphi(y)$. \square

The following regular distributions converge to $\delta(x-a)$ and $\delta(x)$ in $\mathcal{S}'(\mathbb{R})$ as $\epsilon \rightarrow 0^+$ (proofs are simple and left as exercise)

$$\frac{1}{\sqrt{\pi\epsilon}} e^{-\frac{1}{\epsilon}(x-a)^2}, \quad \frac{1}{2\epsilon} \chi_{[a-\epsilon, a+\epsilon]}(x), \quad \frac{2}{\pi\epsilon^2} \sqrt{\epsilon^2 - x^2} \theta(\epsilon^2 - x^2), \quad (25.5)$$

$$\lim_{n \rightarrow \infty} \frac{\sin(nx)}{\pi x} = \delta(x)$$

(Hint: evaluate the integral in Prop.25.2.2 for finite R).

25.2.2 Heaviside's theta function

Consider the functional θ_a , $a \in \mathbb{R}$,

$$\langle \theta_a | \varphi \rangle = \int_a^{\infty} dx \varphi(x) \quad (25.6)$$

It is a regular distribution, with function $\theta(x-a) = \chi_{[a, \infty)}(x)$.

Exercise 25.2.3. Prove the distributional limits ($n \rightarrow \infty$)⁴

- 1) $\chi_{[0, n]} \rightarrow \theta(x)$,
- 2) $f_n(x) = \begin{cases} 0 & x < 0 \\ x^n & x \in [0, 1] \\ x = 1 & x > 1 \end{cases} \rightarrow \theta(x-1)$
- 3) $\frac{1}{e^{nx} + 1} \rightarrow \theta(-x)$.

⁴ The function 3) with $n = \frac{\mu}{k_B T}$ and $x = \frac{E-\mu}{\mu}$ is the Fermi-Dirac distribution, which gives the average number of fermions with energy E , in thermal equilibrium at temperature T and chemical potential $\mu > 0$. The limit distribution, $\theta(\mu - E)$, is the Fermi distribution (the ground state, $T = 0$).

25.2.3 Principal value of $(x - a)^{-1}$

The function $\frac{1}{x-a}$ has a non-integrable singularity in $x = a$ and thus it does not yield a regular distribution. One then defines the “principal value of $\frac{1}{x-a}$ ” as the functional with action

$$\left\langle P \frac{1}{x-a} \mid \varphi \right\rangle = \int_{\mathbb{R}} dx \frac{\varphi(x)}{x-a} \quad (25.7)$$

The principal value integral is:

$$\lim_{\epsilon \rightarrow 0^+} \left(\int_{-\infty}^{a-\epsilon} dx + \int_{a+\epsilon}^{\infty} dx \right) \frac{\varphi(x)}{x-a} = \lim_{\epsilon \rightarrow 0^+} \int_{\epsilon}^{\infty} dx \frac{\varphi(a+x) - \varphi(a-x)}{x} \quad (25.8)$$

the limit $\epsilon \rightarrow 0^+$ exists. Now, use Lagrange’s formula on the interval $\epsilon \leq x \leq 1$, and the triangle inequality on $x \geq 1$:

$$\begin{aligned} \left| \left\langle P \frac{1}{x-a} \mid \varphi \right\rangle \right| &\leq 2(1-\epsilon) \sup_x |\varphi'(x)| + \int_1^{\infty} dx (|\varphi(a+x)| + |\varphi(a-x)|) \\ &\leq 2\|\varphi\|_{0,1} + 2\|\varphi\|_{L^1} \end{aligned}$$

The L^1 norm is majored by seminorms, therefore the principal part is a tempered distribution. \square

25.2.4 The Sokhotski-Plemelj formulae

In alternative to the principal part prescription, one may shift the singularity from the real axis by adding an imaginary part. For finite $\epsilon > 0$ the following are regular distributions, with real parameter a :

$$\varphi \rightarrow \int_{-\infty}^{+\infty} dx \frac{\varphi(x)}{x-a \pm i\epsilon}$$

Let us rewrite the integral as

$$\int_{-\infty}^{+\infty} dx \frac{(x-a)\varphi(x)}{(x-a)^2 + \epsilon^2} \mp i\pi \int_{-\infty}^{+\infty} dx \frac{\epsilon}{\pi} \frac{\varphi(x)}{(x-a)^2 + \epsilon^2}$$

For $\epsilon \rightarrow 0$ the Cauchy distribution tends to $\delta(x - a)$ and the result of the second integral is $\varphi(a)$. In the first integral we split the real axis:

$$\begin{aligned} \int_{-\infty}^{+\infty} dx \frac{(x-a)\varphi(x)}{(x-a)^2 + \epsilon^2} &= \int_{|x-a| > \epsilon} dx \frac{(x-a)\varphi(x)}{(x-a)^2 + \epsilon^2} + \int_{a-\epsilon}^{a+\epsilon} dx \frac{(x-a)\varphi(x)}{(x-a)^2 + \epsilon^2} \\ &= \int_{|x-a| > \epsilon} dx \frac{(x-a)\varphi(x)}{(x-a)^2 + \epsilon^2} + \int_{-1}^{+1} dt \frac{t}{t^2 + 1} \varphi(a + \epsilon t) \end{aligned}$$

In the limit $\epsilon \rightarrow 0$ the first integral is the principal part integral, the second one is zero ($\varphi(a)$ times the integral of an odd function). We obtain the important identities⁵:

$$\lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}} dx \frac{\varphi(x)}{x - a \pm i\epsilon} = \mathcal{P} \int_{\mathbb{R}} dx \frac{\varphi(x)}{x - a} \mp i\pi \varphi(a), \quad \varphi \in \mathcal{S}(\mathbb{R}) \quad (25.9)$$

It is an identity among distributions (with implicit limit $\epsilon \rightarrow 0$ **after** the action on a test function):

$$\boxed{\frac{1}{x - a \pm i\epsilon} = \mathcal{P} \frac{1}{x - a} \mp i\pi \delta(x - a) \quad a \in \mathbb{R}} \quad (25.10)$$

Exercise* 25.2.4. Prove the identity, for real x, y , and $\epsilon, \eta > 0$:

$$\int_{\mathbb{R}} \frac{dx'}{\pi^2} \operatorname{Re} \left[\frac{1}{x' - x + i\epsilon} \right] \operatorname{Re} \left[\frac{1}{x' - y + i\eta} \right] = \frac{1}{\pi} \frac{\epsilon + \eta}{(x - y)^2 + (\epsilon + \eta)^2} \quad (25.11)$$

Therefore, for $x \neq y$ and in the limit $\epsilon + \eta \rightarrow 0^+$:

$$\int \frac{dx'}{\pi^2} \frac{\mathcal{P}}{x' - x} \frac{\mathcal{P}}{x' - y} = \delta(x - y) \quad (25.12)$$

Exercise* 25.2.5 (Hilbert transform).

$$(\mathcal{H}f)(x) = \mathcal{P} \int_{\mathbb{R}} \frac{dx'}{\pi} \frac{f(x')}{x - x'} \quad (25.13)$$

By means of (25.12) show that $(\mathcal{H}^2\varphi)(x) = -\varphi(x)$. Therefore, the solution of the integral equation $\mathcal{H}f = g$ is $f = -\mathcal{H}g$.

⁵ The identities were discovered by Sokhotski in 1873, and proven rigorously about thirty years later by Josip Plemelj in the context of complex integrals.

Exercise 25.2.6. Show that this is a tempered distribution:

$$\langle P_{x^2}^{-1} | \varphi \rangle = \int_{\mathbb{R}} dx \frac{\varphi(x) - \varphi(0)}{x^2} \quad (25.14)$$

25.3 Linear response and Kramers-Krönig relations*

Physical systems are tested by perturbing it with external fields. If the perturbation is weak, the response is a property of the system itself. Notable examples are $D_i = \epsilon_{ij} E_j$, $J_i = \sigma_{ij} E_j$, $M_i = \chi_{ij} H_j$, ... The theory of **linear response** evaluates the variation in time of an observable of a system that is coupled to a weak time-dependent field $\delta\varphi(t)$, in the linear approximation. The physical requirement of *causality*, i.e. the effect on the system may only depend on the field's values at earlier times, implies the general Kramers and Kronig relations for the response function.

Let $g(t)$ be the value at time t of a measurable quantity of the system in presence of the perturbation, and $g_0(t)$ be the value of the same quantity in absence of the perturbation. In the linear approximation, the variation $\delta g(t) = g(t) - g_0(t)$ is linearly related to the external perturbation through a *response function* $R(t, t')$ that only depends on the variables of the unperturbed system:

$$\delta g(t) = \int_{-\infty}^t R(t, t') \delta\varphi(t') dt'$$

The integral involves the history of the system at times less than t because of the physical requirement of causality.

If the properties of the unperturbed system are time-independent (as in thermal equilibrium), the response function depends on $t - t'$. If the upper limit t is replaced by $+\infty$ with the insertion of a theta function, the integral becomes the convolution:

$$\delta g(t) = \int_{-\infty}^{+\infty} \theta(t - t') R(t - t') \delta\varphi(t') dt' \quad (25.15)$$

Hereafter we consider this very common situation.

In frequency space the convolution (25.15) becomes the product of the Fourier transforms⁶, and the linear response takes the simple form of a direct proportionality between response and driving field *at the same frequency*:

$$\boxed{\delta g(\omega) = \chi(\omega) \delta\varphi(\omega)} \quad (25.16)$$

⁶ In physics it is customary to define the Fourier transform of a function of time as $\tilde{f}(\omega) = \int_{\mathbb{R}} dt f(t) e^{i\omega t}$, with inverse $f(t) = \int_{\mathbb{R}} \frac{d\omega}{2\pi} \tilde{f}(\omega) e^{-i\omega t}$. In this section we use this convention.

Some examples were given above (where each quantity depends on ω , with possible further dependence on wave-vector). The response function $\chi(\omega)$ is the *generalized susceptibility*:

$$\chi(\omega) = \int_{\mathbb{R}} dt e^{i\omega t} \theta(t) R(t) = \int_0^{\infty} dt e^{i\omega t} R(t) \quad (25.17)$$

According to a theorem by Paley and Wiener, if $R \in \mathcal{L}^2(0, \infty)$, the function $\chi(\omega)$ is analytic on $\text{Im } \omega \geq 0$. This is a consequence of causality and, in turn, it implies the *Kramers - Kronig relations*. They were obtained independently in 1926 and 1927, and relate the real and imaginary parts of the response function in ω space:

Proposition 25.3.1. *Suppose that $\chi(\omega) \rightarrow 0$ if $|\omega| \rightarrow \infty$; for real ω it is:*

$$\boxed{\text{Re } \chi(\omega) = -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \chi(\omega')}{\omega - \omega'}, \quad \text{Im } \chi(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Re } \chi(\omega')}{\omega - \omega'}} \quad (25.18)$$

Proof. Since $\chi(\omega')$ is analytic in $\text{Im } \omega' > 0$ it is:

$$\int_{\mathbb{R}} d\omega' \frac{\chi(\omega')}{\omega - \omega' - i\epsilon} = 0, \quad \omega \in \mathbb{R}$$

(check: close the path of integration with a semicircle in the upper half plane). The Plemelj-Sokhotski formula gives:

$$0 = \int_{\mathbb{R}} d\omega' \frac{\chi(\omega')}{\omega - \omega'} + i\pi\chi(\omega)$$

Separation of real and imaginary parts gives the relations. □

25.4 Zeros of large- n Hermite polynomials*

Let $x_1 \dots x_n$ be the zeros of the Hermite polynomial $H_n(x)$. They are real and simple. We wish to evaluate their distribution when n is large. The differential equation (11.20), $H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0$, becomes Weber's equation for the Hermite function (19.28) (the equation of the harmonic oscillator in quantum mechanics):

$$-h_n''(x) + (x^2 - 2n - 1)h_n(x) = 0$$

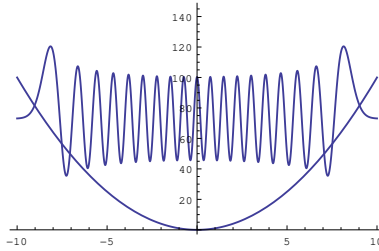


Figure 25.1 The oscillatory part of the Hermite function h_{36} with its 36 real zeros, is confined in the interval $|x| < \sqrt{73}$, between the extreme zeros of h''_{36} . The plot of the function is shifted upwards by 73 to show that the zeros are confined in the parabolic well.

The zeros of $H_n(x)$ are confined in the interval⁷ $x^2 < 2n + 1$. Rescale the zeros $x_i = s_i \sqrt{2n}$, ($i = 1 \dots n$).

The limit distribution of the rescaled zeros is $\rho(s) = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \delta(s - s_i)$ with support $\sigma = [-1, 1]$. We introduce the functions $F_n(z)$ and the limit function:

$$F_n(z) = \frac{1}{n} \sum_{i=1}^n \frac{1}{z - s_i} \quad F(z) = \int_{\sigma} ds \frac{\rho(s)}{z - s} \quad z \notin \sigma$$

For large $|z|$, $F(z)$ behaves as $1/z$ and, by the Sokhotski-Plemelj identity:

$$\rho(s) = \frac{1}{\pi} \text{Im} F(s - i\epsilon) \tag{25.19}$$

The limit function $F(z)$ is obtained from $F_n(z)$ by noting that

$$\frac{H'_n(x)}{H_n(x)} = \sum_{i=1}^n \frac{1}{x - \sqrt{2n} s_i} = \sqrt{\frac{n}{2}} F_n\left(\frac{x}{\sqrt{2n}}\right)$$

A derivative in x and the equation $H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0$ give the Riccati equation $\frac{1}{n} F'_n(z) + F_n^2(z) - 4zF_n(z) + 4 = 0$. In the large- n limit the derivative term is neglected: $F^2(z) - 4zF(z) + 4 = 0$. The solution with correct large z asymptotics is: $F(z) = 2z - 2\sqrt{z^2 - 1}$.

Eq.(25.19) gives the *semicircle law*:

$$\rho(s) = \begin{cases} \frac{2}{\pi} \sqrt{1 - s^2} & \text{if } |s| < 1 \\ 0 & \text{if } |s| > 1 \end{cases} \tag{25.20}$$

⁷ If $x^2 > 2n + 1$, $h_n(x)$ and $h''_n(x)$ have the same sign, and vanish at infinity. As $|x|$ decreases from ∞ , $|h_n(x)|$ increases. For a zero to occur the curvature h''_n must change sign, and then the function may start to point to the real axis and gain a zero.

