

KARL SVOZIL

# MATHEMATICAL METHODS OF THEORETICAL PHYSICS

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# Introduction

THIS IS A THIRD ATTEMPT to provide some written material of a course in mathematical methods of theoretical physics. I have presented this course to an undergraduate audience at the Vienna University of Technology. Only God knows (see Ref. <sup>1</sup> part one, question 14, article 13; and also Ref. <sup>2</sup>, p. 243) if I have succeeded to teach them the subject! I kindly ask the perplexed to please be patient, do not panic under any circumstances, and do not allow themselves to be too upset with mistakes, omissions & other problems of this text. At the end of the day, everything will be fine, and in the long run we will be dead anyway.

I AM RELEASING THIS text to the public domain because it is my conviction and experience that content can no longer be held back, and access to it be restricted, as its creators see fit. On the contrary, we experience a push toward so much content that we can hardly bear this information flood, so we have to be selective and restrictive rather than acquisitive. I hope that there are some readers out there who actually enjoy and profit from the text, in whatever form and way they find appropriate.

SUCH UNIVERSITY TEXTS AS THIS ONE – and even recorded video transcripts of lectures – present a transitory, almost outdated form of teaching. Future generations of students will most likely enjoy *massive open online courses* (MOOCs) that might integrate interactive elements and will allow a more individualized – and at the same time automated – form of learning. What is most important from the viewpoint of university administrations is that (i) MOOCs are cost-effective (that is, cheaper than standard tuition) and (ii) the know-how of university teachers and researchers gets transferred to the university administration and management. In both these ways, MOOCs are the implementation of assembly line methods (first introduced by Henry Ford for the production of affordable cars) in the university setting. They will transform universities and schools as much as the *Ford Motor Company* (NYSE:F) has transformed the car industry.

TO NEWCOMERS in the area of theoretical physics (and beyond) I strongly

*"It is not enough to have no concept, one must also be capable of expressing it."* From the German original in *Karl Kraus, Die Fackel* **697**, 60 (1925): *"Es genügt nicht, keinen Gedanken zu haben: man muss ihn auch ausdrücken können."*

<sup>1</sup> Thomas Aquinas. *Summa Theologica*. Translated by Fathers of the English Dominican Province. Christian Classics Ethereal Library, Grand Rapids, MI, 1981. URL <http://www.ccel.org/ccel/aquinas/summa.html>

<sup>2</sup> Ernst Specker. Die Logik nicht gleichzeitig entscheidbarer Aussagen. *Dialectica*, 14 (2-3):239–246, 1960. DOI: 10.1111/j.1746-8361.1960.tb00422.x. URL <http://dx.doi.org/10.1111/j.1746-8361.1960.tb00422.x>

recommend to consider and acquire two related proficiencies:

- to learn to speak and publish in  $\LaTeX$  and BibTeX.  $\LaTeX$ 's various dialects and formats, such as REVTeX, provide a kind of template for structured scientific texts, thereby assisting you writing and publishing consistently and with methodologic rigour;
- to subscribe to and browse through preprints published at the website [arXiv.org](http://arxiv.org), which provides open access to more than three quarters of a million scientific texts; most of them written in and compiled by  $\LaTeX$ . Over time, this database has emerged as a *de facto* standard from the initiative of an individual researcher working at the *Los Alamos National Laboratory* (the site at which also the first nuclear bomb has been developed and assembled). Presently it happens to be administered by *Cornell University*. I suspect (this is a personal subjective opinion) that (the successors of) [arXiv.org](http://arxiv.org) will eventually bypass if not supersede most scientific journals of today.

It may come as no surprise that this very text is written in  $\LaTeX$  and published by [arXiv.org](http://arxiv.org) under eprint number *arXiv:1203.4558*, accessible freely via <http://arxiv.org/abs/1203.4558>.

MY OWN ENCOUNTER with many researchers of different fields and different degrees of formalization has convinced me that there is no single way of formally comprehending a subject<sup>3</sup>. With regards to formal rigour, there appears to be a rather questionable chain of contempt – all too often theoretical physicists look upon the experimentalists suspiciously, mathematical physicists look upon the theoreticians skeptically, and mathematicians look upon the mathematical physicists dubiously. I have even experienced the distrust formal logicians expressed about their colleagues in mathematics! For an anecdotal evidence, take the claim of a prominent member of the mathematical physics community, who once dryly remarked in front of a fully packed audience, “what other people call ‘proof’ I call ‘conjecture!’”

SO PLEASE BE AWARE that not all I present here will be acceptable to everybody; for various reasons. Some people will claim that I am too confusing and utterly formalistic, others will claim my arguments are in desperate need of rigour. Many formally fascinated readers will demand to go deeper into the meaning of the subjects; others may want some easy-to-identify pragmatic, syntactic rules of deriving results. I apologise to both groups from the onset. This is the best I can do; from certain different perspectives, others, maybe even some tutors or students, might perform much better.

I AM CALLING for more tolerance and a greater unity in physics; as well as for a greater esteem on “both sides of the same effort;” I am also opting for

If you excuse a maybe utterly displaced comparison, this might be tantamount only to studying the Austrian family code (“Ehegesetz”) from \$49 onward, available through <http://www.ris.bka.gv.at/Bundesrecht/> before getting married.

<sup>3</sup> Philip W. Anderson. More is different. *Science*, 177(4047):393–396, August 1972. DOI: 10.1126/science.177.4047.393. URL <http://dx.doi.org/10.1126/science.177.4047.393>

more pragmatism; one that acknowledges the mutual benefits and oneness of theoretical and empirical physical world perceptions. Schrödinger<sup>4</sup> cites Democritus with arguing against a too great separation of the intellect (*διανοία*, *dianoia*) and the senses (*αἰσθησεις*, *aitheseis*). In fragment D 125 from Galen<sup>5</sup>, p. 408, footnote 125, the intellect claims “ostensibly there is color, ostensibly sweetness, ostensibly bitterness, actually only atoms and the void;” to which the senses retort: “Poor intellect, do you hope to defeat us while from us you borrow your evidence? Your victory is your defeat.”

In his 1987 *Abschiedsvorlesung* professor Ernst Specker at the *Eidgenössische Hochschule Zürich* remarked that the many books authored by David Hilbert carry his name first, and the name(s) of his co-author(s) second, although the subsequent author(s) had actually written these books; the only exception of this rule being Courant and Hilbert’s 1924 book *Methoden der mathematischen Physik*, comprising around 1000 densely packed pages, which allegedly none of these authors had really written. It appears to be some sort of collective effort of scholars from the University of Göttingen.

So, in sharp distinction from these activities, I most humbly present my own version of what is important for standard courses of contemporary physics. Thereby, I am quite aware that, not dissimilar with some attempts of that sort undertaken so far, I might fail miserably. Because even if I manage to induce some interest, affection, passion and understanding in the audience – as Danny Greenberger put it, inevitably four hundred years from now, all our present physical theories of today will appear transient<sup>6</sup>, if not laughable. And thus in the long run, my efforts will be forgotten; and some other brave, courageous guy will continue attempting to (re)present the most important mathematical methods in theoretical physics.

INDEED, I HAVE TO ADMIT that in browsing through these notes after a longer time of absence makes me feel uneasy – how complicated, subtle and even incomprehensible my own writings appear! This is a recurring source of frustration. Maybe I am incapable of developing things in a satisfactory, comprehensible manner? Are issues really that complex? I do not want to lure willing & highly spirited young students into blind alleys of unnecessary sophistication! In my darker moments I am reminded of Aurelius Augustinus’ “Confessiones” (Book XI, chapter 25): “*Ei mihi, qui nescio saltem quid nesciam!*”

ALAS, BY KEEPING IN MIND these saddening suspicions, and for as long as we are here on Earth, let us carry on, execute our absurd freedom<sup>7</sup>, and start doing what we are supposed to be doing well; just as Krishna in Chapter XI:32,33 of the *Bhagavad Gita* is quoted for insisting upon Arjuna to fight, telling him to “*stand up, obtain glory! Conquer your enemies, acquire fame and enjoy a prosperous kingdom. All these warriors have already been*

<sup>4</sup> Erwin Schrödinger. *Nature and the Greeks*. Cambridge University Press, Cambridge, 1954

<sup>5</sup> Hermann Diels. *Die Fragmente der Vorsokratiker, griechisch und deutsch*. Weidmannsche Buchhandlung, Berlin, 1906. URL <http://www.archive.org/details/details/diefragmentederv01dieluoft>

German: Nachdem D. [[Demokritos]] sein Mißtrauen gegen die Sinneswahrnehmungen in dem Satze ausgesprochen: ‘Scheinbar (d. i. konventionell) ist Farbe, scheinbar Süßigkeit, scheinbar Bitterkeit: wirklich nur Atome und Leeres’ läßt er die Sinne gegen den Verstand reden: ‘Du armer Verstand, von uns nimmst du deine Beweisstücke und willst uns damit besiegen? Dein Sieg ist dein Fall!’

<sup>6</sup> Imre Lakatos. *Philosophical Papers. 1. The Methodology of Scientific Research Programmes*. Cambridge University Press, Cambridge, 1978

“Alas for me, that I do not at least know the extent of my own ignorance!”

<sup>7</sup> Albert Camus. *Le Mythe de Sisyphe* (English translation: *The Myth of Sisyphus*). 1942

*destroyed by me. You are only an instrument."*



*Part I:*

*Metamathematics and Metaphysics*





# Unreasonable effectiveness of mathematics in the natural sciences

ALL THINGS CONSIDERED, it is mind-boggling why formalized thinking and numbers utilize our comprehension of nature. Even today eminent researchers muse about the “unreasonable effectiveness of mathematics in the natural sciences”<sup>1</sup>.