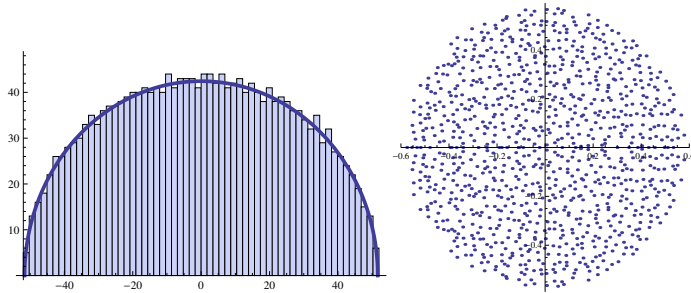


Figure 25.2 Left: histogram of the eigenvalues of two Hermitian matrices of size 1000 with real and imaginary parts of matrix elements chosen uniformly in $[-1,1]$. The Semicircle Law by Wigner is a general feature of eigenvalues of large random real-symmetric or complex-Hermitian matrices with independent identically distributed (i.i.d.) matrix elements. Right: the complex eigenvalues of two non-Hermitian matrices of size 1000 with i.i.d. matrix elements (Circle Law by Ginibre). If the real and imaginary parts have different variance, the distribution is the Elliptic Law.

It is a remarkable fact that the semicircle law also describes the distribution of eigenvalues of Hermitian matrices with random matrix elements, in the large n limit.

25.5 Eigenvalues of random matrices*

A random matrix is an element of an ensemble of matrices with some probability distribution. The matrices may be further restricted to be Hermitian, unitary, positive, banded, ... Interesting question are: what are the statistical properties of the eigenvalues and eigenvectors? To some extent they are universal, i.e. independent of the probability measure: this makes random matrices important.

Random matrices in physics were introduced by Eugene Wigner in the fifties for the statistical properties of sequences of nuclear resonances⁸. Since then, they found many applications: quantum systems with chaotic classical motion (quantum chaos), transport in mesoscopic structures with impurities, spectra of Dirac matrices in QCD, molecular spectra, statistical mechanics on random graphs, random surfaces, etc. The subject is still evolving in several unexpected directions, with beautiful mathematics⁹.

⁸ It was noted that the energy separations s of resonances normalized by an average value, obey the same statistical laws $P(s) \approx s^\beta e^{-ks^2}$ of the normalized separations of eigenvalues of Gaussian random matrices (k is a constant, β is 1 for real symmetric matrices, 2 for complex Hermitian matrices and 4 for quaternionic self-dual). It shows the feature of “level repulsion”: small spacings are rare.

⁹ see: *The Oxford Handbook of Random Matrix Theory*, G. Akemann, J. Baik and P. Di Francesco Editors, Oxford University Press, 2011; M. L. Mehta, *Random Matrices*, 3rd Ed. Elsevier, 2004; F. Haake, *Quantum signatures of chaos*, 3rd Ed. Springer, 2010, and the friendly-readable book by G. Livan, M. Novaes and P. Vivo, *Introduction to random matrices, theory and practice*, online at <https://arxiv.org/pdf/1712.07903.pdf>.

The *Gaussian Unitary Ensemble* (GUE) of matrices consists of Hermitian matrices H_{ij} where H_{ii} , $\text{Re}H_{ij}$ and $\text{Im}H_{ij}$ ($i < j$) are independent random numbers with Gaussian distribution. The probability measure on GUE is

$$p(H)dH \propto \prod_i e^{-nH_{ii}^2} dH_{ii} \prod_{i<j} e^{-2n|H_{ij}|^2} d^2H_{ij} = e^{-n\text{tr}H^2} dH$$

The matrix set and the measure are invariant under the action of the unitary group $H \rightarrow U^\dagger H U$. In place of the matrix elements, the decomposition $H = U^\dagger \Lambda U$ introduces new coordinates: the n real eigenvalues, and $n(n-1)$ parameters for the column eigenvectors which make the matrix U .

The unitary invariance produces the factorization $dH = dU_{\text{Haar}} dp(\Lambda)$, where the first factor is the Haar measure of $\text{SU}(n)$ and dp is the joint probability density for the GUE(n) eigenvalues:

$$p(\lambda_1 \dots \lambda_n) = \frac{1}{Z_n} \prod_{i<j} (\lambda_j - \lambda_i)^2 e^{-n\sum \lambda_i^2} \equiv \frac{1}{Z_n} e^{-n^2 V(\lambda_1 \dots \lambda_n)}$$

$$V(\lambda_1 \dots \lambda_n) = \frac{1}{n} \sum_i \lambda_i^2 - \frac{2}{n^2} \sum_{i<j} \log |\lambda_i - \lambda_j|.$$

with normalization constant $Z_n = \int d\lambda_1 \dots d\lambda_n \exp(-n^2 V)$. The probability density vanishes quadratically when two eigenvalues approach¹⁰ (degenerate eigenvalues are rare, with level repulsion exponent $\beta = 2$).

For large n , the largest contribution to the probability density comes from the set of eigenvalues that minimize the “potential energy” V . It has the interpretation of minimal energy state of a two-dimensional gas of n charged particles that interact via a log potential, in a harmonic well. The minimum solves $\partial V / \partial \lambda_i = 0$:

$$\lambda_i = \frac{2}{n} \sum_{j \neq i} \frac{1}{\lambda_i - \lambda_j} \quad \rightarrow \quad x_i = \sum_{j \neq i} \frac{1}{x_i - x_j}, \quad x_i = \sqrt{\frac{n}{2}} \lambda_i$$

The solution is found by a nice trick by Stieltjes: let $p(x) = (x - x_1) \dots (x - x_n)$. By eq.(9.4) the n conditions for minimum become: $x_i = p''(x_i) / p'(x_i)$ i.e. the polynomial $p''(x) - x p'(x)$ must be zero at $x = x_1, \dots, x_n$. Since it is of degree n , it is proportional to $p(x)$ itself:

$$p''(x) - x p'(x) + n p(x) = 0$$

¹⁰ A simple argument for level repulsion. Let x, y be the real eigenvalues of the 2×2 GUE matrix ($\beta = 2$):

$$\begin{pmatrix} a & b - ic \\ b + ic & d \end{pmatrix}, \quad |x - y| = \sqrt{(a - d)^2 + 4b^2 + 4c^2}$$

To have $x = y$ we need that the random numbers $a - d$, b and c are zero simultaneously: this is very unlikely. For random real symmetric matrices (GOE) it is $c = 0$ and level repulsion is weaker ($\beta = 1$).

The solution is the Hermite polynomial $H_n(x\sqrt{2})$. Therefore, for $n \rightarrow \infty$ the eigenvalues of a random GUE matrix (with probability one) have a *semicircle distribution* with radius determined by the variance of the Gaussian (in this case the radius is $\frac{1}{2}\sqrt{n}$).

25.6 Distributional calculus

Important operations such as conjugation, derivative, Fourier transform, may be extended simply and naturally from well behaved functions (such as test functions or functions associated to regular distributions) to distributions (generalized functions, which may be as awkward as a delta function). The procedure reproduces the steps of this first example.

Complex conjugation has a natural definition if the distribution is regular: if f is the regular distribution $\langle f|\varphi \rangle = \int dx f(x)\varphi(x)$, its complex conjugate is the distribution f^* with action $\langle f^*|\varphi \rangle = \int dx \overline{f(x)}\varphi(x) = \langle f|\overline{\varphi} \rangle$. As the last equality does not depend on f being a regular distribution, it provides the extension: the complex conjugate of a distribution f is the distribution

$$\langle f^*|\varphi \rangle := \overline{\langle f|\overline{\varphi} \rangle} \quad (25.21)$$

Example 25.6.1. *Dirac's delta is real: $\delta_a^* = \delta_a$.*

Along the same line one defines the multiplication of a tempered distribution by a \mathcal{C}^∞ function g that is algebraically bounded with all its derivatives¹¹. It is the tempered distribution

$$\langle gf|\varphi \rangle := \langle f|g\varphi \rangle \quad (25.22)$$

25.6.1 Derivative

Consider a regular distribution with a function $f \in \mathcal{C}^1(\mathbb{R})$. Then f' still defines a regular distribution and integration by parts gives:

$$\langle f'|\varphi \rangle = \int_{-\infty}^{\infty} dx f' \varphi = - \int_{-\infty}^{\infty} dx f \varphi' = - \langle f|\varphi' \rangle.$$

This evaluation suggests the definition of the derivative of *any* distribution:

Definition 25.6.2. The derivative of a distribution f is the distribution f' with action

$$\boxed{\langle f'|\varphi \rangle := - \langle f|\varphi' \rangle} \quad (25.23)$$

¹¹ $g(x) = \cos(e^x)$ is bounded and smooth, but $g'(x)$ is unbounded

As derivation is a continuous operator on $\mathcal{S}(\mathbb{R})$, the derivative of tempered distributions gives tempered distributions, and is linear and continuous on $\mathcal{S}'(\mathbb{R})$. One can evaluate as many derivatives of a distribution as wanted.

Example 25.6.3. *Derivative of Heaviside's functional θ_a .*

By definition: $\langle \theta'_a | \varphi \rangle = - \langle \theta_a | \varphi' \rangle = - \int_a^\infty \varphi'(x) dx = \varphi(a)$. Therefore: $\theta'_a = \delta_a$, or

$$\boxed{\frac{d}{dx} \theta(x-a) = \delta(x-a)}$$

Example 25.6.4. *Derivative of δ_a .* By definition: $\langle \delta'_a | \varphi \rangle = -\varphi'(a)$.

Exercise 25.6.5. Show that: $\frac{d}{dx}|x| = \text{sign}x$, $\langle \delta'_a | \varphi \rangle = -\frac{d}{da} \langle \delta_a | \varphi \rangle$.

Example 25.6.6. *The derivative of $F(x) = \theta(x^2 - m^2)$, $m > 0$, is by definition: $\langle F' | \varphi \rangle = - \int_{-\infty}^{-m} dx \varphi'(x) - \int_m^\infty dx \varphi'(x) = -\varphi(-m) + \varphi(m) = \langle \delta_m - \delta_{-m} | \varphi \rangle$. As an identity among generalized functions one writes:*

$$\frac{d}{dx} \theta(x^2 - m^2) = \delta(x-m) - \delta(x+m).$$

In ordinary calculus one would write: $\frac{d}{dx} \theta(x^2 - m^2) = 2x \delta(x^2 - m^2)$, leading to the conclusion

$$\delta(x^2 - m^2) = \frac{1}{2x} [\delta(x-m) - \delta(x+m)] = \frac{1}{2m} [\delta(x-m) + \delta(x+m)]$$

The example can be generalized to a very useful identity:

Proposition 25.6.7. *Let f be a polynomially bounded function with all its derivatives, with simple zeros x_k . Then:*

$$\boxed{\delta(f(x)) = \sum_{k=1}^n \frac{\delta(x-x_k)}{|f'(x_k)|}} \quad (25.24)$$

Proof. The function $\theta[f(x)]$ is 1 where $f > 0$ and zero elsewhere, and $\langle \theta[f] | \varphi \rangle = \int_{I_1} \varphi(x) dx + \int_{I_2} \varphi(x) dx + \dots$ (where $f(x) > 0$ on each interval I_k). The derivative as a distribution is:

$$\langle \theta'[f] | \varphi \rangle = - \sum_j \int_{I_j} \varphi'(x) dx = - \sum_j [\varphi(b_j) - \varphi(a_j)]$$

where a_j and b_j are the endpoints (that are the roots x_k of f plus, possibly, points at infinity). If an interval is unbounded, $\varphi(\pm\infty) = 0$. We may write:

$$\langle \theta'[f] | \varphi \rangle = \sum_k \varphi(x_k) \text{sign}[f'(x_k)] = \sum_k \int_{\mathbb{R}} dx \frac{\delta(x - x_k)}{|f'(x_k)|} f'(x) \varphi(x)$$

At the same time, the derivative of $\theta[f(x)]$ is $\delta(f(x))f'(x)$. Equality establishes the result, being $f'\varphi$ a test function. □

Example 25.6.8. *It is instructive to evaluate the derivative of the regular distribution $f(x) = \log|x|$. By definition it is*

$$\langle f' | \varphi \rangle = - \int_{\mathbb{R}} dx \log|x| \varphi'(x)$$

An integration by parts would give a non-integrable factor $1/x$. We make progress by removing a neighborhood of $x = 0$, noting that the integral coincides with the following one:

$$\begin{aligned} &= - \lim_{\epsilon \rightarrow 0^+} \left[\int_{-\infty}^{-\epsilon} dx \log(-x) \varphi'(x) + \int_{\epsilon}^{\infty} dx \log x \varphi'(x) \right] \\ &= \lim_{\epsilon \rightarrow 0^+} \log \epsilon [\varphi(\epsilon) - \varphi(-\epsilon)] + \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty} dx \frac{1}{x} \varphi(x) = \int_{-\infty}^{+\infty} dx \frac{1}{x} \varphi(x) \end{aligned}$$

The lesson is that the introduction of an appropriate ϵ may surmount difficulties. Here we identify f' with $P\frac{1}{x}$.

We state but not prove the following characterisation of tempered distributions:

Theorem 25.6.9. *Every tempered distribution is the distributional derivative of finite order of a continuous algebraically bounded function: $f \in \mathcal{S}'(\mathbb{R}) \Leftrightarrow$ there is a continuous function ξ such that $|\xi(x)| \leq C(1 + |x|^n)$ for some C and n , and $k \geq 0$ such that*

$$\langle f | \varphi \rangle = \langle \xi^{(k)} | \varphi \rangle = (-1)^k \int_{-\infty}^{\infty} dx \xi(x) \varphi^{(k)}(x).$$

25.7 Probability densities

The delta and theta functions are very useful in probability theory. Consider a function f of a random variable x with probability density $p(x)$. The probability that f is less than a value F is the measure of the set where the property $f < F$ is fulfilled: $P(f < F) = \int dx p(x) \theta(F - f(x))$. The probability density for the random variable F is $p(F) = \int dx p(x) \delta(F - f(x))$.

Recall that a random variable x has normal distribution N_{μ,σ^2} if the probability density is Gaussian with mean $\langle x \rangle = \mu$ and variance $\langle (x - \mu)^2 \rangle = \sigma^2$:

$$N_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(x - \mu)^2}{2\sigma^2} \right] \tag{25.25}$$

A random variable has Cauchy (or Lorentzian) distribution with parameter $z = \mu + i\delta$ if the probability density is

$$C_{\mu+i\delta}(x) = \frac{\delta}{\pi} \frac{1}{(x - \mu)^2 + \delta^2} \tag{25.26}$$

Here $\langle x \rangle = \mu$ and $p(\mu \pm \delta) = \frac{1}{2}p(\mu)$. The variance is infinite.

Example 25.7.1. If x has distribution N_{μ,σ^2} , the distribution of $s = x^2$ is:

$$p(s) = \int_{-\infty}^{+\infty} dx \delta(s - x^2) N_{\mu,\sigma^2}(x) = \frac{1}{2\sqrt{s}} \left[N_{\mu,\sigma^2}(\sqrt{s}) + N_{\mu,\sigma^2}(-\sqrt{s}) \right]$$

The function is shown in Fig.25.3. The average and variance are: $\bar{s} = \mu^2 + \sigma^2$, $\sigma_s^2 = 2\sigma^2(\sigma^2 + 2\mu^2)$.