Zeno of Elea and Parmenides, for instance, wondered how there can be motion if our universe is either infinitely divisible or discrete. Because, in the dense case (between any two points there is another point), the slightest finite move would require an infinity of actions. Likewise in the discrete case, how can there be motion if everything is not moving at all times<sup>2</sup>?

For the sake of perplexion, take Neils Henrik Abel’s verdict denouncing that (Letter to Holmboe, January 16, 1826<sup>3</sup>), “*divergent series are the invention of the devil, and it is shameful to base on them any demonstration whatsoever.*” This, of course, did neither prevent Abel nor too many other discussants to investigate these devilish inventions.

Indeed, one of the most successful physical theories in terms of predictive powers, perturbative quantum electrodynamics, deals with divergent series<sup>4</sup> which contribute to physical quantities such as mass and charge which have to be “regularized” by subtracting infinities by hand (for an alternative approach, see<sup>5</sup>).

Another, rather burlesque, question is about the physical limit state of a hypothetical lamp with ever decreasing switching cycles discussed by Thomson<sup>6</sup>. If one encodes the physical states of the Thomson lamp by “0” and “1,” associated with the lamp “on” and “off,” respectively, and the switching process with the concatenation of “+1” and “-1” performed so far, then the divergent infinite series associated with the Thomson lamp is the Leibniz series

$$s = \sum_{n=0}^{\infty} (-1)^n = 1 - 1 + 1 - 1 + 1 - \dots \stackrel{A}{=} \frac{1}{1 - (-1)} = \frac{1}{2} \quad (1.1)$$

<sup>1</sup> Eugene P. Wigner. The unreasonable effectiveness of mathematics in the natural sciences. Richard Courant Lecture delivered at New York University, May 11, 1959. *Communications on Pure and Applied Mathematics*, 13:1–14, 1960. DOI: 10.1002/cpa.3160130102. URL <http://dx.doi.org/10.1002/cpa.3160130102>

<sup>2</sup> H. D. P. Lee. *Zeno of Elea*. Cambridge University Press, Cambridge, 1936; Paul Benacerraf. Tasks and supertasks, and the modern Eleatics. *Journal of Philosophy*, LIX(24):765–784, 1962. URL <http://www.jstor.org/stable/2023500>; A. Grünbaum. *Modern Science and Zeno’s paradoxes*. Allen and Unwin, London, second edition, 1968; and Richard Mark Sainsbury. *Paradoxes*. Cambridge University Press, Cambridge, United Kingdom, third edition, 2009. ISBN 0521720796

<sup>3</sup> Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

<sup>4</sup> Freeman J. Dyson. Divergence of perturbation theory in quantum electrodynamics. *Phys. Rev.*, 85(4):631–632, Feb 1952. DOI: 10.1103/PhysRev.85.631. URL <http://dx.doi.org/10.1103/PhysRev.85.631>

<sup>5</sup> Günter Scharf. *Finite Quantum Electrodynamics: The Causal Approach*. Springer, Berlin, Heidelberg, second edition, 1989, 1995

<sup>6</sup> James F. Thomson. Tasks and supertasks. *Analysis*, 15:1–13, October 1954

which is just a particular instance of a geometric series (see below) with the common ratio “-1.” Here, “A” indicates the *Abel sum*<sup>7</sup> obtained from a “continuation” of the geometric series, or alternatively, by  $s = 1 - s$ .

As this shows, formal sums of the Leibnitz type (1.1) require specifications which could make them unique. But has this “specification by continuation” any kind of physical meaning?

In modern days, similar arguments have been translated into the proposal for infinity machines by Blake<sup>8</sup>, p. 651, and Weyl<sup>9</sup>, pp. 41-42, which could solve many very difficult problems by searching through unbounded recursively enumerable cases. To achieve this physically, ultrarelativistic methods suggest to put observers in “fast orbits” or throw them toward black holes<sup>10</sup>.

The Pythagoreans are often cited to have believed that the universe is natural numbers or simple fractions thereof, and thus physics is just a part of mathematics; or that there is no difference between these realms. They took their conception of numbers and world-as-numbers so seriously that the existence of irrational numbers which cannot be written as some ratio of integers shocked them; so much so that they allegedly drowned the poor guy who had discovered this fact. That appears to be a saddening case of a state of mind in which a subjective metaphysical belief in and wishful thinking about one’s own constructions of the world overwhelms critical thinking; and what should be wisely taken as an epistemic finding is taken to be ontologic truth.

The relationship between physics and formalism has been debated by Bridgman<sup>11</sup>, Feynman<sup>12</sup>, and Landauer<sup>13</sup>, among many others. It has many twists, anecdotes and opinions. Take, for instance, Heaviside’s not uncontroversial stance<sup>14</sup> on it:

*I suppose all workers in mathematical physics have noticed how the mathematics seems made for the physics, the latter suggesting the former, and that practical ways of working arise naturally. ... But then the rigorous logic of the matter is not plain! Well, what of that? Shall I refuse my dinner because I do not fully understand the process of digestion? No, not if I am satisfied with the result. Now a physicist may in like manner employ unrigorous processes with satisfaction and usefulness if he, by the application of tests, satisfies himself of the accuracy of his results. At the same time he may be fully aware of his want of infallibility, and that his investigations are largely of an experimental character, and may be repellent to unsympathetically constituted mathematicians accustomed to a different kind of work. [S225]*

Dietrich Küchemann, the ingenious German-British aerodynamicist and one of the main contributors to the wing design of the *Concord* supersonic civil aircraft, tells us<sup>15</sup>

*[Again,] the most drastic simplifying assumptions must be made before we can even think about the flow of gases and arrive at equations which are amenable to treatment. Our whole science lives on highly-idealised concepts and ingenious abstractions and approximations. We should remember this in all*

<sup>7</sup> Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

<sup>8</sup> R. M. Blake. The paradox of temporal process. *Journal of Philosophy*, 23(24): 645–654, 1926. URL <http://www.jstor.org/stable/2013813>

<sup>9</sup> Hermann Weyl. *Philosophy of Mathematics and Natural Science*. Princeton University Press, Princeton, NJ, 1949

<sup>10</sup> Itamar Pitowsky. The physical Church-Turing thesis and physical computational complexity. *Iyyun*, 39:81–99, 1990

<sup>11</sup> Percy W. Bridgman. A physicist’s second reaction to Mengenlehre. *Scripta Mathematica*, 2:101–117, 224–234, 1934

<sup>12</sup> Richard Phillips Feynman. *The Feynman lectures on computation*. Addison-Wesley Publishing Company, Reading, MA, 1996. edited by A.J.G. Hey and R. W. Allen

<sup>13</sup> Rolf Landauer. Information is physical. *Physics Today*, 44(5):23–29, May 1991. DOI: 10.1063/1.881299. URL <http://dx.doi.org/10.1063/1.881299>

<sup>14</sup> Oliver Heaviside. *Electromagnetic theory*. “The Electrician” Printing and Publishing Corporation, London, 1894-1912. URL <http://archive.org/details/electromagnetict02heavrich>

<sup>15</sup> Dietrich Küchemann. *The Aerodynamic Design of Aircraft*. Pergamon Press, Oxford, 1978

*modesty at all times, especially when somebody claims to have obtained “the right answer” or “the exact solution”. At the same time, we must acknowledge and admire the intuitive art of those scientists to whom we owe the many useful concepts and approximations with which we work [page 23].*

The question, for instance, is imminent whether we should take the formalism very seriously and literally, using it as a guide to new territories, which might even appear absurd, inconsistent and mind-boggling; just like Carroll’s *Alice’s Adventures in Wonderland*. Should we expect that all the wild things formally imaginable have a physical realization?

It might be prudent to adopt a contemplative strategy of *evenly-suspended attention* outlined by Freud<sup>16</sup>, who admonishes analysts to be aware of the dangers caused by “*temptations to project, what [the analyst] in dull self-perception recognizes as the peculiarities of his own personality, as generally valid theory into science.*” Nature is thereby treated as a client-patient, and whatever findings come up are accepted as is without any immediate emphasis or judgment. This also alleviates the dangers of becoming embittered with the reactions of “the peers,” a problem sometimes encountered when “surfing on the edge” of contemporary knowledge; such as, for example, Everett’s case<sup>17</sup>.

Jaynes has warned of the “*Mind Projection Fallacy*”<sup>18</sup>, pointing out that “*we are all under an ego-driven temptation to project our private thoughts out onto the real world, by supposing that the creations of one’s own imagination are real properties of Nature, or that one’s own ignorance signifies some kind of indecision on the part of Nature.*”

Note that the formalist Hilbert<sup>19</sup>, p. 170, is often quoted as claiming that nobody shall ever expel mathematicians from the paradise created by Cantor’s set theory. In Cantor’s “naive set theory” definition, “*a set is a collection into a whole of definite distinct objects of our intuition or of our thought. The objects are called the elements (members) of the set.*” If one allows substitution and self-reference<sup>20</sup>, this definition turns out to be inconsistent; that is self-contradictory – for instance Russel’s paradoxical “set of all sets that are not members of themselves” qualifies as set in the Cantorian approach. In praising the set theoretical paradise, Hilbert must have been well aware of the inconsistencies and problems that plagued Cantorian style set theory, but he fully dissented and refused to abandon its stimulus.

Is there a similar pathos also in theoretical physics?

Maybe our physical capacities are limited by our mathematical fantasy alone? Who knows?

For instance, could we make use of the Banach-Tarski paradox<sup>21</sup> as a sort of ideal production line? The Banach-Tarski paradox makes use of the fact that in the continuum “it is (nonconstructively) possible” to transform any given volume of three-dimensional space into any other desired shape, form and volume – in particular also to double the original volume – by

<sup>16</sup> Sigmund Freud. Ratschläge für den Arzt bei der psychoanalytischen Behandlung. In Anna Freud, E. Bibring, W. Hoffer, E. Kris, and O. Isakower, editors, *Gesammelte Werke. Chronologisch geordnet. Achter Band. Werke aus den Jahren 1909–1913*, pages 376–387, Frankfurt am Main, 1999. Fischer

<sup>17</sup> Hugh Everett III. The Everett interpretation of quantum mechanics: Collected works 1955–1980 with commentary. Princeton University Press, Princeton, NJ, 2012. ISBN 9780691145075. URL <http://press.princeton.edu/titles/9770.html>

<sup>18</sup> Edwin Thompson Jaynes. Clearing up mysteries - the original goal. In John Skilling, editor, *Maximum-Entropy and Bayesian Methods: : Proceedings of the 8th Maximum Entropy Workshop, held on August 1-5, 1988, in St. John’s College, Cambridge, England*, pages 1–28. Kluwer, Dordrecht, 1989. URL <http://bayes.wustl.edu/etj/articles/cmystery.pdf>; and Edwin Thompson Jaynes. Probability in quantum theory. In Wojciech Hubert Zurek, editor, *Complexity, Entropy, and the Physics of Information: Proceedings of the 1988 Workshop on Complexity, Entropy, and the Physics of Information, held May - June, 1989, in Santa Fe, New Mexico*, pages 381–404. Addison-Wesley, Reading, MA, 1990. ISBN 9780201515091. URL <http://bayes.wustl.edu/etj/articles/prob.in.qm.pdf>

<sup>19</sup> David Hilbert. Über das Unendliche. *Mathematische Annalen*, 95(1):161–190, 1926. DOI: 10.1007/BF01206605. URL <http://dx.doi.org/10.1007/BF01206605>; and Georg Cantor. Beiträge zur Begründung der transfiniten Mengenlehre. *Mathematische Annalen*, 46(4):481–512, November 1895. DOI: 10.1007/BF02124929. URL <http://dx.doi.org/10.1007/BF02124929>  
German original: “*Aus dem Paradies, das Cantor uns geschaffen, soll uns niemand vertreiben können.*”

Cantor’s German original: “*Unter einer “Menge” verstehen wir jede Zusammenfassung  $M$  von bestimmten wohlunterschiedenen Objekten  $m$  unsrer Anschauung oder unseres Denkens (welche die*

transforming finite subsets of the original volume through isometries, that is, distance preserving mappings such as translations and rotations. This, of course, could also be perceived as a merely abstract paradox of infinity, somewhat similar to Hilbert's hotel.

By the way, Hilbert's hotel <sup>22</sup> has a countable infinity of hotel rooms. It is always capable to accommodate a newcomer by shifting all other guests residing in any given room to the room with the next room number. Maybe we will never be able to build an analogue of Hilbert's hotel, but maybe we will be able to do that one far away day.

After all, science finally succeeded to do what the alchemists sought for so long: we are capable of producing gold from mercury <sup>23</sup>.



<sup>22</sup> Rudy Rucker. *Infinity and the Mind*. Birkhäuser, Boston, 1982

Anton Zeilinger has quoted Tony Klein as saying that "every system is a perfect simulacrum of itself."

<sup>23</sup> R. Sherr, K. T. Bainbridge, and H. H. Anderson. Transmutation of mercury by fast neutrons. *Physical Review*, 60(7):473–479, Oct 1941. DOI: 10.1103/PhysRev.60.473. URL <http://dx.doi.org/10.1103/PhysRev.60.473>

## 2

### *Methodology and proof methods*

FOR MANY THEOREMS there exist many proofs. Consider this: the 4th edition of *Proofs from THE BOOK*<sup>1</sup> lists six proofs of the infinity of primes (chapter 1). Chapter 19 refers to nearly a hundred proofs of the fundamental theorem of algebra, that every nonconstant polynomial with complex coefficients has at least one root in the field of complex numbers.

WHICH PROOFS, if there exist many, somebody chooses or prefers is often a question of taste and elegance, and thus a subjective decision. Some proofs are constructive<sup>2</sup> and computable<sup>3</sup> in the sense that a construction method is presented. Tractability is not an entirely different issue<sup>4</sup> – note that even “higher” polynomial growth of temporal requirements, or of space and memory resources, of a computation with some parameter characteristic for the problem, may result in a solution which is unattainable “for all practical purposes” (fapp)<sup>5</sup>.

FOR THOSE OF US with a rather limited amount of storage and memory, and with a lot of troubles and problems, it is quite consoling that it is not (always) necessary to be able to memorize all the proofs that are necessary for the deduction of a particular corollary or theorem which turns out to be useful for the physical task at hand. In some cases, though, it may be necessary to keep in mind the assumptions and derivation methods that such results are based upon. For example, how many readers may be able to immediately derive the simple power rule for derivation of polynomials – that is, for any real coefficient  $a$ , the derivative is given by  $(r^a)' = ar^{a-1}$ ? While I suspect that not too many may be able to derive this formula without consulting additional help (a help: one could use the *binomial theorem*), many of us would nevertheless acknowledge to be aware of, and be able and happy to apply, this rule.

STILL ANOTHER ISSUE is whether it is better to have a proof of a “true” mathematical statement rather than none. And what is truth – can it

<sup>1</sup> Martin Aigner and Günter M. Ziegler. *Proofs from THE BOOK*. Springer, Heidelberg, four edition, 1998-2010. ISBN 978-3-642-00855-9. URL <http://www.springerlink.com/content/978-3-642-00856-6>

<sup>2</sup> Douglas Bridges and F. Richman. *Varieties of Constructive Mathematics*. Cambridge University Press, Cambridge, 1987; and E. Bishop and Douglas S. Bridges. *Constructive Analysis*. Springer, Berlin, 1985

<sup>3</sup> Oliver Aberth. *Computable Analysis*. McGraw-Hill, New York, 1980; Klaus Weihrauch. *Computable Analysis. An Introduction*. Springer, Berlin, Heidelberg, 2000; and Vasco Brattka, Peter Hertling, and Klaus Weihrauch. A tutorial on computable analysis. In S. Barry Cooper, Benedikt Löwe, and Andrea Sorbi, editors, *New Computational Paradigms: Changing Conceptions of What is Computable*, pages 425–491. Springer, New York, 2008

<sup>4</sup> Georg Kreisel. A notion of mechanistic theory. *Synthese*, 29:11–26, 1974. DOI: 10.1007/BF00484949. URL <http://dx.doi.org/10.1007/BF00484949>; Robin O. Gandy. Church's thesis and principles for mechanics. In J. Barwise, H. J. Kreiser, and K. Kunen, editors, *The Kleene Symposium. Vol. 101 of Studies in Logic and Foundations of Mathematics*, pages 123–148. North Holland, Amsterdam, 1980; and Itamar Pitowsky. The physical Church-Turing thesis and physical computational complexity. *Iyyun*, 39:81–99, 1990

<sup>5</sup> John S. Bell. Against 'measurement'. *Physics World*, 3:33–41, 1990. URL <http://physicsworldarchive.iop.org/summary/pwa-xml/3/8/phwv3i8a26>

be some revelation, a rare gift, such as seemingly in Śrīnivāsa Aiyangār Rāmānujan's case? A related issue is knowledge acquired by revelation or by some authority; say, by some *oracle*. Oracles occur in modern computer science, but only as idealized concepts whose physical realization is highly questionable if not forbidden.

SOME PROOF METHODS, among others, which are used today, are:

1. (indirect) proof by contradiction;
2. proof by mathematical induction;
3. direct proof;
4. proof by construction;
5. nonconstructive proof.

LET US CONSIDER SOME CONCRETE EXAMPLES and instances of the perplexing varieties of proof methods used today. A typical proof by contradiction is about the irrationality of  $\sqrt{2}$  (see also Ref. <sup>6</sup>, p. 128).

Suppose that  $\sqrt{2}$  is rational (false); that is  $\sqrt{2} = \frac{n}{m}$  for some  $n, m \in \mathbb{N}$ . Suppose further that  $n$  and  $m$  are coprime; that is, that they have no common positive (integer) divisor other than 1 or, equivalently, suppose that their greatest common (integer) divisor is 1. Squaring the (wrong) assumption  $\sqrt{2} = \frac{n}{m}$  yields  $2 = \frac{n^2}{m^2}$  and thus  $n^2 = 2m^2$ . We have two different cases: either  $n$  is odd, or  $n$  is even.

case 1: suppose that  $n$  is odd; that is  $n = (2k+1)$  for some  $k \in \mathbb{N}$ ; and thus  $n^2 = 4k^2 + 2k + 1$  is again odd (the square of an odd number is odd again); but that cannot be, since  $n^2$  equals  $2m^2$  and thus should be even; hence we arrive at a contradiction.

case 2: suppose that  $n$  is even; that is  $n = 2k$  for some  $k \in \mathbb{N}$ ; and thus  $4k^2 = 2m^2$  or  $2k^2 = m^2$ . Now observe that by assumption,  $m$  cannot be even (remember  $n$  and  $m$  are coprime, and  $n$  is assumed to be even), so  $m$  must be odd. By the same argument as in case 1 (for odd  $n$ ), we arrive at a contradiction. By combining these two exhaustive cases 1 & 2, we arrive at a complete contradiction; the only consistent alternative being the irrationality of  $\sqrt{2}$ .