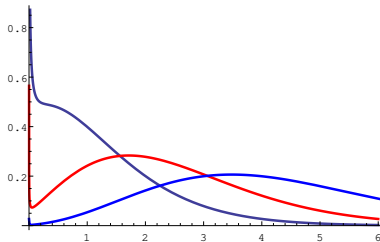


Figure 25.3 The distribution of x^2 , where x is normally distributed with $\sigma = 0.5$, $\mu = 1$ (black), $\mu = 1.5$ (red) and $\mu = 2$ (blue)

Example 25.7.2. If x and y have normal distributions with zero mean N_{0,σ^2} the probability density of $X = x/y$ is:

$$\begin{aligned} p(X) &= \int dx dy p(x)p(y)\delta(X - \frac{x}{y}) = \int dx dy p(x)p(y)|y|\delta(x - Xy) \\ &= \frac{1}{2\pi\sigma^2} \int dy |y| e^{-\frac{1}{2\sigma^2}(1+X^2)y^2} = \frac{1}{\pi} \frac{1}{X^2 + 1} \end{aligned}$$

This is the Cauchy probability distribution with zero mean.

Example 25.7.3 (Chi-square distribution). If x_1, \dots, x_N are independent random variables with same distribution N_{0, σ^2} , the probability density of $X = x_1^2 + \dots + x_N^2$ is

$$\begin{aligned}\chi_N^2(X) &= \frac{1}{(2\pi\sigma^2)^{N/2}} \int d^N x e^{-\frac{1}{2\sigma^2} \|x\|^2} \delta(X - \|x\|^2) \\ &= \frac{1}{(2\pi\sigma^2)^{N/2}} e^{-X/2\sigma^2} \int d^N x \delta(X - \|x\|^2) \\ &= \frac{1}{(2\pi\sigma^2)^{N/2}} e^{-X/2\sigma^2} \Omega_{N-1} \int_0^\infty dr r^{N-1} \delta(X - r^2)\end{aligned}$$

where $\Omega_{N-1} = 2\pi^{N/2}/\Gamma(N/2)$ is the surface of the sphere $\|x\| = 1$ in \mathbb{R}^N (see ex.12.3.2). Now use $\delta(X - r^2) = \frac{1}{2\sqrt{X}} \delta(r - \sqrt{X})$ and obtain

$$\chi_N^2(X) = \frac{1}{2\sigma^2 \Gamma(N/2)} \left[\frac{X}{2\sigma^2} \right]^{\frac{N}{2}-1} \exp\left[-\frac{X}{2\sigma^2}\right]$$

Example 25.7.4 (Central limit theorem). Consider N independent random variables x_j with same distribution $p(x)$. The sum of such variables is a random variable with distribution $p(s) = \int dx_1 \dots dx_N p(x_1) \dots p(x_N) \delta(s - \sum_i x_i)$. Now represent the delta function as a Fourier integral and obtain:

$$p(s) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{-iks} \left[\int dx p(x) e^{ikx} \right]^N \quad (25.27)$$

The function in parenthesis defines the characteristic function $\chi_p(k)$ of $p(x)$. If p is integrable, the function χ_p is bounded by $\|p\|_1 = 1$, is continuous, and decays at infinity (Riemann-Lebesgue theorem). Its power N decays even faster. For large N , because of fast decay of $\chi_p^N(k)$, the integral is controlled by the small k values, where

$$\chi_p(k) = 1 + ik\langle x \rangle - \frac{1}{2}k^2\langle x^2 \rangle + \dots \approx e^{ik\mu - \frac{1}{2}k^2(\langle x^2 \rangle - \mu^2)} + \dots$$

Up to terms negligible for large N , we gain the characteristic function of the normal distribution:

$$\chi_N(k) = \frac{1}{\sqrt{2\pi\sigma^2}} \int dx e^{-\frac{(x-\mu)^2}{2\sigma^2} + ikx} = e^{-\frac{1}{2}k^2\sigma^2 + ik\mu}$$

For the sum of normally distributed random variables the integral (25.27) is exactly done for any N , and gives the normal distribution with mean $\bar{s} = N\mu$, variance $\sigma_s^2 = N\sigma^2$:

$$p(s) = \frac{1}{\sqrt{2\pi N\sigma^2}} \exp\left[-\frac{(s - N\mu)^2}{2N\sigma^2}\right] \quad (25.28)$$

As discussed, for large N this results holds also for the sum of N independent identical random variables that are not Gaussian, with mean μ and variance σ^2 .

Exercise 25.7.5. Particles are uniformly distributed in a unit square. Show that the probability for a particle to have distance r from a corner is

$$p(r) = r \times \begin{cases} \frac{\pi}{2} & r < 1 \\ \frac{\pi}{2} - 2\arccos\frac{1}{r} & 1 \leq r \leq \sqrt{2} \end{cases}$$

Exercise 25.7.6. 1) If x is Cauchy-distributed with parameter $z = \mu + i\delta$, then $1/x$ is Cauchy-distributed with parameter $1/\bar{z}$.

2) If x_1 and x_2 are Cauchy-distributed with parameters z_1 and z_2 , then $x_1 + x_2$ is Cauchy-distributed with parameter $z_1 + z_2$ (use the theorem of residues).

Exercise 25.7.7. The eigenvalues of random matrices in GUE(2) have joint distribution $p(\lambda_1, \lambda_2) = \frac{1}{\pi}(\lambda_1 - \lambda_2)^2 e^{-\lambda_1^2 - \lambda_2^2}$. Show that the distribution of level spacings $s = |\lambda_1 - \lambda_2|$ is: $p(s) = \sqrt{\frac{2}{\pi}} s^2 e^{-s^2/2}$. Then, evaluate $\langle s \rangle$ and show that the normalized spacing $S = s/\langle s \rangle$ has distribution¹² (Wigner surmise)

$$p(S) = \frac{32}{\pi^2} S^2 \exp\left(-\frac{4}{\pi} S^2\right)$$

The Wigner surmise for symmetric, hermitian and quaternionic matrices has been thoroughly applied as reference for the spectral properties of quantum systems with chaotic classical behaviour.

25.7.1 Fourier transform

To extend the Fourier transform to distributions, start from regular functionals. Suppose that both f and $\mathcal{F}f$ are functions that produce regular distributions (for example f is in

¹² Fritz Haake, Quantum Signatures of Chaos, Springer

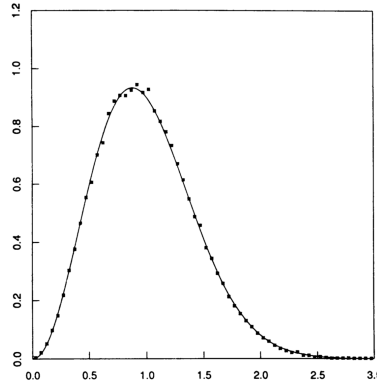


Figure 25.4 The normalized distribution of the spacings of 10^5 zeros of the Riemann function $\zeta(z)$ on the line $\text{Im}z = \frac{1}{2}$ and the Wigner surmise (from: A. M. Odlyzko, On the distribution of spacings between zeros of the Zeta function, *Mathematics of Computation* 48 (1987) 273–308).

\mathcal{S}). Then:

$$\begin{aligned} \langle \mathcal{F} f | \varphi \rangle &= \int_{\mathbb{R}} dx (\mathcal{F} f)(x) \varphi(x) = \int_{\mathbb{R}} dx \varphi(x) \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{-ikx} f(k) \\ &= \int_{\mathbb{R}} dk f(k) \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \varphi(x) = \langle f | \mathcal{F} \varphi \rangle \end{aligned}$$

The extension to all distributions is:

Definition 25.7.8. The Fourier transform of a tempered distribution f is the distribution $\mathcal{F} f$ with action

$$\boxed{\langle \mathcal{F} f | \varphi \rangle := \langle f | \mathcal{F} \varphi \rangle} \tag{25.29}$$

Proposition 25.7.9. The Fourier transform $\mathcal{F} : \mathcal{S}'(\mathbb{R}) \rightarrow \mathcal{S}'(\mathbb{R})$ is invertible ($\mathcal{F} \mathcal{F}^{-1} f = f$) and continuous.

Proof. Continuity and the inversion property are exported from the same properties in $\mathcal{S}(\mathbb{R})$: $\langle \mathcal{F}^{-1} \mathcal{F} f | \varphi \rangle = \langle \mathcal{F} f | \mathcal{F}^{-1} \varphi \rangle = \langle f | \mathcal{F} \mathcal{F}^{-1} \varphi \rangle = \langle f | \varphi \rangle$.

Since the Fourier transform is linear, it is enough to check continuity in the origin: let $f_n \rightarrow 0$ in $\mathcal{S}'(\mathbb{R})$ then $\langle \mathcal{F} f_n | \varphi \rangle = \langle f_n | \mathcal{F} \varphi \rangle \rightarrow 0$ i.e. $\mathcal{F} f_n \rightarrow 0$. □

Example 25.7.10. Fourier transform of δ_a .

$$\langle \mathcal{F} \delta_a | \varphi \rangle = \langle \delta_a | \mathcal{F} \varphi \rangle = (\mathcal{F} \varphi)(a) = \int_{\mathbb{R}} dx \frac{e^{-iax}}{\sqrt{2\pi}} \varphi(x).$$

The Fourier transform of Dirac's delta is the regular distribution with function:

$$\boxed{(\mathcal{F} \delta_a)(x) = \frac{e^{-iax}}{\sqrt{2\pi}}} \quad (25.30)$$

In particular: $1 = \sqrt{2\pi} \mathcal{F} \delta_0 (= \sqrt{2\pi} \mathcal{F}^{-1} \delta_0)$.

The same result is obtained by exploiting the continuity of the Fourier transform, acting on a regular approximation of δ_a . For example:

$$u_\epsilon(x) = \frac{1}{\pi} \frac{\epsilon}{(x-a)^2 + \epsilon^2}, \quad (\mathcal{F} u_\epsilon)(x) = \frac{1}{\sqrt{2\pi}} e^{-\epsilon|x-ia|} \quad (25.31)$$

As a family of regular distributions, for $\epsilon \rightarrow 0$ the sequence u_ϵ converges to δ_a . The sequence of Fourier transforms also converges in \mathcal{S}' and the limit is (25.30).

Example 25.7.11. The following approximation of the delta function is useful:

$$\boxed{\lim_{N \rightarrow \infty} \frac{\sin(Nx)}{\pi x} = \delta_0} \quad (25.32)$$

A simple proof based on continuity of the Fourier transform: since $\chi_{[-N,N]} \rightarrow 1$ in $\mathcal{S}'(\mathbb{R})$, then $\mathcal{F} \chi_{[-N,N]} \rightarrow \sqrt{2\pi} \delta_0$.

Example 25.7.12.

$$\mathcal{F} x^n = i^n \sqrt{2\pi} \delta_0^{(n)} \quad (25.33)$$

$\langle \mathcal{F} x^n | \varphi \rangle = \langle 1 | x^n \mathcal{F} \varphi \rangle = (-i)^n \langle 1 | \mathcal{F} \varphi^{(n)} \rangle$. Since $1 = \sqrt{2\pi} \mathcal{F} \delta_0$, it is: $\langle \mathcal{F} x^n | \varphi \rangle = (-i)^n \sqrt{2\pi} \langle \delta_0 | \varphi^{(n)} \rangle = i^n \sqrt{2\pi} \langle \delta_0^{(n)} | \varphi \rangle$

Example 25.7.13. The discrete Laplacian of a function $u_{\mathbf{n}}$ on the hypercubic lattice, $\mathbf{n} \in \mathbb{Z}^d$, is

$$(Du)_{\mathbf{n}} = 2du_{\mathbf{n}} - \sum_{\langle \mathbf{n}, \mathbf{n}' \rangle} u_{\mathbf{n}'}$$

where the sum is on the $2d$ nearest neighbour lattice points of \mathbf{n} . The eigenvectors are $u_{\mathbf{n}} = \exp(i\mathbf{n} \cdot \mathbf{p})$, with eigenvalues $E(\mathbf{p}) = 2d - (2 \cos p_1 + \dots + 2 \cos p_d)$, where $0 \leq p \leq 2\pi$. The spectral density is

$$p_d(E) = \int_0^{2\pi} \frac{dp_1}{2\pi} \dots \int_0^{2\pi} \frac{dp_d}{2\pi} \delta(E - E(\mathbf{p}))$$

Now express the delta function as a Fourier integral:

$$\begin{aligned}
 p_d(E) &= \int_0^{2\pi} \frac{dp_1}{2\pi} \dots \int_0^{2\pi} \frac{dp_d}{2\pi} \int \frac{dk}{2\pi} e^{ik(E-E(\mathbf{p}))} \\
 &= \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(E-2d)} \left[\int_0^{2\pi} \frac{dp}{2\pi} e^{2ik\cos p} \right]^d \\
 &= \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(E-2d)} J_0(2k)^d
 \end{aligned}$$

where J_0 is a Bessel function, eq.(13.5). Since J_0 is even, the integral becomes:

$$p_d(E) = \int_0^{\infty} \frac{dk}{\pi} \cos[k(E-2d)] J_0(2k)^d \tag{25.34}$$

The support is the interval $[0, 4d]$. The integral in $d = 1, 2$ is found in tables of integrals. The numerical evaluation for $d = 3$ is shown in Fig.25.5.

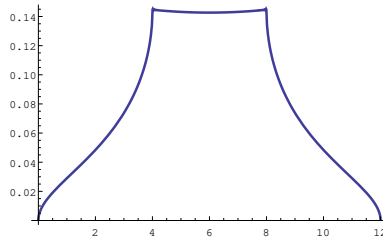


Figure 25.5 The density of eigenvalues of the discrete Laplacian in $d = 3$.

Example 25.7.14. Fourier transform of $P \frac{1}{x-a}$.

$$\langle \mathcal{F} \frac{P}{x-a} | \varphi \rangle = \int \frac{dx}{x-a} \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} e^{-ikx} \varphi(k) = \lim_{R \rightarrow \infty} \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} \varphi(k) e^{-ika} \int_{-R}^{+R} \frac{dx}{x} e^{-ikx}.$$

The interval $[-R, R]$ is specified to exchange the integrals. The principal-valued integral is evaluated in \mathbb{C} with appropriate contour:

$$\int_{-R}^{+R} \frac{dx}{x} e^{-ikx} = \text{sign}(k) \left[-i\pi + i \int_0^{\pi} d\theta e^{i|k|Re^{i\theta}} \right].$$

The second term, coming from the semi-circle, is bounded in modulus and yields an integral with $\varphi(k)$ that vanishes for $R \rightarrow \infty$. Then:

$$(\mathcal{F}P \frac{1}{x-a})(k) = -i\sqrt{\frac{\pi}{2}} \operatorname{sign}(k) e^{-ika} \quad (25.35)$$

Example 25.7.15. Fourier transform of θ_a .

$$\langle \mathcal{F}\theta_a | \varphi \rangle = \langle \theta_a | \mathcal{F}\varphi \rangle = \int_a^\infty dx \int_{\mathbb{R}} \frac{dy}{\sqrt{2\pi}} e^{-ixy} \varphi(y)$$

Since integrals cannot be exchanged, introduce a convergence factor and consider the Fourier transform of the distributions $\theta_{a,\epsilon}(x) = e^{-\epsilon x} \theta_a(x)$ ($\epsilon > 0$). As $\theta_{a,\epsilon} \rightarrow \theta_a$ and the Fourier transform is continuous in \mathcal{S}' , it is

$$\begin{aligned} \langle \mathcal{F}\theta_a | \varphi \rangle &= \lim_{\epsilon \rightarrow 0^+} \int_a^\infty dx e^{-\epsilon x} \int_{\mathbb{R}} \frac{dy}{\sqrt{2\pi}} e^{-ixy} \varphi(y) \\ &= \int_{\mathbb{R}} dy \varphi(y) \int_a^\infty \frac{dx}{\sqrt{2\pi}} e^{-ixy - \epsilon x} = \int_{\mathbb{R}} dy \frac{1}{i\sqrt{2\pi}} \frac{e^{-iay}}{y - i\epsilon} \varphi(y) \end{aligned}$$

In the last line it is understood that the limit $\epsilon \rightarrow 0^+$ is taken. The limit can be done after the action on a test function is evaluated (this is the meaning of convergence of distributions). We obtain $\mathcal{F}\theta_a$ as a limit of regular distributions:

$$(\mathcal{F}\theta_a)(x) = \frac{1}{i\sqrt{2\pi}} \frac{e^{-iax}}{x - i\epsilon}. \quad (25.36)$$

Inversion gives a useful representation of Heaviside's function:

$$\theta(x-a) = \int_{-\infty}^{\infty} \frac{dk}{2\pi i} \frac{e^{ik(x-a)}}{k - i\epsilon} = i \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{-ik(x-a)}}{k + i\epsilon} \quad (25.37)$$

Exercise 25.7.16. Consider the functional

$$\langle F_N | \varphi \rangle = \frac{1}{N} \sum_{k=0}^{N-1} \varphi\left(\frac{k}{N}\right), \quad \varphi \in \mathcal{S}(\mathbb{R})$$

Is it a tempered distribution? Does the sequence $\{F_N\}$ converge to a distribution? Evaluate $\{\mathcal{F}F_N\}$. Does the sequence converge in $\mathcal{S}'(\mathbb{R})$ for $N \rightarrow \infty$?

Exercise 25.7.17 (Fourier transform of the sign-function). *Show that*

$$(\mathcal{F} \operatorname{sign})(x) = -i\sqrt{\frac{2}{\pi}} \operatorname{P} \frac{1}{x} \tag{25.38}$$

Exercise 25.7.18. *Evaluate the Fourier transform of $(x - a); e^{-i\omega x}$ ($\omega \in \mathbb{R}$).*

Exercise 25.7.19. *What is the Plemelj-Sokhotski identity after Fourier transform?*

25.8 Linear operators on distributions*

We'll prove that the Hermite functions are a complete orthonormal system in $L^2(\mathbb{R})$. Then the Schwartz space $\mathcal{S}(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, i.e. any square-integrable function is the limit of a L^2 norm-convergent sequence of rapidly decreasing functions.

By Riesz's theorem $L^2(\mathbb{R})$ is self-dual, i.e. a function f may also represent a linear continuous functional on $L^2(\mathbb{R})$ and thus as tempered distribution (up to conjugation): $\langle f|\varphi \rangle = (\bar{f}|\varphi)$. Let us check continuity:

$$|\langle f|\varphi \rangle|^2 = |(\bar{f}|\varphi)|^2 \leq \|f\|_2^2 \|\varphi\|_2^2 \leq \|f\|_2^2 \pi \|\varphi\|_{00} (\|\varphi\|_{00} + \|\varphi\|_{20})$$

for all test functions. This hierarchy is the Gel'fand triplet: $\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R})$. It is useful for extending an operator with domain $\mathcal{S}(\mathbb{R})$ to an operator on $\mathcal{S}'(\mathbb{R})$, and give meaning to expansions of L^2 functions in terms of generalized functions.

Suppose that the operator $\hat{A} : \mathcal{S}(\mathbb{R}) \rightarrow \mathcal{S}(\mathbb{R})$ is linear and continuous (convergent sequences are mapped to convergent sequences). If f is a tempered distribution, the functional $\varphi \rightarrow \langle f|\hat{A}\varphi \rangle$ is a tempered distribution. The operator \hat{A} induces an "adjoint" operator $A' : \mathcal{S}'(\mathbb{R}) \rightarrow \mathcal{S}'(\mathbb{R})$

$$\langle A'f|\varphi \rangle = \langle f|\hat{A}\varphi \rangle, \quad f \in \mathcal{S}'(\mathbb{R}), \varphi \in \mathcal{S}(\mathbb{R}) \tag{25.39}$$

25.8.1 Generalized eigenvectors

$f_\lambda \in \mathcal{S}'$ is a "generalized eigenvector" of \hat{A} if it solves the eigenvalue equation $A'f_\lambda = \lambda f_\lambda$ i.e.

$$\langle f_\lambda|\hat{A}\varphi \rangle = \lambda \langle f_\lambda|\varphi \rangle \quad \forall \varphi \in \mathcal{S}(\mathbb{R}). \tag{25.40}$$

Example 25.8.1. *The operator $(\hat{Q}_0\varphi)(x) = x\varphi(x)$ leaves \mathcal{S} invariant and is continuous; the corresponding operator Q'_0 acts on distributions as multiplication by the algebraically bounded function x .*

The eigenvalue equation $Q'_0f_\lambda = \lambda f_\lambda$, i.e. $\langle f_\lambda|\hat{Q}_0\varphi \rangle = \lambda \langle f_\lambda|\varphi \rangle \forall \varphi$ has solution for any real λ : $f_\lambda = \delta_\lambda$. Note the "completeness" property of the generalized eigenvectors with respect

to the inner product:

$$(\varphi_1|\varphi_2)_2 = \int_{\mathbb{R}} d\lambda \overline{\langle \delta_\lambda|\varphi_1 \rangle} \langle \delta_\lambda|\varphi_2 \rangle.$$

Example 25.8.2. The operator $\hat{P}_0\varphi = -i\varphi'$ leaves \mathcal{S} invariant and is continuous. The operator P'_0 on distributions is $\langle P'_0 f|\varphi \rangle = \langle f|-i\varphi' \rangle = i \langle f'|\varphi \rangle$, i.e. $P'_0 f = i f'$. The eigenvalue equation $P'_0 e_\lambda = \lambda e_\lambda$ is solved by $e_\lambda(x) = e^{-i\lambda x}/\sqrt{2\pi}$, $\lambda \in \mathbb{R}$ (Im $\lambda \neq 0$ gives exponentially divergent functions, which do not give regular distributions). The chosen normalization is such that $\langle e_\lambda|\varphi \rangle = (\mathcal{F}\varphi)(\lambda)$. Note the completeness property:

$$(\varphi_1|\varphi_2)_2 = (\mathcal{F}\varphi_1|\mathcal{F}\varphi_2)_2 = \int_{\mathbb{R}} d\lambda \overline{\langle e_\lambda|\varphi_1 \rangle} \langle e_\lambda|\varphi_2 \rangle.$$

Remark 25.8.3. An operator \hat{A} with domain $\mathcal{S}(\mathbb{R})$ is densely defined in $L^2(\mathbb{R})$. The adjoint \hat{A}^\dagger exists, and $(A^\dagger f|\varphi) = (f|A\varphi)$, $\forall f \in \mathcal{D}(A^\dagger)$, $\forall \varphi \in \mathcal{S}(\mathbb{R})$. By viewing $A^\dagger f$ and f as elements of the dual space $L^2(\mathbb{R})^*$, and thus as distributions, we rewrite the property of the adjoint as $\langle (A^\dagger f)^*|\varphi \rangle = \langle f^*|A\varphi \rangle$, i.e. $\langle (A^\dagger f^*)^*|\varphi \rangle = \langle f|A\varphi \rangle$. Therefore, for distributions that are functions $f \in \mathcal{D}(A^\dagger)$ it is $A'f = (A^\dagger f^*)^*$. With this rule, A' is an extension of A^\dagger to \mathcal{S}' .

Chapter 26

Green Functions*

Green functions are an important tool for solving inhomogeneous linear differential equations. Let us begin with examples.

26.1 The Helmholtz equation

The inhomogeneous Helmholtz or Yukawa static equation $(\nabla_{\mathbf{x}}^2 - m^2)\varphi(\mathbf{x}) = -4\pi\rho(\mathbf{x})$ contains a local linear operator and a source ρ . For $m = 0$ it is the Poisson equation for the electrostatic potential generated by a charge distribution.

The standard approach to the inhomogeneous equation is to exploit linearity and begin by solving the equation with a point-source¹

$$(\nabla_{\mathbf{x}}^2 - m^2)G(\mathbf{x}, \mathbf{y}) = -4\pi\delta(\mathbf{x} - \mathbf{y})$$

This is the *fundamental equation*, and a solution is a *Green function* of the operator. Evidently, this equation is meaningful in the space of distributions. Two solutions differ by a solution of the homogeneous equation.

With the Green function, a particular solution of the inhomogeneous problem with source ρ is

$$\varphi(\mathbf{x}) = \int d\mathbf{y} G(\mathbf{x}, \mathbf{y}) \rho(\mathbf{y})$$

Since the operator is local and the delta-source is translation-invariant, the Green function depends on $\mathbf{x} - \mathbf{y}$, and can be found via Fourier transform. With the conventions of

¹ $\delta(\mathbf{x} - \mathbf{y}) = \delta(x_1 - y_1)\delta(x_2 - y_2)\delta(x_3 - y_3)$, where x_i and y_i are the Cartesian components.

physicists for functions of space coordinates:

$$G(\mathbf{x}-\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} G(\mathbf{k})$$

$$\delta(\mathbf{x}-\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}$$

In \mathbf{k} -space the equation is algebraic: $-(k^2 + m^2)G(\mathbf{k}) = -4\pi$. Back to coordinates $\mathbf{r} = \mathbf{x} - \mathbf{y}$:

$$G(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{4\pi}{k^2 + m^2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= 2\pi \int_0^\infty \frac{k^2 dk}{(2\pi)^3} \frac{4\pi}{k^2 + m^2} \int_0^\pi \sin\theta d\theta e^{ikr \cos\theta}$$

$$= \int_0^\infty \frac{k^2 dk}{\pi} \frac{1}{k^2 + m^2} \frac{e^{ikr} - e^{-ikr}}{ikr} = \frac{1}{r} \int_{-\infty}^\infty \frac{k dk}{i\pi} \frac{e^{ikr}}{k^2 + m^2}$$

with simple poles $k = \pm im$. Since $r > 0$ the path is closed in the upper half-plane, and

$$G(r) = \frac{\exp(-mr)}{r}$$

This is the Green function of the Yukawa operator (it is the static Yukawa potential), the one that decays at infinity. Other Green functions differ from it by a solution of the homogeneous equation. With $m = 0$ it is the familiar Coulomb potential².

The solution of the inhomogeneous problem is:

$$\varphi(\mathbf{x}) = \int d\mathbf{y} \frac{\exp(-m|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|} \rho(\mathbf{y}) \quad (26.1)$$

Note that the translation-invariance of the Green function gives the solution as a convolution.

26.2 The forced undamped oscillator

$$\ddot{x}(t) + \Omega^2 x(t) = F(t)$$

The general solution is the sum of a solution of the homogeneous equation, $x_0(t) = A\cos(\Omega t) + B\sin(\Omega t)$, and a particular solution $x_p(t)$. The latter is obtained via a Green

² If $m = 0$ from the start, the poles would have been on the real axis but, in the sense of distributions, one freely modifies k^2 to $k^2 + \epsilon^2$, with $\epsilon = 0$ in the end.

function, $x_p(t) = \int ds G(t, s) F(s)$ that solves

$$\frac{d^2}{dt^2} G(t, s) + \Omega^2 G(t, s) = \delta(t - s)$$

Here the Green function is a function of $t - s$. In Fourier space the variable conjugated to time is ω and the following sign convention is used:

$$G(t - s) = \int_{\mathbb{R}} \frac{d\omega}{2\pi} G(\omega) e^{-i\omega(t-s)}$$

The equation for $G(\omega)$ is algebraic: $(-\omega^2 + \Omega^2)G(\omega) = 1$. Then:

$$G(t - s) = - \int_{\mathbb{R}} \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-s)}}{\omega^2 - \Omega^2} = \int_{\mathbb{R}} \frac{d\omega}{4\pi\Omega} e^{-i\omega(t-s)} \left[\frac{1}{\omega + \Omega} - \frac{1}{\omega - \Omega} \right]$$

The poles $\pm\Omega$ are real. They have to be pushed off the real axis by adding imaginary parts $\pm i\epsilon$. Each sign combination gives a different Green function. They differ by solutions of the homogeneous equation.

The choice with all poles in the lower half-plane (poles $\pm\Omega - i\epsilon$) defines the **retarded Green function** (the reason for this name will become clear):

$$G^R(t - s) = \int_{\mathbb{R}} \frac{d\omega}{4\pi\Omega} e^{-i\omega(t-s)} \left[\frac{1}{\omega + \Omega + i\epsilon} - \frac{1}{\omega - \Omega + i\epsilon} \right]$$

If $t < s$ the path is closed in $\text{Im } \omega > 0$ and the integral is zero. If $t > s$ the path encloses both poles:

$$\begin{aligned} G^R(t - s) &= \theta(t - s) \frac{-2\pi i}{4\pi\Omega} [e^{i\Omega(t-s)} - e^{-i\Omega(t-s)}] \\ &= \theta(t - s) \frac{1}{\Omega} \sin[\Omega(t - s)] \end{aligned}$$

The particular solution with the retarded Green function

$$x_p(t) = \frac{1}{\Omega} \int_{-\infty}^t ds \sin[\Omega(t - s)] F(s)$$

has the property of causality: its value at time t only depends on the forcing field at earlier times. This makes the retarded Green function of special importance in physics.