For the sake of mentioning a mathematical proof method which does not have any “constructive” or algorithmic flavour, consider a proof of the following theorem: “There exist irrational numbers  $x, y \in \mathbb{R} - \mathbb{Q}$  with  $x^y \in \mathbb{Q}$ .”

Consider the following proof:

case 1:  $\sqrt{2}^{\sqrt{2}} \in \mathbb{Q}$ ;

case 2:  $\sqrt{2}^{\sqrt{2}} \notin \mathbb{Q}$ , then  $\sqrt{2}^{\sqrt{2}^{\sqrt{2}}} = \left(\sqrt{2}^{\sqrt{2}}\right)^{\sqrt{2}} = (\sqrt{2})^{(\sqrt{2}\sqrt{2})} = \sqrt{2}^2 = 2 \in \mathbb{Q}$ .

The proof assumes the *law of the excluded middle*, which excludes all other cases but the two just listed. The question of which one of the two

<sup>6</sup> Claudi Alsina and Roger B. Nelsen. *Charming proofs. A journey into elegant mathematics*. The Mathematical Association of America (MAA), Washington, DC, 2010. ISBN 978-0-88385-348-1/hbk



cases is correct; that is, which number is rational, remains unsolved in the context of the proof. – Actually, a proof that case 2 is correct and  $\sqrt{2}^{\sqrt{2}}$  is a transcendental was only found by Gelfond and Schneider in 1934!

THERE EXIST ANCIENT and yet rather intuitive – but sometimes distracting and erroneous – informal notions of proof. An example <sup>7</sup> is the Babylonian notion to “prove” arithmetical statements by considering “large number” cases of algebraic formulae such as (Chapter V of Ref. <sup>8</sup>), for  $n \geq 1$ ,

$$\sum_{i=1}^n i^2 = \frac{1}{3} (1 + 2n) \sum_{i=1}^n i. \quad (2.1)$$

The Babylonians convinced themselves that it is correct maybe by first cautiously inserting small numbers; say,  $n = 1$ :

$$\sum_{i=1}^1 i^2 = 1^2 = 1, \text{ and}$$

$$\frac{1}{3} (1 + 2) \sum_{i=1}^1 i = \frac{3}{3} \cdot 1 = 1,$$

and  $n = 3$ :

$$\sum_{i=1}^3 i^2 = 1 + 4 + 9 = 14, \text{ and}$$

$$\frac{1}{3} (1 + 6) \sum_{i=1}^3 i = \frac{7}{3} (1 + 2 + 3) = \frac{7 \times 6}{3} = 14;$$

and then by taking the bold step to test this identity with something bigger, say  $n = 100$ , or something “*real big*,” such as the *Bell number prime* 1298074214633706835075030044377087 (check it out yourself); or something which “looks random” – although randomness is a very elusive quality, as *Ramsey theory* shows – thus coming close to what is a *probabilistic proof*.

As naive and silly this babylonian “proof” method may appear at first glance – for various subjective reasons (e.g. you may have some suspicions with regards to particular deductive proofs and their results; or you simply want to check the correctness of the deductive proof) it can be used to “convince” students and ourselves that a result which has derived deductively is indeed applicable and viable. We shall make heavy use of these kind of intuitive examples. As long as one always keeps in mind that this inductive, merely anecdotal, method is necessary but not sufficient (sufficiency is, for instance, guaranteed by mathematical induction) it is quite all right to go ahead with it.

MATHEMATICAL INDUCTION presents a way to ascertain certain identities, or relations, or estimations in a two-step rendition that represents a

The Gelfond-Schneider theorem states that, if  $n$  and  $m$  are algebraic numbers that is, if  $n$  and  $m$  are roots of a non-zero polynomial in one variable with rational or equivalently, integer, coefficients with  $n \neq 0, 1$  and if  $m$  is not a rational number, then any value of  $n^m = e^{m \log n}$  is a transcendental number.

<sup>7</sup> M. Baaz. Über den allgemeinen Gehalt von Beweisen. In *Contributions to General Algebra*, volume 6, pages 21–29, Vienna, 1988. Hölder-Pichler-Tempsky

<sup>8</sup> Otto Neugebauer. *Vorlesungen über die Geschichte der antiken mathematischen Wissenschaften. 1. Band: Vorgriechische Mathematik*. Springer, Berlin, 1934. page 172

Ramsey theory can be interpreted as expressing that *there is no true randomness*, irrespective of the method used to produce it; or, stated differently by Motzkin, a “*complete disorder is an impossibility. Any structure will necessarily contain an orderly substructure.*”

Alexander Soifer. Ramsey theory before ramsey, prehistory and early history: An essay in 13 parts. In Alexander Soifer, editor, *Ramsey Theory*, volume 285 of *Progress in Mathematics*, pages 1–26. Birkhäuser Boston, 2011. ISBN 978-0-8176-8091-6. DOI: 10.1007/978-0-8176-8092-3\_1. URL [http://dx.doi.org/10.1007/978-0-8176-8092-3\\_1](http://dx.doi.org/10.1007/978-0-8176-8092-3_1)



potential infinity of steps by (i) directly verifying some formula “babylonically,” that is, by direct insertion for some “small number” called the *basis of induction*, and then (ii) by verifying the *inductive step*. For any finite number  $m$ , we can then inductively verify the expression by starting with the basis of induction, which we have explicitly checked, and then taking successive values of  $n$  until  $m$  is reached.

For a demonstration of induction, consider again the babylonian example (2.1) mentioned earlier. In the first step (i), a basis is easily verified by taking  $n = 1$ . In the second step (ii), we substitute  $n + 1$  for  $n$  in (2.1), thereby obtaining

$$\begin{aligned}
 \sum_{i=1}^{n+1} i^2 &= \frac{1}{3} [1 + 2(n+1)] \sum_{i=1}^{n+1} i, \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n + 2) \left[ \sum_{i=1}^n i + (n+1) \right], \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i + \underbrace{\frac{2}{3} \sum_{i=1}^n i + \frac{1}{3} (3 + 2n)(n+1)}_{\frac{n(n+1)}{2}}, \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i + \frac{n(n+1)}{3} + \frac{2n^2 + 3n + 2n + 3}{3}, \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i + \frac{n^2 + n}{3} + \frac{2n^2 + 5n + 3}{3}, \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i + \frac{3n^2 + 6n + 3}{3}, \\
 \sum_{i=1}^n i^2 + (n+1)^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i + \underbrace{n^2 + 2n + 1}_{(n+1)^2}, \\
 \sum_{i=1}^n i^2 &= \frac{1}{3} (1 + 2n) \sum_{i=1}^n i.
 \end{aligned} \tag{2.2}$$

In that way, we can think of validating any finite case  $n = m$  by inductively verifying successive values of  $n$  from  $n = 1$  onwards, until  $m$  is reached.

THE CONTEMPORARY notion of proof is formalized and algorithmic. Around 1930 mathematicians could still hope for a “mathematical theory of everything” which consists of a finite number of axioms and algorithmic derivation rules by which all true mathematical statements could formally be derived. In particular, as expressed in Hilbert’s 2nd problem [Hilbert, 1902], it should be possible to prove the consistency of the axioms of arithmetic. Hence, Hilbert and other formalists dreamed, any such formal system (in German “Kalkül”) consisting of axioms and derivation rules, might represent “the essence of all mathematical truth.” This approach, as curageous as it appears, was doomed.

GÖDEL<sup>9</sup>, TARSKI<sup>10</sup>, and Turing<sup>11</sup> put an end to the formalist program.

<sup>9</sup> Kurt Gödel. Über formal unentscheidbare Sätze der Principia Mathematica und verwandter Systeme. *Monatshefte für Mathematik und Physik*, 38(1):173–198, 1931. DOI: 10.1007/s00605-006-0423-7. URL <http://dx.doi.org/10.1007/s00605-006-0423-7>

<sup>10</sup> Alfred Tarski. Der Wahrheitsbegriff in den Sprachen der deduktiven Disziplinen. *Akademie der Wissenschaften in Wien. Mathematisch-naturwissenschaftliche*

They coded and formalized the concepts of proof and computation in general, equating them with algorithmic entities. Today, in times when universal computers are everywhere, this may seem no big deal; but in those days even coding was challenging – in his proof of the undecidability of (Peano) arithmetic, Gödel used the uniqueness of prime decompositions to explicitly code mathematical formulæ!

FOR THE SAKE of exploring (algorithmically) these ideas let us consider the sketch of Turing's proof by contradiction of the unsolvability of the halting problem. The halting problem is about whether or not a computer will eventually halt on a given input, that is, will evolve into a state indicating the completion of a computation task or will stop altogether. Stated differently, a solution of the halting problem will be an algorithm that decides whether another arbitrary algorithm on arbitrary input will finish running or will run forever.

The scheme of the proof by contradiction is as follows: the existence of a hypothetical halting algorithm capable of solving the halting problem will be *assumed*. This could, for instance, be a subprogram of some suspicious supermacro library that takes the code of an arbitrary program as input and outputs 1 or 0, depending on whether or not the program halts. One may also think of it as a sort of oracle or black box analyzing an arbitrary program in terms of its symbolic code and outputting one of two symbolic states, say, 1 or 0, referring to termination or nontermination of the input program, respectively.