For example, if $F(t) = 0$ for $t < 0$ and $F(t) = F_0 \sin \omega t$ for $t > 0$ it is

$$x_p(t) = \frac{F_0}{\Omega^2 - \omega^2} \left[\sin(\omega t) - \frac{\omega}{\Omega} \sin(\Omega t) \right]$$

The motion is a superposition of oscillations with forcing frequency ω and natural frequency Ω . If $\omega = (1 + \epsilon)\Omega$, for $\epsilon \rightarrow 0$ the expression becomes a resonance (an amplitude grows linearly in time):

$$x_p(t) = \frac{F_0}{2\Omega^2} \sin(\Omega t) - \frac{F_0}{2\Omega} t \cos(\Omega t).$$

26.3 Wave equation with source

The wave equation with source ρ is

$$\square \varphi(x) = -4\pi \rho(x) \quad (26.2)$$

$$\square = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \nabla^2 \quad (26.3)$$

where $x = (ct, \mathbf{x})$, and \square is the d'Alembertian operator (or wave operator). The Green function (or "fundamental solution") of the wave operator is the distribution that solves

$$\square_x G(x, x') = -4\pi \delta_4(x - x') \quad (26.4)$$

Then, the general solution is $\varphi(x) = \varphi_0(x) + \varphi_P(x)$, where φ_0 solves the homogeneous equation $\square_x \varphi_0 = 0$, and $\varphi_P(x) = \int d^4 x' G(x, x') \rho(x')$ is a particular solution.

The Green function is not unique. Its determination can be dictated by physics. For example *causality* requires that the field φ_P at time t cannot depend on values of the source ρ at times $t' > t$ (actually, because of the finite wave speed c , the effect is further delayed). Being the equation (26.4) translation-invariant, we solve it by the Fourier expansion

$$G(x, x') = \int \frac{d^4 k}{(2\pi)^4} e^{ik \cdot (x - x')} G(k)$$

where $k = (\mathbf{k}, \omega/c)$, $k \cdot x = \mathbf{k} \cdot \mathbf{x} - \omega t$.

In Fourier space eq.(26.4) is algebraic: $(|\mathbf{k}|^2 - \omega^2/c^2)G(\mathbf{k}, \omega) = 4\pi$. Therefore

$$G(x, x') = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi c} e^{-i\omega(t-t')} \frac{(-4\pi c^2)}{\omega^2 - |\mathbf{k}|^2 c^2}$$

The integral is singular with poles at $\omega = \pm |\mathbf{k}|c$. This is no problem: we are dealing with distributions, and small epsilons may be introduced to shift poles off the real axis. As this can be done in different ways, there are different Green functions.

Causality determines one choice of the signs. If $t' > t$ the integration path closes in the upper half-plane (this ensures exponential decay on the semicircle); if we require that $G(x, x') = 0$ for $t' > t$, no poles must be encircled, i.e. the two poles must be in the lower

half plane. This choice defines the *retarded* Green function:

$$\begin{aligned}
 G^R(x, x') &= \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \frac{(-4\pi c)}{(\omega + i\epsilon)^2 - |\mathbf{k}|^2 c^2} \\
 &= \theta(t-t') \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \frac{4\pi i}{2|\mathbf{k}|} \left[e^{-i|\mathbf{k}|c(t-t')} - e^{i|\mathbf{k}|c(t-t')} \right] \\
 &= \theta(t-t') \int_0^{\infty} \frac{2\pi k^2 dk}{(2\pi)^3} \frac{4\pi i}{2k} \left[e^{-ikc(t-t')} - e^{ikc(t-t')} \right] \int_{-\pi}^{\pi} \sin\theta d\theta e^{ik|\mathbf{x}-\mathbf{x}'|\cos\theta} \\
 &= \frac{\theta(t-t')}{|\mathbf{x}-\mathbf{x}'|} \int_0^{\infty} \frac{dk}{2\pi} \left[e^{-ikc(t-t')} - e^{ikc(t-t')} \right] \left[e^{ik|\mathbf{x}-\mathbf{x}'|} - e^{-ik|\mathbf{x}-\mathbf{x}'|} \right]
 \end{aligned}$$

There are four terms. A change $k \rightarrow -k$ for two of them gives

$$\begin{aligned}
 G^R(x, x') &= \frac{\theta(t-t')}{|\mathbf{x}-\mathbf{x}'|} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \left[e^{-ik[c(t-t')-|\mathbf{x}-\mathbf{x}'|]} - e^{-ik[c(t-t')+|\mathbf{x}-\mathbf{x}'|]} \right] \\
 &= \frac{\theta(t-t')}{|\mathbf{x}-\mathbf{x}'|} \left[\delta[c(t-t')-|\mathbf{x}-\mathbf{x}'|] - \delta[c(t-t')+|\mathbf{x}-\mathbf{x}'|] \right]
 \end{aligned}$$

The second delta function, with $t > t'$ is zero. Then

$$G^R(x, x') = \theta(t-t') \frac{\delta(|\mathbf{x}-\mathbf{x}'| - c(t-t'))}{|\mathbf{x}-\mathbf{x}'|}$$

The delta function has support on the spherical surface centred in \mathbf{x}' with radius $c(t-t') > 0$, increasing with t .

The causal field with source $\rho(\mathbf{x}', t')$ is a continuous superposition of such spherical waves being emitted at every point of the source at earlier times delayed by the finite speed of the wave:

$$\begin{aligned}
 \varphi_P(\mathbf{x}, t) &= \int d\mathbf{x}' \int_{-\infty}^t dt' \frac{\delta(|\mathbf{x}-\mathbf{x}'| - c(t-t'))}{|\mathbf{x}-\mathbf{x}'|} \rho(\mathbf{x}', t') \\
 &= \int d\mathbf{x}' \frac{\rho(\mathbf{x}', t - \frac{1}{c}|\mathbf{x}-\mathbf{x}'|)}{c|\mathbf{x}-\mathbf{x}'|}
 \end{aligned} \tag{26.5}$$

26.4 Green functions as distributions.

Let $A : \mathcal{S}(\mathbb{R}) \rightarrow \mathcal{S}(\mathbb{R})$ be a linear continuous operator. A Green function G_S of A is a distribution that solves the equation $\langle G_S | A\varphi \rangle = \langle A' G_S | \varphi \rangle = \varphi(s)$, for any test function i.e.

$$A' G_S = \delta_s, \quad s \in \mathbb{R}$$

In terms of generalized functions it is $\int dx G_s(x)(A\varphi)(x) = \varphi(s)$. The inhomogeneous equation $\hat{A}\varphi = \psi$ has the particular solution

$$\varphi(s) = \langle G_s | \psi \rangle = \int dx G_s(x) \psi(x)$$

Proof. $\varphi(s) = \langle \delta_s | \varphi \rangle = \langle A' G_s | \varphi \rangle = \langle G_s | \hat{A}\varphi \rangle = \langle G_s | \psi \rangle$. □

A second Green function would produce a particular solution that differs by a solution of the homogeneous equation $A\varphi = 0$.

Example 26.4.1. *The Green functions of $\hat{P}_0\varphi = -i\varphi'$ solve $P'_0 G_t = \delta_t$, i.e. $i\partial_s G_t(s) = \delta(s-t)$, where s is the variable of the generalized function.*

- $G_t^R(s) = i\theta(t-s)$ yields the retarded solution of $-i\varphi'(t) = \psi(t)$:

$$\varphi^R(t) = i \int_{\mathbb{R}} ds \theta(t-s) \psi(s) = i \int_{-\infty}^t ds \psi(s)$$

where φ^R is built with values of the source ψ at earlier times.

- $G_t^A(s) = -i\theta(s-t)$ yields the advanced solution:

$$\varphi^A(t) = -i \int_{\mathbb{R}} ds \theta(s-t) \psi(s) = -i \int_t^{\infty} ds \psi(s)$$

The difference $G_t^R(s) - G_t^A(s) = i$ is a constant (solution of the homogeneous equation).

Chapter 27

Fourier Transform II

The Fourier transform \mathcal{F} and antitransform \mathcal{F}^{-1} were studied in detail in $\mathcal{S}(\mathbb{R})$ and extended to the dual space of tempered distributions. It is of great interest to investigate the properties of \mathcal{F} as operators on the spaces $L^p(\mathbb{R})$, $p = 1, 2$. Many properties continue to hold in higher dimension.

27.1 Fourier transform in $L^1(\mathbb{R})$

The Fourier transform

$$(\mathcal{F}f)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ikx} f(x), \quad k \in \mathbb{R}$$

is well defined on the whole space $\mathcal{L}^1(\mathbb{R})$, and $|\mathcal{F}f(k)| \leq \frac{1}{\sqrt{2\pi}} \|f\|_1 \quad \forall k \in \mathbb{R}$. Therefore \mathcal{F} is a linear operator from $L^1(\mathbb{R})$ to bounded functions.

The Fourier transform of a characteristic function

$$(\mathcal{F}\chi_{[a,b]})(k) = \int_a^b \frac{dx}{\sqrt{2\pi}} e^{-ikx} = \sqrt{\frac{2}{\pi}} \frac{\sin[\frac{b-a}{2}k]}{k} e^{-i\frac{b+a}{2}k}$$

is bounded, continuous, and vanishes for $|k| \rightarrow \infty$.

The same properties hold true for step functions σ (linear combinations of a finite number of characteristic functions of finite intervals). Step functions are a dense subset of $L^1(\mathbb{R})$. This anticipates the fundamental theorem:

Theorem 27.1.1 (Riemann - Lebesgue). *If $f \in \mathcal{L}^1(\mathbb{R})$ then $\mathcal{F}f$ is bounded, continuous, and vanishes at infinity:*

$$\boxed{\lim_{|k| \rightarrow \infty} |(\mathcal{F}f)(k)| = 0} \tag{27.1}$$

Proof. If σ_n is a sequence of step functions and $\sigma_n \rightarrow f$ in L^1 , then $\mathcal{F}\sigma_n \rightarrow \mathcal{F}f$ uniformly: $|(\mathcal{F}f)(k) - (\mathcal{F}\sigma_n)(k)| = |\mathcal{F}(f - \sigma_n)(k)| \leq \frac{1}{\sqrt{2\pi}} \|f - \sigma_n\|_1$ for all k . Since $\mathcal{F}\sigma_n$ are continuous, also $\mathcal{F}f$ is continuous¹.

$\forall \epsilon$ there is a step function σ_ϵ such that $\|f - \sigma_\epsilon\|_1 < \epsilon$. Since $|\mathcal{F}\sigma_\epsilon|$ vanishes at infinity, there is R_ϵ such that for all $|k| > R_\epsilon$ it is $|(\mathcal{F}\sigma_\epsilon)(k)| < \epsilon$. Then, for $|k| > R_\epsilon$ it is: $|(\mathcal{F}f)(k)| \leq |(\mathcal{F}(f - \sigma_\epsilon))(k)| + |(\mathcal{F}\sigma_\epsilon)(k)| \leq \frac{1}{\sqrt{2\pi}} \|f - \sigma_\epsilon\|_1 + |(\mathcal{F}\sigma_\epsilon)(k)| < \epsilon$ (up to a finite constant). \square

Remark 27.1.2. *The set where $\mathcal{F}\chi_{[a,b]}(x) \neq 0$ has infinite measure. This is true in general: if $f \in \mathcal{L}^1(\mathbb{R})$ and the Lebesgue measures of the sets where $|f| \neq 0$ and $|\mathcal{F}f| \neq 0$ are both finite, then $f = 0$ a.e.²*

Exercise 27.1.3. *Find the condition for an integrable real function to have a real Fourier transform.*

Since the Fourier transform is bounded, the following integrals exist and are equal (Fubini's theorem applies):

$$\int_{\mathbb{R}} dk \overline{(\mathcal{F}f)(k)} g(k) = \int_{\mathbb{R}} dk \overline{f(k)} (\mathcal{F}^{-1}g)(k) \tag{27.2}$$

Theorem 27.1.4 (Inversion). *If both f and $\mathcal{F}f$ are $\mathcal{L}^1(\mathbb{R})$, then $\mathcal{F}\mathcal{F}^{-1}f = f$.*

Proposition 27.1.5. *The convolution product of $f, g \in \mathcal{L}^1(\mathbb{R})$*

$$(f * g)(x) = \int_{\mathbb{R}} dy f(x - y)g(y) \tag{27.3}$$

*is a function in $\mathcal{L}^1(\mathbb{R})$ with norm $\|f * g\|_1 \leq \|f\|_1 \|g\|_1$, and*

$$\mathcal{F}(f * g) = \sqrt{2\pi} (\mathcal{F}f)(\mathcal{F}g) \tag{27.4}$$

The product $$ is commutative, associative and distributive.*

Proof. $\int_{\mathbb{R}} dx |(f * g)(x)| \leq \int_{\mathbb{R}} dx \int_{\mathbb{R}} dy |f(x - y)| |g(y)| = \|f\|_1 \|g\|_1$ after a shift $x' = x - y$. The Fourier transform of $f * g$ exists in \mathcal{L}^1 , and

$$\mathcal{F}(f * g)(k) = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-ik(x-y)} \int_{\mathbb{R}} f(x - y)g(y)e^{iky} = \sqrt{2\pi} (\mathcal{F}f)(k)(\mathcal{F}g)(k)$$

¹ If f_n is a sequence of continuous functions and $f_n \rightarrow f$ uniformly, then f is continuous (proof: $|f(x) - f(y)| \leq |f(x) - f_n(x)| + |f(y) - f_n(y)| + |f_n(x) - f_n(y)| \leq 3\epsilon$ for n large enough and $|y - x| < \delta_\epsilon$).

² M. Benedicks, *On Fourier transforms of functions supported on sets of finite Lebesgue measure*, Math. Anal. Appl. **106** (1985) 180–183. The theorem holds in any dimension.

□

Example 27.1.6. Solve the integral equation $\int_{-\infty}^{+\infty} dy e^{-|x-y|} f(y) = g(x)$.

The Fourier transform gives $(\mathcal{F} f)(k) = \frac{1}{2}(1+k^2)(\mathcal{F} g)(k)$. Now antitransform:

$$f(x) = \frac{1}{2}g(x) + \frac{1}{2} \int_{\mathbb{R}} \frac{dk}{\sqrt{2\pi}} k^2 e^{ikx} (\mathcal{F} g)(k) = \frac{1}{2}[g(x) - g''(x)].$$

Example 27.1.7. The linear operator on $\mathcal{L}^1(\mathbb{R})$

$$(\hat{T}f)(x) = \int_{-\infty}^{+\infty} dy \frac{f(y)}{\cosh(x-y)}$$

acts as a convolution, then $\hat{T}f \in \mathcal{L}^1$ and it is $\|\hat{T}f\|_1 \leq \|\text{sech}\|_1 \|f\|_1$, where $\|\text{sech}\|_1 = \int_{-\infty}^{+\infty} \frac{dx}{\cosh x} = \pi$. Since $\cosh(x) > 0$, we have equality for $f > 0$: $\|\hat{T}f\|_1 = \pi \|f\|_1$. The sup-norm is $\|\hat{T}\| = \pi$.