On the basis of this *hypothetical halting algorithm* one constructs another *diagonalization program* as follows: on receiving some arbitrary *input program* code as input, the diagonalization program consults the *hypothetical halting algorithm* to find out whether or not this input program halts; on receiving the answer, it does the *opposite*: If the hypothetical halting algorithm decides that the input program *halts*, the diagonalization program does *not halt* (it may do so easily by entering an infinite loop). Alternatively, if the hypothetical halting algorithm decides that the input program does *not halt*, the diagonalization program will *halt* immediately.

The diagonalization program can be forced to execute a paradoxical task by receiving *its own program code* as input. This is so because, by considering the diagonalization program, the hypothetical halting algorithm steers the diagonalization program into *halting* if it discovers that it *does not halt*; conversely, the hypothetical halting algorithm steers the diagonalization program into *not halting* if it discovers that it *halts*.

The complete contradiction obtained in applying the *diagonalization program* to its own code proves that this program and, in particular, the hypothetical halting algorithm cannot exist.

A universal computer can in principle be embedded into, or realized by, certain physical systems designed to universally compute. Assuming

unbounded space and time, it follows by reduction that there exist physical observables, in particular, forecasts about whether or not an embedded computer will ever halt in the sense sketched earlier, that are provably undecidable.

Thus, a clear distinction should be made between *determinism* (such as *computable evolution laws*) on the one hand, and *predictability* on the other hand <sup>12</sup>.

More quantitatively, we can argue that there exist deterministic physical systems whose behaviour is so “complex” that it cannot be characterized by any “shortcut” or prediction. Take, as an example, the *busy beaver function* <sup>13</sup> of  $n$  addressing the following question: suppose one considers all programs (on a particular computer) up to length (in terms of the number of symbols)  $n$ . What is the *largest number* producible by such a program before halting?

Consider a related question: what is the upper bound of running time – or, alternatively, recurrence time – of a program of length  $n$  bits before terminating or, alternatively, recurring? An answer to this question will explain just how long we have to wait for the most time-consuming program of length  $n$  bits to halt. That, of course, is a worst-case scenario. Many programs of length  $n$  bits will have halted long before the maximal halting time. We mention without proof <sup>14</sup> that this bound can be represented by the busy beaver function.

By reduction to the halting time, lower bounds for the recurrence of certain “complex” physical behaviors can be obtained. In particular, for deterministic systems representable by  $n$  bits and capable of carrying universal computation, the maximal recurrence time grows faster than any computable number of  $n$ . This bound from below for possible behaviors may be interpreted quite generally as a measure of the impossibility to predict and forecast such behaviors by algorithmic means. That is, by reduction to the halting problem <sup>15</sup> we conclude that the general forecast and induction problems are both unsolvable by algorithmic means.



<sup>12</sup> Patrick Suppes. The transcendental character of determinism. *Midwest Studies In Philosophy*, 18(1):242–257, 1993. DOI: 10.1111/j.1475-4975.1993.tb00266.x. URL <http://dx.doi.org/10.1111/j.1475-4975.1993.tb00266.x>

<sup>13</sup> Tibor Rado. On non-computable functions. *The Bell System Technical Journal*, XLI(41)(3):877–884, May 1962; and A. K. Dewdney. Computer recreations: A computer trap for the busy beaver, the hardest-working Turing machine. *Scientific American*, 251(2):19–23, August 1984

<sup>14</sup> Gregory J. Chaitin. Information-theoretic limitations of formal systems. *Journal of the Association of Computing Machinery*, 21:403–424, 1974. URL <http://www.cs.auckland.ac.nz/CDMTCS/chaitin/acm74.pdf>; and Gregory J. Chaitin. Computing the busy beaver function. In T. M. Cover and B. Gopinath, editors, *Open Problems in Communication and Computation*, page 108. Springer, New York, 1987. DOI: 10.1007/978-1-4612-4808-8\_28. URL [http://dx.doi.org/10.1007/978-1-4612-4808-8\\_28](http://dx.doi.org/10.1007/978-1-4612-4808-8_28)

<sup>15</sup> Karl Svozil. Physical unknowables. In Matthias Baaz, Christos H. Papadimitriou, Hilary W. Putnam, and Dana S. Scott, editors, *Kurt Gödel and the Foundations of Mathematics*, pages 213–251. Cambridge University Press, Cambridge, UK, 2011. URL <http://arxiv.org/abs/physics/0701163>

### 3

## *Numbers and sets of numbers*

THE CONCEPT OF NUMBERING THE UNIVERSE is far from trivial. In particular it is far from trivial which number schemes are appropriate. In the pythagorean tradition the natural numbers appear to be most natural. Actually Leibnitz (among others like Bacon before him) argues that just two number, say, “0” and “1,” are enough to creat all of other numbers, and thus all of the Universe <sup>1</sup>.

EVERY PRIMARY EMPIRICAL EVIDENCE seems to be based on some click in a detector: either there is some click or there is none. Thus every empirical physical evidence is composed from such elementary events.

Thus binary number codes are in good, albeit somewhat accidental, accord with the intuition of most experimentalists today. I call it “accidental” because quantum mechanics does not favour any base; the only criterium is the number of mutually exclusive measurement outcomes which determines the dimension of the linear vector space used for the quantum description model – two mutually exclusive outcomes would result in a Hilbert space of dimension two, three mutually exclusive outcomes would result in a Hilbert space of dimension three, and so on.

THERE ARE, of course, many other sets of numbers imagined so far; all of which can be considered to be encodable by binary digits. One of the most challenging number schemes is that of the real numbers <sup>2</sup>. It is totally different from the natural numbers insofar as there are undenumerably many reals; that is, it is impossible to find a one-to-one function – a sort of “translation” – from the natural numbers to the reals.

Cantor appears to be the first having realized this. In order to proof it, he invented what is today often called *Cantor's diagonalization technique*, or just diagonalization. It is a proof by contradiction; that is, what shall be disproved is assumed; and on the basis of this assumption a complete contradiction is derived.

For the sake of contradiction, assume for the moment that the set of

<sup>1</sup> Karl Svozil. Computational universes. *Chaos, Solitons & Fractals*, 25(4):845–859, 2006a. DOI: 10.1016/j.chaos.2004.11.055. URL <http://dx.doi.org/10.1016/j.chaos.2004.11.055>

<sup>2</sup> S. Drobot. *Real Numbers*. Prentice-Hall, Englewood Cliffs, New Jersey, 1964; and Edmund Hlawka. Zum Zahlbegriff. *Philosophia Naturalis*, 19:413–470, 1982

reals is denumerable. (This assumption will yield a contradiction.) That is, the enumeration is a one-to-one function  $f : \mathbb{N} \rightarrow \mathbb{R}$  (wrong), i.e., to any  $k \in \mathbb{N}$  exists some  $r_k \in \mathbb{R}$  and *vice versa*. No algorithmic restriction is imposed upon the enumeration, i.e., the enumeration may or may not be effectively computable. For instance, one may think of an enumeration obtained *via* the enumeration of computable algorithms and by assuming that  $r_k$  is the output of the  $k$ 'th algorithm. Let  $0.d_{k1}d_{k2}\cdots$  be the successive digits in the decimal expansion of  $r_k$ . Consider now the *diagonal* of the array formed by successive enumeration of the reals,

$$\begin{array}{ccccccc} r_1 & = & 0.d_{11} & d_{12} & d_{13} & \cdots & \\ r_2 & = & 0.d_{21} & d_{22} & d_{23} & \cdots & \\ r_3 & = & 0.d_{31} & d_{32} & d_{33} & \cdots & \\ \vdots & & \vdots & \vdots & \vdots & \ddots & \end{array} \quad (3.1)$$

yielding a new real number  $r_d = 0.d_{11}d_{22}d_{33}\cdots$ . Now, for the sake of contradiction, construct a new real  $r'_d$  by changing each one of these digits of  $r_d$ , avoiding zero and nine in a decimal expansion. This is necessary because reals with different digit sequences are equal to each other if one of them ends with an infinite sequence of nines and the other with zeros, for example  $0.0999\ldots = 0.1\ldots$ . The result is a real  $r' = 0.d'_1d'_2d'_3\cdots$  with  $d'_n \neq d_{nn}$ , which differs from each one of the original numbers in at least one (i.e., in the “diagonal”) position. Therefore, there exists at least one real which is not contained in the original enumeration, contradicting the assumption that *all* reals have been taken into account. Hence,  $\mathbb{R}$  is not denumerable.

Bridgman has argued <sup>3</sup> that, from a physical point of view, such an argument is operationally unfeasible, because it is physically impossible to process an infinite enumeration; and subsequently, quasi on top of that, a digit switch. Alas, it is possible to recast the argument such that  $r'_d$  is finitely created up to arbitrary operational length, as the enumeration progresses.

<sup>3</sup> Percy W. Bridgman. A physicist's second reaction to Mengenlehre. *Scripta Mathematica*, 2:101–117, 224–234, 1934



*Part II:*

*Linear vector spaces*



## Finite-dimensional vector spaces

VECTOR SPACES are prevalent in physics; they are essential for an understanding of mechanics, relativity theory, quantum mechanics, and statistical physics.

### 4.1 Basic definitions

In what follows excerpts from Halmos' beautiful treatment "Finite-Dimensional Vector Spaces" will be reviewed<sup>1</sup>. Of course, there exist zillions of other very nice presentations, among them Greub's "Linear algebra," and Strang's "Introduction to Linear Algebra," among many others, even freely downloadable ones<sup>2</sup> competing for your attention.

The more physically oriented notation in Mermin's book on quantum information theory<sup>3</sup> is adopted. Vectors are typed in bold face, or in Dirac's "bra-ket" notation. Thereby, the vector  $\mathbf{x}$  is identified with the "ket vector"  $|\mathbf{x}\rangle$ . The vector  $\mathbf{x}^*$  from the dual space (see Section 4.8 on page 28) is identified with the "bra vector"  $\langle\mathbf{x}|$ . Dot (scalar or inner) products between two vectors  $\mathbf{x}$  and  $\mathbf{y}$  in Euclidean space are then denoted by  $\langle\mathbf{bra}|\mathbf{c}|\mathbf{ket}\rangle$  form; that is, by  $\langle\mathbf{x}|\mathbf{y}\rangle$ .

The overline sign stands for complex conjugation; that is, if  $a = \Re a + i\Im a$  is a complex number, then  $\bar{a} = \Re a - i\Im a$ .

Unless stated differently, only finite-dimensional vector spaces are considered.

For an  $n \times m$  matrix  $\mathbf{A}$  we shall use the *index notation*

$$\mathbf{A} \equiv \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{pmatrix} \equiv a_{ij}. \quad (4.1)$$

A *matrix multiplication* (written with or without dot)  $\mathbf{A} \cdot \mathbf{B} = \mathbf{AB}$  of an  $n \times m$  matrix  $\mathbf{A} \equiv a_{ij}$  with an  $m \times l$  matrix  $\mathbf{B} \equiv b_{pq}$  can then be written as an  $n \times l$  matrix  $\mathbf{A} \cdot \mathbf{B} \equiv a_{ij}b_{jk}$ ,  $1 \leq i \leq n$ ,  $1 \leq j \leq m$ ,  $1 \leq k \leq l$ . Here the

"I would have written a shorter letter, but I did not have the time." (Literally: "I made this [letter] very long, because I did not have the leisure to make it shorter.")  
Blaise Pascal, *Provincial Letters: Letter XVI* (English Translation)

"Perhaps if I had spent more time I should have been able to make a shorter report..."  
James Clerk Maxwell, Document 15, p. 426

Elisabeth Garber, Stephen G. Brush, and C. W. Francis Everitt. *Maxwell on Heat and Statistical Mechanics: On "Avoiding All Personal Enquiries" of Molecules*. Associated University Press, Cranbury, NJ, 1995. ISBN 0934223343

<sup>1</sup> Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

<sup>2</sup> Werner Greub. *Linear Algebra*, volume 23 of *Graduate Texts in Mathematics*. Springer, New York, Heidelberg, fourth edition, 1975; Gilbert Strang. *Introduction to linear algebra*. Wellesley-Cambridge Press, Wellesley, MA, USA, fourth edition, 2009. ISBN 0-9802327-1-6. URL <http://math.mit.edu/linearalgebra/>; Howard Homes and Chris Rorres. *Elementary Linear Algebra: Applications Version*. Wiley, New York, tenth edition, 2010; Seymour Lipschutz and Marc Lipson. *Linear algebra*. Schaum's outline series. McGraw-Hill, fourth edition, 2009; and Jim Hefferon. *Linear algebra*. 320-375, 2011. URL <http://joshua.smcvt.edu/linearalgebra/html/book.pdf>

<sup>3</sup> David N. Mermin. Lecture notes on quantum computation. 2002-2008. URL <http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html>; and David N. Mermin. *Quantum Computer Science*. Cambridge University Press, Cambridge, 2007. ISBN 9780521876582. URL <http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html>



*Einstein summation convention* has been used, which requires that, when an index variable appears twice in a single term, one has to sum over all of the possible index values. Stated differently, if  $\mathbf{A}$  is an  $n \times m$  matrix and  $\mathbf{B}$  is an  $m \times l$  matrix, their matrix product  $\mathbf{AB}$  is an  $n \times l$  matrix, in which the  $m$  entries across the rows of  $\mathbf{A}$  are multiplied with the  $m$  entries down the columns of  $\mathbf{B}$ .

Often, a *vector* will be coded – with respect to a basis or coordinate system (see below) – as an  $n$ -tuple of numbers; which in turn can be interpreted as either a  $1 \times n$  matrix (row vector), or a  $n \times 1$  matrix (column vector). We can then write certain terms very compactly (alas often misleadingly). Suppose, for instance, that  $\mathbf{x} \equiv (x_1, x_2, \dots, x_n)$  and  $\mathbf{y} \equiv (y_1, y_2, \dots, y_n)$  are two (row) vectors (with respect to a given basis). Then,  $x_i y_j a_{ij} \equiv \mathbf{x} \mathbf{A} \mathbf{y}^T$  can (somewhat superficially) be represented as a matrix multiplication of a row vector with a matrix and a column vector yielding a scalar; which in turn can be interpreted as a  $1 \times 1$  matrix. Here “ $T$ ” indicates transposition;

that is,  $\mathbf{y}^T \equiv \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$  represents a column vector (with respect to a particular basis).

#### 4.1.1 Fields of real and complex numbers

In physics, scalars occur either as real or complex numbers. Thus we shall restrict our attention to these cases.

A *field*  $\langle \mathbb{F}, +, \cdot, -, ^{-1}, 0, 1 \rangle$  is a set together with two operations, usually called *addition* and *multiplication*, denoted by “ $+$ ” and “ $\cdot$ ” (often “ $a \cdot b$ ” is identified with the expression “ $ab$ ” without the center dot) respectively, such that the following conditions (or, stated differently, axioms) hold:

- (i) closure of  $\mathbb{F}$  with respect to addition and multiplication: for all  $a, b \in \mathbb{F}$ , both  $a + b$  and  $ab$  are in  $\mathbb{F}$ ;
- (ii) associativity of addition and multiplication: for all  $a, b$ , and  $c$  in  $\mathbb{F}$ , the following equalities hold:  $a + (b + c) = (a + b) + c$ , and  $a(bc) = (ab)c$ ;
- (iii) commutativity of addition and multiplication: for all  $a$  and  $b$  in  $\mathbb{F}$ , the following equalities hold:  $a + b = b + a$  and  $ab = ba$ ;
- (iv) additive and multiplicative identity: there exists an element of  $\mathbb{F}$ , called the additive identity element and denoted by  $0$ , such that for all  $a$  in  $\mathbb{F}$ ,  $a + 0 = a$ . Likewise, there is an element, called the multiplicative identity element and denoted by  $1$ , such that for all  $a$  in  $\mathbb{F}$ ,  $1 \cdot a = a$ . (To exclude the trivial ring, the additive identity and the multiplicative identity are required to be distinct.)

- (v) additive and multiplicative inverses: for every  $a$  in  $\mathbb{F}$ , there exists an element  $-a$  in  $\mathbb{F}$ , such that  $a + (-a) = 0$ . Similarly, for any  $a$  in  $\mathbb{F}$  other than 0, there exists an element  $a^{-1}$  in  $\mathbb{F}$ , such that  $a \cdot a^{-1} = 1$ . (The elements  $+(-a)$  and  $a^{-1}$  are also denoted  $-a$  and  $\frac{1}{a}$ , respectively.) Stated differently: subtraction and division operations exist.
- (vi) Distributivity of multiplication over addition: For all  $a, b$  and  $c$  in  $\mathbb{F}$ , the following equality holds:  $a(b + c) = (ab) + (ac)$ .

#### 4.1.2 Vectors and vector space

Vector spaces are merely structures allowing the sum (addition) of objects called “vectors,” and multiplication of these objects by scalars; thereby remaining in this structure. That is, for instance, the “coherent superposition”  $\mathbf{a} + \mathbf{b} \equiv |\mathbf{a} + \mathbf{b}\rangle$  of two vectors  $\mathbf{a} \equiv |\mathbf{a}\rangle$  and  $\mathbf{b} \equiv |\mathbf{b}\rangle$  can be guaranteed to be a vector. At this stage, little can be said about the length or relative direction or orientation of these “vectors.” Algebraically, “vectors” are elements of vector spaces. Geometrically a vector may be interpreted as “a quantity which is usefully represented by an arrow”<sup>4</sup>.

A *linear vector space*  $\langle \mathfrak{V}, +, \cdot, -, 0, 1 \rangle$  is a set  $\mathfrak{V}$  of elements called *vectors*, here denoted by bold face symbols such as  $\mathbf{a}, \mathbf{x}, \mathbf{v}, \mathbf{w}, \dots$ , or, equivalently, denoted by  $|\mathbf{a}\rangle, |\mathbf{x}\rangle, |\mathbf{v}\rangle, |\mathbf{w}\rangle, \dots$ , satisfying certain conditions (or, stated differently, axioms); among them, with respect to addition of vectors:

- (i) commutativity,
- (ii) associativity,
- (iii) the uniqueness of the origin or null vector  $0$ , as well as
- (iv) the uniqueness of the negative vector;

with respect to multiplication of vectors with scalars associativity:

- (v) the existence of a unit factor 1; and
- (vi) distributivity with respect to scalar and vector additions; that is,

$$\begin{aligned} (\alpha + \beta)\mathbf{x} &= \alpha\mathbf{x} + \beta\mathbf{x}, \\ \alpha(\mathbf{x} + \mathbf{y}) &= \alpha\mathbf{x} + \alpha\mathbf{y}, \end{aligned} \tag{4.2}$$

with  $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$  and scalars  $\alpha, \beta \in \mathbb{F}$ , respectively.