By the convolution theorem (see (14.26) for a Fourier transform):

$$(\mathcal{F} \hat{T}f)(k) = \sqrt{2\pi} \frac{\pi}{\cosh(\frac{\pi}{2}k)} (\mathcal{F} f)(k)$$

The operator \hat{T} is invertible if $\hat{T}f = 0$ implies $f = 0$. This is true, as the Fourier transform implies $\mathcal{F}f = 0$ i.e. $f = 0$. The inverse operator is defined on continuous functions such that $(\mathcal{F} \hat{T}f)(k) \cosh(\frac{\pi}{2}k)$ is integrable.

27.2 Fourier transform in $L^2(\mathbb{R})$

Hermite functions h_n belong to $\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R})$. The following theorem has various interesting implications:

Theorem 27.2.1. The Hermite functions h_n are an orthonormal complete set in $L^2(\mathbb{R})$.

Proof. The generating function of Hermite functions is (24.7):

$$h(x, z) = \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{2^n n!}} h_n(x) = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{x^2}{2} + zx - \frac{z^2}{4}}$$

Suppose that there is $f \in L^2$ such that $(h_m | f) = 0$ for all m . This implies that $\int dx h(x, z) f(x) = 0$ for all z . For $z = -ik$, up to irrelevant factors, it is

$$0 = \int_{\mathbb{R}} \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2 - ikx} f(x) = (\mathcal{F} g)(k), \quad g(x) = e^{-\frac{1}{2}x^2} f(x)$$

The function g belongs to $\mathcal{L}^1(\mathbb{R})$ (Schwarz inequality) and its Fourier transform is zero. Then $g \in \text{Ker } \mathcal{F}$, but $\text{Ker } \mathcal{F} = \{0\}$ by the inversion theorem in L^1 . Then $g = 0$ i.e. $f = 0$. \square

Since \mathcal{F} is isometric on $\mathcal{S}(\mathbb{R})$ ($\|\mathcal{F}\varphi\|_2 = \|\varphi\|_2$) and the Schwartz space is dense in L^2 , the operator \mathcal{F} may be extended to a unitary operator \hat{F} on $L^2(\mathbb{R})$. The explicit construction exploits the property of h_n to be eigenstates of \hat{F} and to form an orthonormal complete set.

Consider the expansion $f = \sum_n (h_n|f) h_n$; then $f_N = \sum_{n \leq N} (h_n|f) h_n$ is a Cauchy sequence of functions in $\mathcal{S}(\mathbb{R})$ that is norm-convergent to f . It is $\mathcal{F} f_N = \sum_{n \leq N} (-i)^n h_n (h_n|f)$. This new sequence is again a Cauchy sequence. Its limit defines the **Fourier-Plancherel operator**

$$\hat{F}f = \sum_{n=0}^{\infty} (-i)^n (h_n|f) h_n \tag{27.5}$$

The inverse transform \mathcal{F}^{-1} extends uniquely to the adjoint \hat{F}^\dagger .

Another way to evaluate the Fourier transform of $f \in \mathcal{L}^2$ is to consider the functions $\chi_{[-R,R]} f \in \mathcal{L}^1(\mathbb{R}) \cap \mathcal{L}^2(\mathbb{R})$. On such functions $\hat{F} = \mathcal{F}$ and, since \hat{F} is continuous:

$$(\hat{F}f)(k) = \text{l.i.m.}_{R \rightarrow \infty} \int_{-R}^R \frac{dx}{\sqrt{2\pi}} e^{-ikx} f(x)$$

where l.i.m. is "limit in the mean", i.e. in L^2 -norm.

Remark 27.2.2. *The Hermite functions solve Weber's differential equation (19.29). As such, they are the eigenfunctions of the number operator $\hat{N} = \frac{1}{2}(\hat{P}^2 + \hat{Q}^2 - 1)$: $\hat{N}h_n = nh_n$, $n \in \mathbb{N}$. The operator is the generator in $L^2(\mathbb{R})$ of the one-parameter unitary group*

$$\hat{U}(\theta) = e^{-i\theta \hat{N}} = \sum_{n=0}^{\infty} e^{-in\theta} (h_n|\cdot) h_n$$

with domain $\mathcal{D}(\hat{N}) = \{f : \sum_{n=0}^{\infty} n^2 |(h_n|f)|^2 < \infty\}$. The group describes the 2π -periodic evolution in time θ of the quantum harmonic oscillator. Both \hat{N} and $\hat{U}(\theta)$ leave $\mathcal{S}(\mathbb{R})$ invariant. It is $\hat{U}(\frac{\pi}{2}) = \hat{F}$, $\hat{U}(-\frac{\pi}{2}) = \hat{F}^{-1} = \hat{F}^\dagger$. $\hat{U}(\pi)$ is the parity operator.

This is a nice characterization of test functions and tempered distributions in terms of Hermite functions:

Proposition 27.2.3 (Vladimirov³).

$$\varphi \in \mathcal{S}(\mathbb{R}) \iff \sum_{n=0}^{\infty} n^{2k} |(h_n|\varphi)|^2 < \infty \quad \forall k \in \mathbb{N} \quad (27.6)$$

$$F \in \mathcal{S}'(\mathbb{R}) \iff \exists C, p > 0 \text{ s.t. } |< F|h_n >| \leq C(1+n)^p, \quad \forall n \quad (27.7)$$

27.2.1 Completeness of the Fourier basis

The Fourier transform of a function in $\mathcal{S}(\mathbb{R})$ can be written as

$$(\mathcal{F}\varphi)(k) = \int_{\mathbb{R}} dx \overline{u_k(x)} \varphi(x) = < \overline{u}_k | \varphi >, \quad u_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}, \quad k \in \mathbb{R}$$

where $< \overline{u}_k | >$ is the action of a regular distribution. By the inversion theorem it is:

$$\boxed{\varphi(x) = \int_{\mathbb{R}} dk < \overline{u}_k | \varphi > u_k(x)} \quad (27.8)$$

Since the Schwartz space is dense in L^2 , the relation shows the *completeness* of the continuous system of functions $\{u_k\}$. They are the eigenfunctions of the derivative operator on distributions, which extends the self-adjoint unbounded operator \hat{P} .

³ V. Vladimirov, *Le distribuzioni nella fisica matematica*, Mir (1981).

Chapter 28

Laplace Transform*

28.1 The Laplace integral

The theory of the Laplace transform is here deduced from the theory of Fourier transform. The Fourier transform exists for integrable functions: this is restrictive in applications, for it leaves out several useful functions. However, a non-integrable function $f(x)$ multiplied by e^{-cx} may become integrable on $x \geq 0$ for a suitable value $c > 0$. At the same time, to avoid problems at the other end of the real line, one restricts the function to be zero for $x < 0$.

If for a suitable value c the integral is finite

$$\int_0^{\infty} dx e^{-cx} |f(x)| < \infty \tag{28.1}$$

the Fourier integral of the function

$$\begin{cases} \sqrt{2\pi} e^{-cx} f(x) & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases}$$

exists, and is: $\int_0^{\infty} dx e^{-x(c+ik)} f(x)$. By the Riemann-Lebesgue theorem, the Fourier integral is a continuous bounded function that decays to zero at infinity.

By setting $z = c + ik$, the integral remains well defined for $\text{Re } z > c$, and in such range it is the Laplace transform of f :

$$\boxed{(\mathcal{L}f)(z) = \int_0^{\infty} dx f(x) e^{-zx}} \tag{28.2}$$

The integral is bounded in modulus by (28.1):

$$|(\mathcal{L}f)(z)| \leq \int_0^\infty dx e^{-x\operatorname{Re}z} |f(x)| \leq \int_0^\infty dx e^{-cx} |f(x)|.$$

Theorem 28.1.1. $(\mathcal{L}f)(z)$ is holomorphic in $\operatorname{Re} z > c$ and

$$\frac{d^n}{dz^n}(\mathcal{L}f)(z) = (-1)^n (\mathcal{L}x^n f)(z) \quad (28.3)$$

Proof. Let's show that the following limit $h \rightarrow 0$ exists:

$$\begin{aligned} & \left| \frac{(\mathcal{L}f)(z+h) - (\mathcal{L}f)(z)}{h} + (\mathcal{L}xf)(z) \right| = \left| \int_0^\infty dx e^{-xz} f(x) \left[\frac{e^{-hx} - 1}{h} + x \right] \right| \\ & \leq \int_0^\infty dx e^{-x\operatorname{Re}z} |f(x)| \left| \frac{e^{-hx} - 1}{h} + x \right| \leq \frac{|h|}{2} \int_0^\infty dx e^{-x(\operatorname{Re}z - |h|)} x^2 |f(x)| \rightarrow 0 \end{aligned}$$

where the following inequality is used

$$\left| \frac{e^{-hx} - 1}{h} + x \right| = \left| h \int_0^x dy \int_0^y ds e^{-sh} \right| \leq |h| \int_0^x dy y e^{y|\operatorname{Re}h|} \leq \frac{1}{2} |h| x^2 e^{x|\operatorname{Re}h|}$$

Being $\mathcal{L}f$ holomorphic, all derivatives exist in its domain. □

These properties are proven without difficulty:

$$\mathcal{L}(af + bg)(z) = a\mathcal{L}f(z) + b\mathcal{L}g(z) \quad (\text{linearity}) \quad (28.4)$$

$$\overline{(\mathcal{L}f)(z)} = (\mathcal{L}\bar{f})(\bar{z}) \quad (28.5)$$

$$(\mathcal{L}f')(z) = -f(0) + z(\mathcal{L}f)(z) \quad (28.6)$$

$$(\mathcal{L}f'')(z) = -f'(0) - zf(0) + z^2(\mathcal{L}f)(z) \quad (28.7)$$

$$(\mathcal{L}e^{-ax}f)(z) = (\mathcal{L}f)(z+a). \quad (28.8)$$

Some simple Laplace transforms:

$$(\mathcal{L}[e^{\alpha x}])(z) = \frac{1}{z - \alpha}, \quad \operatorname{Re} z > \operatorname{Re} \alpha \quad (28.9)$$

$$(\mathcal{L}[\sin \omega x])(z) = \frac{\omega}{z^2 + \omega^2}, \quad \operatorname{Re} z > 0 \quad (28.10)$$

$$(\mathcal{L}[\cos \omega x])(z) = \frac{z}{z^2 + \omega^2}, \quad \operatorname{Re} z > 0 \quad (28.11)$$

$$(\mathcal{L}[x^{a-1}])(z) = \int_0^\infty dx e^{-zx} x^{a-1} = \frac{\Gamma(a)}{z^a}, \quad \operatorname{Re} a > 0, \operatorname{Re} z > 0 \quad (28.12)$$

Logs and powers are accounted with $a \rightarrow a + \epsilon$, and expanding in ϵ :

$$x^{a-1+\epsilon} = x^{a-1} [1 + \epsilon \log x + \frac{1}{2} \epsilon^2 (\log x)^2 + \dots]$$

$$\Gamma(a + \epsilon) = \Gamma(a) [1 + \epsilon \psi(a) + \frac{1}{2} \epsilon^2 \psi_2(a) + \dots]$$

where $\psi(z)$ is the digamma function etc. By equating equal powers of ϵ one obtains ($\operatorname{Re} z > 0$):

$$(\mathcal{L}[x^{a-1} \log x])(z) = \frac{\Gamma(a)}{z^a} [\psi(a) - \operatorname{Log} z] \quad (28.13)$$

$$(\mathcal{L}[x^{a-1} \log^2 x])(z) = \frac{\Gamma(a)}{z^a} [\psi_2(a) - 2\psi(a) \operatorname{Log} z - \operatorname{Log}^2 z] \quad (28.14)$$

28.2 Inversion

The Laplace transform can be inverted. With $f(x) = 0$ for $x < 0$, recall the correspondence: $(\mathcal{F}[\sqrt{2\pi} e^{-ax} f(x)])(k) = (\mathcal{L}f)(a + ik)$, where $a > c$. If, as a function of k , it is $(\mathcal{L}f)(a + ik) \in \mathcal{L}^1(\mathbb{R})$, the Fourier transform can be inverted:

$$\sqrt{2\pi} e^{-ax} f(x) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} (\mathcal{L}f)(a + ik) e^{ikx}.$$

The formula transforms into: $f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{(a+ik)x} (\mathcal{L}f)(a + ik)$. Put $z = a + ik$, $dz = idk$ and the inversion formula is obtained:

$$\boxed{f(x) = \int_{a-i\infty}^{a+i\infty} \frac{dz}{2\pi i} e^{zx} (\mathcal{L}f)(z)} \quad (28.15)$$

The line of integration is parallel to the imaginary axis with $a > c$.

The function $(\mathcal{L}f)(z)$ is analytic for $\text{Re } z > c$. If it is meromorphic for $\text{Re } z < c$, the computation of the integral can be done by the Residue Theorem, by closing the integration path by a semicircle in $\text{Re } z < c$ surrounding the poles (Bromwich's contour).

28.3 Hankel's representation of Γ

The antitransform of $(\mathcal{L}[x^{a-1}])(z)$ is

$$x^{a-1} = \Gamma(a) \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} e^{zx} z^{-a}$$

where $c > 0$ is arbitrary. For $x = 1$ Hankel's integral representation of the Gamma function is obtained:

$$\boxed{\frac{1}{\Gamma(a)} = \int_{\epsilon-i\infty}^{\epsilon+i\infty} \frac{dz}{2\pi i} e^z z^{-a}} \tag{28.16}$$

The path of integration can be deformed to the loop shown in fig. 28.1.

If $a = n$ the singularity is a pole in the origin, the loop may be deformed to a circle, and the Residue Theorem gives $\Gamma(n) = (n - 1)!$.

If $a \neq n$ the evaluation of the loop integral gives an important identity of the Gamma function. Let $z^a = e^{a\text{Log}z}$; the loop runs along the cut of discontinuity of the Log: $\text{Log}(x \pm i\epsilon) = \log|x| \pm i\pi$ for $x < 0$. Then:

$$\begin{aligned} \frac{1}{\Gamma(a)} &= \int_{loop} \frac{dz}{2\pi i} e^{z-a\text{Log}z} = \int_{-\infty}^0 \frac{dx}{2\pi i} e^x \left[e^{-a\text{Log}(x-i\epsilon)} - e^{-a\text{Log}(x+i\epsilon)} \right] \\ &= \frac{\sin(\pi a)}{\pi} \int_0^\infty dx e^{-x} x^{-a} = \frac{\sin(\pi a)}{\pi} \Gamma(1-a) \end{aligned}$$

$$\boxed{\Gamma(a)\Gamma(1-a) = \frac{\pi}{\sin \pi a}} \tag{28.17}$$

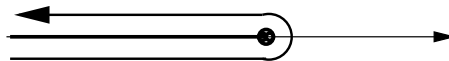


Figure 28.1 Hankel's loop for $1/\Gamma(a)$.