Examples of vector spaces are:

- (i) The set  $\mathbb{C}$  of complex numbers:  $\mathbb{C}$  can be interpreted as a complex vector space by interpreting as vector addition and scalar multiplication as the usual addition and multiplication of complex numbers, and with  $0$  as the null vector;

For proofs and additional information see §2 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

<sup>4</sup> Gabriel Weinreich. *Geometrical Vectors (Chicago Lectures in Physics)*. The University of Chicago Press, Chicago, IL, 1998

In order to define *length*, we have to engage an additional structure, namely the *norm*  $\|\mathbf{a}\|$  of a vector  $\mathbf{a}$ . And in order to define relative *direction* and *orientation*, and, in particular, *orthogonality* and *collinearity* we have to define the *scalar product*  $\langle \mathbf{a} | \mathbf{b} \rangle$  of two vectors  $\mathbf{a}$  and  $\mathbf{b}$ .

- (ii) The set  $\mathbb{C}^n$ ,  $n \in \mathbb{N}$  of  $n$ -tuples of complex numbers: Let  $\mathbf{x} = (x_1, \dots, x_n)$  and  $\mathbf{y} = (y_1, \dots, y_n)$ .  $\mathbb{C}^n$  can be interpreted as a complex vector space by interpreting the ordinary addition  $\mathbf{x} + \mathbf{y} = (x_1 + y_1, \dots, x_n + y_n)$  and the multiplication  $\alpha \mathbf{x} = (\alpha x_1, \dots, \alpha x_n)$  by a complex number  $\alpha$  as vector addition and scalar multiplication, respectively; the null tuple  $\mathbf{0} = (0, \dots, 0)$  is the neutral element of vector addition;
- (iii) The set  $\mathfrak{P}$  of all polynomials with complex coefficients in a variable  $t$ :  $\mathfrak{P}$  can be interpreted as a complex vector space by interpreting the ordinary addition of polynomials and the multiplication of a polynomial by a complex number as vector addition and scalar multiplication, respectively; the null polynomial is the neutral element of vector addition.

## 4.2 Linear independence

A set  $\mathfrak{S} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\} \subset \mathfrak{V}$  of vectors  $\mathbf{x}_i$  in a linear vector space is *linearly independent* if  $\mathbf{x}_i \neq \mathbf{0} \forall 1 \leq i \leq k$ , and additionally, if either  $k = 1$ , or if no vector in  $\mathfrak{S}$  can be written as a linear combination of other vectors in this set  $\mathfrak{S}$ ; that is, there are no scalars  $\alpha_j$  satisfying  $\mathbf{x}_i = \sum_{1 \leq j \leq k, j \neq i} \alpha_j \mathbf{x}_j$ .

Equivalently, if  $\sum_{i=1}^k \alpha_i \mathbf{x}_i = \mathbf{0}$  implies  $\alpha_i = 0$  for each  $i$ , then the set  $\mathfrak{S} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$  is linearly independent.

Note that the vectors of a basis are linear independent and “maximal” insofar as any inclusion of an additional vector results in a linearly dependent set; that is, this additional vector can be expressed in terms of a linear combination of the existing basis vectors; see also Section 4.4 on page 22.

## 4.3 Subspace

A nonempty subset  $\mathfrak{M}$  of a vector space is a *subspace* or, used synonymously, a *linear manifold*, if, along with every pair of vectors  $\mathbf{x}$  and  $\mathbf{y}$  contained in  $\mathfrak{M}$ , every linear combination  $\alpha \mathbf{x} + \beta \mathbf{y}$  is also contained in  $\mathfrak{M}$ .

If  $\mathfrak{U}$  and  $\mathfrak{V}$  are two subspaces of a vector space, then  $\mathfrak{U} + \mathfrak{V}$  is the subspace spanned by  $\mathfrak{U}$  and  $\mathfrak{V}$ ; that is, it contains all vectors  $\mathbf{z} = \mathbf{x} + \mathbf{y}$ , with  $\mathbf{x} \in \mathfrak{U}$  and  $\mathbf{y} \in \mathfrak{V}$ .

$\mathfrak{M}$  is the *linear span*

$$\mathfrak{M} = \text{span}(\mathfrak{U}, \mathfrak{V}) = \text{span}(\mathbf{x}, \mathbf{y}) = \{\alpha \mathbf{x} + \beta \mathbf{y} \mid \alpha, \beta \in \mathbb{F}, \mathbf{x} \in \mathfrak{U}, \mathbf{y} \in \mathfrak{V}\}. \quad (4.3)$$

A generalization to more than two vectors and more than two subspaces is straightforward.

For every vector space  $\mathfrak{V}$ , the vector space containing only the null vector, and the vector space  $\mathfrak{V}$  itself are subspaces of  $\mathfrak{V}$ .

For proofs and additional information see §10 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

### 4.3.1 Scalar or inner product

A *scalar* or *inner* product presents some form of measure of “distance” or “apartness” of two vectors in a linear vector space. It should not be confused with the bilinear functionals (introduced on page 28) that connect a vector space with its dual vector space, although for real Euclidean vector spaces these may coincide, and although the scalar product is also bilinear in its arguments. It should also not be confused with the tensor product introduced on page 36.

An inner product space is a vector space  $\mathfrak{V}$ , together with an inner product; that is, with a map  $\langle \cdot | \cdot \rangle : \mathfrak{V} \times \mathfrak{V} \longrightarrow \mathbb{F}$  (usually  $\mathbb{F} = \mathbb{C}$  or  $\mathbb{F} = \mathbb{R}$ ) that satisfies the following three conditions (or, stated differently, axioms) for all vectors and all scalars:

- (i) Conjugate symmetry:  $\langle \mathbf{x} | \mathbf{y} \rangle = \overline{\langle \mathbf{y} | \mathbf{x} \rangle}$ .
- (ii) Linearity in the first argument:

$$\langle \alpha \mathbf{x} + \beta \mathbf{y} | \mathbf{z} \rangle = \alpha \langle \mathbf{x} | \mathbf{z} \rangle + \beta \langle \mathbf{y} | \mathbf{z} \rangle.$$

- (iii) Positive-definiteness:  $\langle \mathbf{x} | \mathbf{x} \rangle \geq 0$ ; with equality if and only if  $\mathbf{x} = \mathbf{0}$ .

Note that from the first two properties, it follows that the inner product is *antilinear*, or synonymously, *conjugate-linear*, in its first argument:

$$\langle \alpha \mathbf{x} + \beta \mathbf{y} | \mathbf{z} \rangle = \overline{\alpha} \langle \mathbf{x} | \mathbf{z} \rangle + \overline{\beta} \langle \mathbf{y} | \mathbf{z} \rangle.$$

The *norm* of a vector  $\mathbf{x}$  is defined by

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x} | \mathbf{x} \rangle} \quad (4.4)$$

One example is the *dot product*

$$\langle \mathbf{x} | \mathbf{y} \rangle = \sum_{i=1}^n \overline{x_i} y_i \quad (4.5)$$

of two vectors  $\mathbf{x} = (x_1, \dots, x_n)$  and  $\mathbf{y} = (y_1, \dots, y_n)$  in  $\mathbb{C}^n$ , which, for real Euclidean space, reduces to the well-known dot product  $\langle \mathbf{x} | \mathbf{y} \rangle = x_1 y_1 + \dots + x_n y_n = \|\mathbf{x}\| \|\mathbf{y}\| \cos \angle(\mathbf{x}, \mathbf{y})$ .

It is mentioned without proof that the most general form of an inner product in  $\mathbb{C}^n$  is  $\langle \mathbf{x} | \mathbf{y} \rangle = \mathbf{y} \mathbf{A} \mathbf{x}^\dagger$ , where the symbol “ $\dagger$ ” stands for the *conjugate transpose* (also denoted as *Hermitian conjugate* or *Hermitian adjoint*), and  $\mathbf{A}$  is a positive definite Hermitian matrix (all of its eigenvalues are positive).

Two nonzero vectors  $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$ ,  $\mathbf{x}, \mathbf{y} \neq \mathbf{0}$  are *orthogonal*, denoted by “ $\mathbf{x} \perp \mathbf{y}$ ” if their scalar product vanishes; that is, if

$$\langle \mathbf{x} | \mathbf{y} \rangle = 0. \quad (4.6)$$

Let  $\mathfrak{E}$  be any set of vectors in an inner product space  $\mathfrak{V}$ . The symbol

$$\mathfrak{E}^\perp = \{ \mathbf{x} | \langle \mathbf{x} | \mathbf{y} \rangle = 0, \mathbf{x} \in \mathfrak{V}, \forall \mathbf{y} \in \mathfrak{E} \} \quad (4.7)$$

For proofs and additional information see §61 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

For real, Euclidean vector spaces, this function is symmetric; that is  $\langle \mathbf{x} | \mathbf{y} \rangle = \langle \mathbf{y} | \mathbf{x} \rangle$ .

denotes the set of all vectors in  $\mathfrak{V}$  that are orthogonal to every vector in  $\mathfrak{E}$ .

Note that, regardless of whether or not  $\mathfrak{E}$  is a subspace,  $\mathfrak{E}^\perp$  is a subspace. Furthermore,  $\mathfrak{E}$  is contained in  $(\mathfrak{E}^\perp)^\perp = \mathfrak{E}^{\perp\perp}$ . In case  $\mathfrak{E}$  is a subspace, we call  $\mathfrak{E}^\perp$  the *orthogonal complement* of  $\mathfrak{E}$ .

The following *projection theorem* is mentioned without proof. If  $\mathfrak{M}$  is any subspace of a finite-dimensional inner product space  $\mathfrak{V}$ , then  $\mathfrak{V}$  is the direct sum of  $\mathfrak{M}$  and  $\mathfrak{M}^\perp$ ; that is,  $\mathfrak{M}^{\perp\perp} = \mathfrak{M}$ .