28.4 Convolution

The Fourier transform of the convolution of two functions is the product of their Fourier transforms and a factor $\sqrt{2\pi}$. Because of the relation between Fourier and Laplace transforms, a similar property is expected for the Laplace transform.

Consider two functions of the type considered so far, $\sqrt{2\pi}\theta(x)e^{-ax}f(x)$ and $\sqrt{2\pi}\theta(x)e^{-ax}g(x)$, where the vanishing condition for $x < 0$ is written explicitly. Let's write their convolution product according to the theory of Fourier transform:

$$\begin{aligned} & \int_{-\infty}^{\infty} dy [\sqrt{2\pi}\theta(y)f(y)e^{-ay}] [\sqrt{2\pi}\theta(x-y)g(x-y)e^{-a(x-y)}] \\ &= 2\pi e^{-ax} \int_0^x dy f(y)g(x-y) \end{aligned}$$

This integral defines the convolution product of two Laplace-transformable functions:

$$(f * g)(x) = \int_0^x dy f(y)g(x-y) \quad (28.18)$$

Exercise 28.4.1. Show that the convolution product is commutative.

Theorem 28.4.2 (Convolution theorem).

$$\boxed{\int_0^x dy f(y)g(x-y) = \int_{a-i\infty}^{a+i\infty} \frac{dz}{2\pi i} e^{zx} (\mathcal{L}f)(z)(\mathcal{L}g)(z)} \quad (28.19)$$

Proof. We use results of the theory of Fourier transform. By the convolution theorem for the Fourier transform, it is

$$\begin{aligned} & 2\pi e^{-ax} \int_0^x dy f(y)g(x-y) \\ &= \sqrt{2\pi} \mathcal{F}^{-1} \left(\mathcal{F} [\sqrt{2\pi}\theta(y)f(y)e^{-ay}] \mathcal{F} [\sqrt{2\pi}\theta(y)g(y)e^{-ay}] \right) (x) \\ &= \int_{-\infty}^{\infty} dk e^{ikx} (\mathcal{L}f)(a+ik)(\mathcal{L}g)(a+ik) \end{aligned}$$

Therefore:

$$\int_0^x dy f(y)g(x-y) = \int_{\mathbb{R}} \frac{dk}{2\pi} e^{(a+ik)x} (\mathcal{L}f)(a+ik)(\mathcal{L}g)(a+ik)$$

Now put $z = a + ik$, $dz = idk$. □

Example 28.4.3. Consider the inhomogeneous equation

$$\begin{cases} f''(t) + \omega^2 f(t) = g(t) \\ f(0) = A, \quad f'(0) = B \end{cases}$$

The Laplace transform yields the algebraic equation $(z^2 + \omega^2)(\mathcal{L}f)(z) - f'(0) - zf(0) = (\mathcal{L}g)(z)$, with solution

$$(\mathcal{L}f)(z) = \frac{(\mathcal{L}g)(z) + B + Az}{z^2 + \omega^2}.$$

To obtain f one inverts a Laplace transform:

$$\begin{aligned} f(t) &= \mathcal{L}^{-1} \left(\mathcal{L}[g](t) \frac{\mathcal{L}[\sin \omega t]}{\omega} + B \frac{\mathcal{L}[\sin \omega t]}{\omega} + A \mathcal{L}[\cos \omega t] \right) \\ &= \int_0^t dt' \frac{\sin \omega(t-t')}{\omega} g(t') + f_{\text{hom}}(t), \end{aligned}$$

where $f_{\text{hom}}(t) = \frac{B}{\omega} \sin(\omega t) + A \cos(\omega t)$ solves the homogeneous equation. The particular solution exhibits the causality property: its value at time t is determined by the values of the forcing field at earlier times.

28.5 The Mellin transform

In analogy with the construction of the Laplace transform, the Fourier identity

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ikx} \int_{-\infty}^{\infty} dy e^{iky} f(y)$$

is formally modified to define the useful Mellin transform¹.

In the identity put $x = \log s$ and $y = \log t$:

$$f(\log s) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} s^{-ik} \int_0^{\infty} dt t^{ik-1} f(\log t)$$

Let $z = c + ik$, $dz = idk$: $s^{-c} f(\log s) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} s^{-z} \int_0^{\infty} dt t^{z-1} t^{-c} f(\log t)$; rename $f(\log s) s^{-c}$ as $f(s)$. Then: $f(s) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} s^{-z} \int_0^{\infty} dt t^{z-1} f(t)$.

¹ for a nice introduction see: <https://www.cs.purdue.edu/homes/spa/papers/chap9.ps>. A specialised book is: Yu.A. Brychkov, O.I. Marichev, N.V. Svischenko, Handbook of Mellin transforms, CRC Press.

The Mellin transform of a function is:

$$\boxed{(\mathcal{M} f)(z) = \int_0^{\infty} dx x^{z-1} f(x)} \quad (28.20)$$

It exists for $|(\mathcal{M} f)(z)| \leq \int_0^{\infty} dx |f(x)| x^{\operatorname{Re} z - 1} < \infty$, which means that z is bounded in some strip of the complex plane. The inversion formula is

$$f(x) = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} x^{-z} (\mathcal{M} f)(z) \quad (28.21)$$

The Mellin transform of e^{-x} is $\Gamma(z)$, and is defined for $\operatorname{Re} z > 0$.

Exercise 28.5.1. Prove the properties:

$$(\mathcal{M} xf)(z) = (\mathcal{M} f)(z+1) \quad (28.22)$$

$$(\mathcal{M} f')(z) = -(z-1)(\mathcal{M} f)(z-1) \quad (28.23)$$

$$(\mathcal{M} x^n D^n f)(z) = (-1)^n (z-n) \dots (z-1) (\mathcal{M} f)(z) \quad (28.24)$$

$$\int_0^{\infty} dx |f(x)|^2 = \int_{c-i\infty}^{c+i\infty} \frac{dz}{2\pi i} |\mathcal{M} f(z)|^2 \quad (\text{Parseval identity}) \quad (28.25)$$

$$(\mathcal{M} fg)(z) = \int_{c-i\infty}^{c+i\infty} \frac{dz'}{2\pi i} (\mathcal{M} f)(z') (\mathcal{M} g)(z-z') \quad (28.26)$$

Ramanujan had a favourite formula², that Hardy stated as a theorem. It is named “Master theorem” and discloses difficult results.

Let $g(z)$ be analytic in $H_\delta = \{\operatorname{Re} z > -\delta\}$, $0 < \delta < 1$, such that $|g(z)| < C \exp(Px + A|y|)$ for $A < \pi$ and all $z \in H_\delta$, then:

$$\int_0^{\infty} dx x^{s-1} \sum_{k=0}^{\infty} (-1)^k g(k) x^k = \frac{\pi}{\sin(\pi s)} g(-s), \quad 0 < \operatorname{Re} s < \delta.$$

An easy application is $g(k) = 1/k!$, that gives eq.(28.17).

² This theorem will be an instrument by which at least some of the definite integrals whose values are at present not known can be evaluated ... Ramanujan's Notebooks, part 1, Springer, page 298.

Chapter 29

Gaussian Integrals, Grassmann Variables*

The chapter is an introduction to useful tools that are frequently used in statistics, statistical and theoretical physics of particles and condensed matter.

29.1 Gaussian integrals

For a strictly positive real matrix P (i.e. $\mathbf{x}^t P \mathbf{x} > 0$ for all \mathbf{x}) of size $n \times n$, the Gaussian integral in n real variables is

$$Z_0 = \int d\mathbf{x} e^{-\frac{1}{2}\mathbf{x}^t P \mathbf{x}} = \frac{(2\pi)^{n/2}}{\sqrt{\det P}} \quad (29.1)$$

Proof. Diagonalize P by an orthogonal transformation, $P = R^T \Lambda R$, where Λ is the diagonal matrix of eigenvalues $\lambda_j > 0$. Change variable: $\mathbf{x}' = R\mathbf{x}$. R is the Jacobian of the linear transformation and has unit determinant. The integral factors in n Gaussian integrals of one variable: $\int dx'_j \exp(-\frac{1}{2}\lambda_j x'^2_j) = \sqrt{2\pi/\lambda_j}$. \square

The normalized function

$$p(\mathbf{x}) = \frac{1}{Z_0} e^{-\frac{1}{2}\mathbf{x}^t P \mathbf{x}}$$

is a probability density for real vectors, i.e. $p(\mathbf{x}) d\mathbf{x}$ is the probability that a vector has components in the cube $d\mathbf{x}$ centred in \mathbf{x} in \mathbb{R}^n .

To evaluate average values it is useful to introduce a “source” $\mathbf{y} \in \mathbb{R}^n$:

$$Z[\mathbf{y}] = \int d\mathbf{x} e^{-\frac{1}{2}\mathbf{x}^t P \mathbf{x} + \mathbf{y}^t \mathbf{x}} = \frac{(2\pi)^{n/2}}{\sqrt{\det P}} e^{\frac{1}{2}\mathbf{y}^t P^{-1} \mathbf{y}} \quad (29.2)$$

Proof. Make the shift $\mathbf{x}' = \mathbf{x} - P^{-1}\mathbf{y}$. □

With this integral one evaluates average values of products of vector components. For example:

$$\langle x_r x_s \rangle = \frac{1}{Z_0} \int d\mathbf{x} e^{-\frac{1}{2}\mathbf{x}^t P \mathbf{x}} x_r x_s = \frac{1}{Z_0} \left. \frac{\partial^2 Z[\mathbf{y}]}{\partial y_r \partial y_s} \right|_{\mathbf{y}=0} = (P^{-1})_{rs} \tag{29.3}$$

A probability density for vectors in \mathbb{C}^n requires a positive definite matrix that may be Hermitian or real symmetric. The normalization is

$$Z_0 = \int d^2\mathbf{z} e^{-\mathbf{z}^\dagger P \mathbf{z}} = \frac{\pi^n}{\det P} \tag{29.4}$$

where $z = x + iy$, $d^2z = dx dy$ and $d^2\mathbf{z} = d^2z_1 \dots d^2z_n$.

Proof. Diagonalize P by a unitary transformation $P = U^\dagger \Lambda U$, where Λ is the diagonal matrix of eigenvalues $\lambda_j > 0$, and make the change $\mathbf{z}' = U\mathbf{z}$. U has unit determinant. The integral factors in n Gaussian integrals of complex variable that are evaluated in polar coordinates: $Z_0 = \prod_{j=1}^n \int d^2z' \exp(-\lambda_j |z'|^2) = \prod_{j=1}^n 2\pi \int_0^\infty r dr \exp(-\lambda_j r^2) = \prod_{j=1}^n (\pi/\lambda_j)$. □

If a matrix H is complex Hermitian (or real symmetric) but not positive definite, one has a different type of integrals, with a convergence factor $a > 0$,

$$Z_0 = \int d^2\mathbf{z} e^{-a\mathbf{z}^\dagger \mathbf{z} - i\mathbf{z}^\dagger H \mathbf{z}} = \frac{(-i\pi)^n}{\det(H - ia)} \tag{29.5}$$

The parameter a can be small but nonzero.

Proof. Let $H = U^\dagger \Lambda U$ and put $\mathbf{z}' = U\mathbf{z}$. The integral factors in n complex integrals: $\prod_j \int d^2z \exp[-(a + i\lambda_j)|z|^2] = \prod_j \pi/(a + i\lambda_j)$. □

This result is similar to that with a positive matrix, but requires the imaginary exponent. The formulas (29.1) and (29.5) are useful integral representations of the square root of the determinant or of the determinant of positive matrices *in the denominator* of a fraction. Now we introduce a formalism that, among its many applications, provides the determinant *in the numerator*.

29.1.1 Grassmann variables

Grassmann variables are not variables in the usual sense. They are symbols (or units) that anticommute and form the basis of an algebra.

Consider n Grassmann units $\theta_1, \dots, \theta_n$ characterized by the property

$$\theta_i \theta_j + \theta_j \theta_i = 0, \quad \theta_j^2 = 0 \tag{29.6}$$

With such units one builds products $\theta_i\theta_j\dots\theta_m$. If two or more factors are equal the product is zero; a nonzero product has at most length n . The product of an even number of units commutes with the units.

A product can always be brought to the order by which units were numbered

$$(-1)^\sigma \theta_i\theta_j\dots\theta_m, \quad i < j < \dots < m$$

σ is the number of anticommutations done to order the product or, equivalently, the parity 0 (even) or 1 (odd) of the permutation. For example: $\theta_5\theta_9\theta_4\theta_1 = -\theta_1\theta_4\theta_5\theta_9$ (the permutation $(5, 9, 4, 1) \rightarrow (1, 4, 5, 9)$ is odd).

Besides the Grassmann units one adds the unit 1, which commutes with all the θ_j . With $n = 3$ there are 2^3 ordered products:

$$1, \theta_1, \theta_2, \theta_3, \theta_1\theta_2, \theta_1\theta_3, \theta_2\theta_3, \theta_1\theta_2\theta_3$$

With n Grassmann units and the unity 1 there are 2^n ordered products. They arise from the following expansion, where the 2^n terms are given a label:

$$(1 + \theta_1)(1 + \theta_2)\dots(1 + \theta_n) = \sum_{\alpha} \Theta_{\alpha} \quad (29.7)$$

α is the sequence of the numbers of the units in the product. For example: $\Theta_0 = 1$, $\Theta_{2,4} = \theta_2\theta_4$. A product $\Theta_{\alpha}\Theta_{\alpha'}$ is either zero (one or more factors in common) or is an element $\pm\Theta_{\alpha''}$ (the sign arises because of ordering of the factors). The number of digits in α'' is the sum of the numbers of digits in α and α' .

The independent products are a basis for a (real) complex **Grassmann algebra**, with elements

$$f(\theta_1, \dots, \theta_n) = \sum_{\alpha} f_{\alpha} \Theta_{\alpha}, \quad f_{\alpha} \in \mathbb{C}$$

In this notation an element appears as a “function” of the Grassmann “variables”, but it is merely a linear combination of Grassmann basis with real or complex coefficients. The elements of the algebra can be added in the obvious way and multiplied. For example, with terms written in ordered form:

$$(f_0 + f_2\theta_2 + f_{123}\theta_1\theta_2\theta_3)(g_1\theta_1 + g_2\theta_2) = f_0g_1\theta_1 + f_0g_2\theta_2 - f_2g_1\theta_1\theta_2$$

A power series always truncates; for example $e^{a\theta_1\theta_2} = 1 + a\theta_1\theta_2$. In the next example, the fact that even products of different Grassmann units commute, gives the usual property of

the exponential:

$$\begin{aligned} e^{a\theta_1\theta_2+b\theta_3\theta_4} &= 1 + a\theta_1\theta_2 + b\theta_3\theta_4 + ab\theta_1\theta_2\theta_3\theta_4 \\ &= (1 + a\theta_1\theta_2)(1 + b\theta_3\theta_4) \\ &= e^{a\theta_1\theta_2}e^{b\theta_3\theta_4} \end{aligned}$$

29.1.2 Grassmann integrals

On the Grassmann algebra one defines a formal integral¹ by the rules:

- $\int d\theta_i 1 = 0$, $\int d\theta_i \theta_i = 1$;
- the symbols $d\theta_j$ anticommute with each other and with Grassmann units;
- the integral is linear.

Example 29.1.1. 1) $\int d\theta_1(f_0 + f_1\theta_1 + f_2\theta_2 + f_{12}\theta_1\theta_2) = f_1 + f_{12}\theta_2$;
2) $\iint d\theta_1 d\theta_2(f_0 + f_1\theta_1 + f_2\theta_2 + f_{12}\theta_1\theta_2) = -f_{12} \int d\theta_1 \theta_1 \int d\theta_2 \theta_2 = -f_{12}$.

Proposition 29.1.2. If η_1, \dots, η_n and $\theta_1, \dots, \theta_n$ are Grassmann units:

$$\int d\theta_1 \dots d\theta_n e^{\eta_1\theta_1 + \dots + \eta_n\theta_n} = (-1)^n \eta_1 \dots \eta_n \quad (29.8)$$

Proof. Note that $e^{\eta_1\theta_1 + \dots + \eta_n\theta_n} = e^{\eta_1\theta_1} \dots e^{\eta_n\theta_n} = (1 + \eta_1\theta_1) \dots (1 + \eta_n\theta_n)$. The factors commute with the symbols $d\theta_j$:

$$\begin{aligned} \int d\theta_1 \dots d\theta_n (1 + \eta_1\theta_1) \dots (1 + \eta_n\theta_n) &= \int d\theta_1 (1 + \eta_1\theta_1) \dots \int d\theta_n (1 + \eta_n\theta_n) \\ &= \int d\theta_1 \eta_1 \theta_1 \dots \int d\theta_n \eta_n \theta_n = (-1)^n \eta_1 (\int d\theta_1 \theta_1) \dots \eta_n (\int d\theta_n \theta_n). \end{aligned} \quad \square$$

Now consider the variant:

Proposition 29.1.3. Let M be a $n \times n$ real or complex matrix and η_1, \dots, η_n anticommuting units:

$$\int d\theta_1 \dots d\theta_n e^{\sum_{ij} \eta_i M_{ij} \theta_j} = (-1)^n (\det M) \eta_1 \dots \eta_n \quad (29.9)$$

Proof. By (29.9) the value of the integral is $(-1)^n (\eta_{j_1} M_{j_1,1}) \dots (\eta_{j_n} M_{j_n,n})$, where repeated indices are summed. In expanding the sum, a product $\eta_{j_1} \dots \eta_{j_n}$ cannot contain two equal factors. Then the products can only contain permutations of $\eta_1 \dots \eta_n$ up to signs $(-1)^\sigma$ i.e. the multi-index sum reduces to a sum on permutations. Finally, $\sum_{\pi} (-1)^\sigma M_{\pi_1,1} \dots M_{\pi_n,n}$ is precisely $\det M$. \square

¹ Felix A. Berezin, The method of second quantization, Nauka Moscow 1965

The factors η_j in the result of the integral (29.9) can be removed by further integrations. The sign $(-1)^n$ is absorbed in the change M to $-M$:

$$\int d\eta_n \dots d\eta_1 d\theta_1 \dots d\theta_n e^{-\sum_{ij} \eta_i M_{ij} \theta_j} = \det M$$

The usual notation is to write the units η_j as $\bar{\theta}_j$. Since $d\bar{\theta}_1 d\theta_1$ etc. commute with everything, we rewrite the integral in the final form

$$\boxed{\int d\bar{\theta}_1 d\theta_1 \dots d\bar{\theta}_n d\theta_n e^{-\sum_{ij} \bar{\theta}_i M_{ij} \theta_j} = \det M} \quad (29.10)$$

In analogy with commuting fields (see the Bargmann space 19.7 of holomorphic functions), the Russian physicist Felix Berezin (1931–1980) introduced an inner product as a Grassmann integral, and the operators of multiplication and derivation by a Grassmann unit². Grassmann fields are used to fulfil the Pauli principle in the construction of the path integral for fermions, in quantum field theory and in superconductivity.

As an application of Gaussian integrals of commuting and anticommuting variables, let us consider the problem of the spectral density of random matrices.

29.1.3 Spectral density of random matrices

Let H be a $n \times n$ Hermitian random matrix, meaning that its independent matrix elements are distributed according to some probability. Its real eigenvalues x_k are then random, and we wish to evaluate their probability distribution:

$$\rho(x) = \left\langle \frac{1}{n} \sum_k \delta(x - x_k) \right\rangle$$

where the average is done over the matrices of the ensemble. The resolvent matrix is $G(z) = (z - H)^{-1}$. With $z = x - i\epsilon$ the trace is:

$$\text{tr} G(x + i\epsilon) = \sum_k \frac{1}{x - x_k - i\epsilon}$$

By the Plemelj-Sokhotski identity we obtain a useful relation for the averaged density of the eigenvalues:

$$\rho(x) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \text{Im} \left\langle \frac{1}{n} \text{tr} G(x - i\epsilon) \right\rangle \quad (29.11)$$

² There are analogies with the Bargmann space 19.7, where variables commute. For a presentation see J. Zinn-Justin, Path integrals in quantum mechanics, Oxford Univ. Press 1989.

On the other hand, $\det(z - H) = \prod(z - x_k)$ and:

$$\sum_k \frac{1}{z - x_k} = -\det(z - H) \frac{d}{dz} \frac{1}{\det(z - H)} = -\frac{d}{dz} \frac{\det(z' - H)}{\det(z - H)} \Big|_{z'=z}$$

The ensemble average (29.11) is then evaluated by averaging the ratio of determinants. This is performed by expressing both determinants as integrals in commuting variables z_j and Grassmann variables $\bar{\theta}_j, \theta_j$, with equations (29.5) and (29.10):

$$(-i)^n \frac{\det(x' - H)}{\det(x - i\epsilon - H)} = \int \prod_{k=1}^n d\bar{\theta}_k d\theta_k \frac{d^2 z_k}{\pi} e^{-\bar{\theta}(x' - H)\theta - i\mathbf{z}^\dagger(x - i\epsilon - H)\mathbf{z}} \tag{29.12}$$

After the ensemble average of the factor $\langle \exp[\bar{\theta}H\theta + i\mathbf{z}^\dagger H\mathbf{z}] \rangle$, one remains with an integral on the auxiliary variables that is no longer Gaussian. To proceed, in general, the large n limit is appealed. An exception is the Lloyd model. Perhaps it is the simplest exact evaluation of an average on disorder.

The Lloyd model

In 1969 P. Lloyd introduced a model for a particle on a lattice with a random potential at each site for the study of the Anderson localisation in 3D. The potential is a random variable with Cauchy disorder. The rare feature is that the average spectral density may be analytically evaluated³.

The evaluation is here done for $H = H_0 + V$, where H_0 is any Hermitian matrix of size n and V is a diagonal matrix with elements v_j distributed according to the Cauchy distribution:

$$p(v) = \frac{\delta}{\pi} \frac{1}{v^2 + \delta^2} \tag{29.13}$$

The larger is δ , the greater is disorder.

To evaluate the average of (29.12) we need the integrals (here $s > 0$)

$$\int_{-\infty}^{+\infty} dv p(v) e^{ivs} = e^{-\delta s}, \quad \int_{-\infty}^{+\infty} dv p(v) v e^{ivs} = i\delta e^{-\delta s}$$

³ P. Lloyd, *Exactly solvable model of electronic states in a three-dimensional disordered Hamiltonian: non-existence of localised states*, J. Phys. C **2** n.2 (1969) 1717–1725.

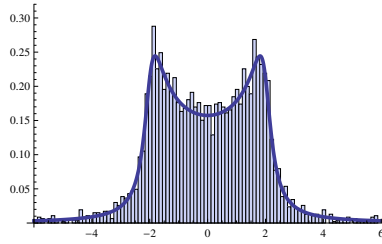


Figure 29.1 The analytic distribution of eigenvalues of the Laplacian in $d=1$, with Cauchy diagonal (Lloyd model, $\delta = 0.3$), eq.(29.16). The histogram is the distribution for a single Lloyd matrix of size 4000. The (van Hove) singularities of the free model in ± 2 are smoothed by disorder, that also adds tails to the sharp band $[-2, 2]$.

The average of (29.12) is done on the factor

$$\begin{aligned} \left\langle e^{\sum_j v_j (\bar{\theta}_j \theta_j + i|z_j|^2)} \right\rangle &= \prod_{j=1 \dots n} \int d v p(v) e^{i v |z_j|^2} (1 + v \bar{\theta}_j \theta_j) \\ &= \prod_{j=1 \dots n} e^{-\delta |z_j|^2} (1 + i \delta \bar{\theta}_j \theta_j) = e^{-\delta \sum_j (|z_j|^2 + i \bar{\theta}_j \theta_j)} \end{aligned}$$

$$\begin{aligned} \left\langle \frac{\det(x' - H)}{\det(x + i\epsilon - H)} \right\rangle &= \int \prod_{k=1}^n d\bar{\theta}_k d\theta_k \frac{d^2 z_k}{-i\pi} e^{-\bar{\theta}(x' - H_0 - i\delta)\theta - i z_k^\dagger (x - H_0 - i\delta) z_k} \\ &= \frac{\det(x' - H_0 - i\delta)}{\det(x - H_0 - i\delta)} \end{aligned}$$

Then $\rho(x) = \frac{1}{\pi} \text{Im} \frac{1}{n} \text{tr} G_0(x - i\delta)$ where $G_0(z)$ is the resolvent of H_0 .

If λ_k are the eigenvalues of H_0 , the spectrum of H averaged on Cauchy disorder is a superposition of Cauchy distributions centred on the eigenvalues of H_0 :

$$\rho(x) = \frac{1}{n} \sum_{k=1 \dots n} \frac{1}{\pi} \frac{\delta}{(x - \lambda_k)^2 + \delta^2} \tag{29.14}$$

If H_0 is the adjacency matrix for the cubic lattice \mathbb{Z}^d , the spectral density per unit volume is (25.34), with support $[-2d, 2d]$:

$$\rho_0(\lambda) = \int_0^\infty \frac{ds}{\pi} J_0(2s)^d \cos(\lambda s)$$

The spectral density of the Lloyd model $H_0 + V$ is a convolution integral,

$$\rho(x) = \int_{-\infty}^{+\infty} d\lambda \frac{\delta}{\pi} \frac{\rho_0(\lambda)}{(x-\lambda)^2 + \delta^2} = \int_0^\infty \frac{ds}{\pi} J_0(2s)^d e^{-\delta s} \cos(xs) \quad (29.15)$$

The integral for $d = 1$ is known, and is plotted in fig.29.1:

$$\rho(x) = \frac{1}{\pi\sqrt{2}} \frac{\sqrt{4 + \delta^2 - x^2 + \sqrt{(4 + \delta^2 - x^2)^2 + 4x^2\delta^2}}}{\sqrt{(4 + \delta^2 - x^2)^2 + 4x^2\delta^2}} \quad (29.16)$$

Several problems characterized by disorder, as random matrix theory, transport in disordered potential, the Anderson metal-insulator transition, random graphs, glasses, are studied by these techniques⁴. They are often dubbed supersymmetric because they symmetrically involve commuting and anticommuting variables. An alternative, not simpler, is the Replica Method.

⁴ E. Brézin, *Grassmann variables and supersymmetry in the theory of disordered systems* (VIII Sitges Conf. 1984), Lect. Notes Phys. **216** (1985) 115–123. It is reported in the textbook C. Itzykson and J. M. Drouffe, *Théorie statistique des champs*, vol.2 p.274, Editions du CNRS (1989). A nice reference is F Haake, *Quantum signatures of chaos*, Springer.

Appendix

Figures and sources

These figures are my own drawings: 2-1, 3-1, 3-2, 5-2, 7-1, 8-1, 13-1, 14-1, 14-4a, 14-4b, 28-1.

These plots were produced with Wolfram Mathematica13 (a formidable tool!): 2-2a, 2-2b, 3-3, 4-1a, 4-1b, 4-2, 5-3a, 5-3b, 5-4, 6-1, 6-2, 6-3, 6-4a, 6-4b, 6-5, 11-1, 11-2, 11-3, 11-4, 12-1, 13-2, 14-2, 14-3, 15-1, 15-2, 18-1, 19-3, 20-1, 20-2, 20-3, 20-4, 20-5a, 20-5b, 20-8, 20-9, 20-10a, 25-1, 25-2a, 25-2b, 25-3, 25-5, 29-1.

These figures were taken from the WEB:

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- 5-1a: Pierre A. Cauchy, <https://library.si.edu/image-gallery/73510>, Image by Ch. H. Reutlinger - Smithsonian Inst. Libraries.
- 5-1b: Karl Weierstrass, <https://mathshistory.st-andrews.ac.uk/Biographies/Weierstrass/>
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- 24-2: Izrail Gelfand, <https://www.israelmgelfand.com/bio.html>, also in <https://mathshistory.st-andrews.ac.uk/Biographies/Gelfand/>
- 25-4: from: A. M. Odlyzko, On the distribution of spacings between zeros of the Zeta function, Mathematics of Computation 48 (1987) 273-308.

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These are textbooks that I found particularly useful and inspiring (others are specified in the text).

Complex analysis:

- L. V. Ahlfors, *Complex Analysis*, McGraw-Hill;
 J. Bak and D. J. Newman, *Complex Analysis*, UTM Springer;
 R. P. Boas, *Invitation to complex analysis*, MAA textbooks;
 P. Henrici, *Applied and computational complex analysis*, Wiley;
 A. I. Markushevich, *Theory of functions of a complex variable*, Chelsea.

Functional analysis:

- Ph. Blanchard and E. Brüning, *Mathematical Methods in Physics: Distributions, Hilbert space operators, and Variational methods*, Birkhäuser;
 W. Cheney, *Analysis for applied mathematics*, Springer;
 A. Kolmogorov and S. Fomine, *Éléments de la théorie des fonctions et de l'analyse fonctionnelle*, Éditions de Moscou (also in Dover edition);
 M. Reed and B. Simon, *Functional Analysis*, Academic Press.

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Luca Guido Molinari

Mathematical Methods for Physics

This textbook has been used by the author for many years in his class of Mathematical Methods of Physics. It covers several topics that are considered necessary for the training of physicists. Group theory and differential equations are covered in specific courses. Its main features are the style, less formal than mathematics texts, and the presence of numerous examples from the field of physics.

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