For the sake of an example, suppose  $\mathfrak{V} = \mathbb{R}^2$ , and take  $\mathfrak{E}$  to be the set of all vectors spanned by the vector  $(1, 0)$ ; then  $\mathfrak{E}^\perp$  is the set of all vectors spanned by  $(0, 1)$ .

See page 20 for a definition of subspace.

#### 4.3.2 Hilbert space

A (quantum mechanical) *Hilbert space* is a linear vector space  $\mathfrak{V}$  over the field  $\mathbb{C}$  of complex numbers (sometimes only  $\mathbb{R}$  is used) equipped with vector addition, scalar multiplication, and some inner (scalar) product. Furthermore, *closure* is an additional requirement, but nobody has made operational sense of that so far: If  $\mathbf{x}_n \in \mathfrak{V}$ ,  $n = 1, 2, \dots$ , and if  $\lim_{n,m \rightarrow \infty} (\mathbf{x}_n - \mathbf{x}_m, \mathbf{x}_n - \mathbf{x}_m) = 0$ , then there exists an  $\mathbf{x} \in \mathfrak{V}$  with  $\lim_{n \rightarrow \infty} (\mathbf{x}_n - \mathbf{x}, \mathbf{x}_n - \mathbf{x}) = 0$ .

Infinite dimensional vector spaces and continuous spectra are non-trivial extensions of the finite dimensional Hilbert space treatment. As a heuristic rule – which is not always correct – it might be stated that the sums become integrals, and the Kronecker delta function  $\delta_{ij}$  defined by

$$\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j, \\ 1 & \text{for } i = j. \end{cases} \quad (4.8)$$

becomes the Dirac delta function  $\delta(x - y)$ , which is a generalized function in the continuous variables  $x, y$ . In the Dirac bra-ket notation, unity is given by  $\mathbf{1} = \int_{-\infty}^{+\infty} |x\rangle\langle x| dx$ . For a careful treatment, see, for instance, the books by Reed and Simon <sup>5</sup>.

#### 4.4 Basis

We shall use bases of vector spaces to formally represent vectors (elements) therein.

A (linear) *basis* [or a *coordinate system*, or a *frame (of reference)*] is a set  $\mathfrak{B}$  of linearly independent vectors such that every vector in  $\mathfrak{V}$  is a linear combination of the vectors in the basis; hence  $\mathfrak{B}$  spans  $\mathfrak{V}$ .

What particular basis should one choose? *A priori* no basis is privileged over the other. Yet, in view of certain (mutual) properties of elements of some bases (such as orthogonality or orthonormality) we shall prefer (s)ome over others.

Note that a vector is some directed entity with a particular length, oriented in some (vector) “space.” It is “laid out there” in front of our eyes, as

<sup>5</sup> Michael Reed and Barry Simon. *Methods of Mathematical Physics I: Functional Analysis*. Academic Press, New York, 1972; and Michael Reed and Barry Simon. *Methods of Mathematical Physics II: Fourier Analysis, Self-Adjointness*. Academic Press, New York, 1975

For proofs and additional information see §7 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

it is: some directed entity. *A priori*, this space, in its most primitive form, is not equipped with a basis, or synonymously, frame of reference, or reference frame. Insofar it is not yet coordinatized. In order to formalize the notion of a vector, we have to code this vector by “coordinates” or “components” which are the coefficients with respect to a (de)composition into basis elements. Therefore, just as for numbers (e.g., by different numeral bases, or by prime decomposition), there exist many “competing” ways to code a vector.

Some of these ways appear to be rather straightforward, such as, in particular, the *Cartesian basis*, also synonymously called the *standard basis*. It is, however, not in any way *a priori* “evident” or “necessary” what should be specified to be “the Cartesian basis.” Actually, specification of a “Cartesian basis” seems to be mainly motivated by physical inertial motion – and thus identified with some inertial frame of reference – “without any friction and forces,” resulting in a “straight line motion at constant speed.” (This sentence is cyclic, because heuristically any such absence of “friction and force” can only be operationalized by testing if the motion is a “straight line motion at constant speed.”) If we grant that in this way straight lines can be defined, then Cartesian bases in Euclidean vector spaces can be characterized by orthogonal (orthogonality is defined *via* vanishing scalar products between nonzero vectors) straight lines spanning the entire space. In this way, we arrive, say for a planar situation, at the coordinates characterized by some basis  $\{(0, 1), (1, 0)\}$ , where, for instance, the basis vector “(1, 0)” literally and physically means “a unit arrow pointing in some particular, specified direction.”

Alas, if we would prefer, say, cyclic motion in the plane, we might want to call a frame based on the polar coordinates  $r$  and  $\theta$  “Cartesian,” resulting in some “Cartesian basis”  $\{(0, 1), (1, 0)\}$ ; but this “Cartesian basis” would be very different from the Cartesian basis mentioned earlier, as “(1, 0)” would refer to some specific unit radius, and “(0, 1)” would refer to some specific unit angle (with respect to a specific zero angle). In terms of the “straight” coordinates (with respect to “the usual Cartesian basis”)  $x, y$ , the polar coordinates are  $r = \sqrt{x^2 + y^2}$  and  $\theta = \tan^{-1}(y/x)$ . We obtain the original “straight” coordinates (with respect to “the usual Cartesian basis”) back if we take  $x = r \cos \theta$  and  $y = r \sin \theta$ .

Other bases than the “Cartesian” one may be less suggestive at first; alas it may be “economical” or pragmatical to use them; mostly to cope with, and adapt to, the *symmetry* of a physical configuration: if the physical situation at hand is, for instance, rotationally invariant, we might want to use rotationally invariant bases – such as, for instance, polar coordinates in two dimensions, or spherical coordinates in three dimensions – to represent a vector, or, more generally, to code any given representation of a physical entity (e.g., tensors, operators) by such bases.

## 4.5 Dimension

The *dimension* of  $\mathfrak{V}$  is the number of elements in  $\mathfrak{B}$ .

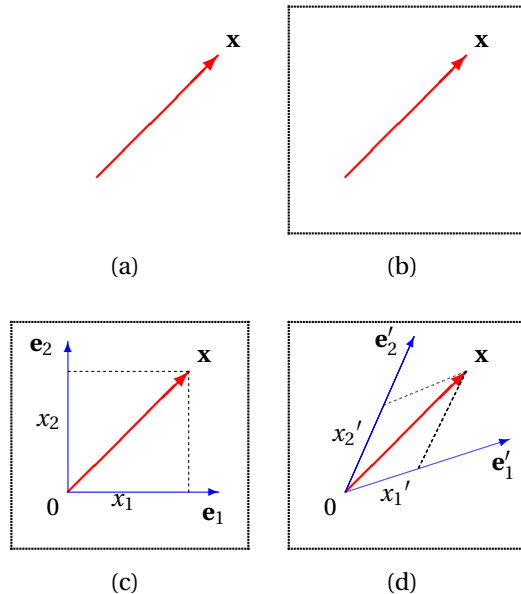
All bases  $\mathfrak{B}$  of  $\mathfrak{V}$  contain the same number of elements.

A vector space is finite dimensional if its bases are finite; that is, its bases contain a finite number of elements.

In quantum physics, the dimension of a quantized system is associated with the *number of mutually exclusive measurement outcomes*. For a spin state measurement of an electron along a particular direction, as well as for a measurement of the linear polarization of a photon in a particular direction, the dimension is two, since both measurements may yield two distinct outcomes which we can interpret as vectors in two-dimensional Hilbert space, which, in Dirac's bra-ket notation <sup>6</sup>, can be written as  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , or  $|+\rangle$  and  $|-\rangle$ , or  $|H\rangle$  and  $|V\rangle$ , or  $|0\rangle$  and  $|1\rangle$ , or  $|\text{happy}\rangle$  and  $|\text{sad}\rangle$ , respectively.

## 4.6 Coordinates

The coordinates of a vector with respect to some basis represent the coding of that vector in that particular basis. It is important to realize that, as bases change, so do coordinates. Indeed, the changes in coordinates have to “compensate” for the bases change, because the same coordinates in a different basis would render an altogether different vector. Figure 4.1 presents some geometrical demonstration of these thoughts, for your contemplation.



For proofs and additional information see §8 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

<sup>6</sup> Paul A. M. Dirac. *The Principles of Quantum Mechanics*. Oxford University Press, Oxford, 1930

For proofs and additional information see §46 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Figure 4.1: Coordinatization of vectors: (a) some primitive vector; (b) some primitive vectors, laid out in some space, denoted by dotted lines (c) vector coordinates  $x_1$  and  $x_2$  of the vector  $\mathbf{x} = (x_1, x_2) = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2$  in a standard basis; (d) vector coordinates  $x'_1$  and  $x'_2$  of the vector  $\mathbf{x} = (x'_1, x'_2) = x'_1 \mathbf{e}'_1 + x'_2 \mathbf{e}'_2$  in some nonorthogonal basis.

Elementary high school tutorials often condition students into believing

that the components of the vector “is” the vector, rather than emphasizing that these components *represent* or *encode* the vector with respect to some (mostly implicitly assumed) basis. A similar situation occurs in many introductions to quantum theory, where the span (i.e., the onedimensional linear subspace spanned by that vector)  $\{\mathbf{y} \mid \mathbf{y} = \alpha \mathbf{x}, \alpha \in \mathbb{C}\}$ , or, equivalently, for orthogonal projections, the *projection* (i.e., the projection operator; see also page 41)  $\mathbf{E}_{\mathbf{x}} = \mathbf{x}^T \otimes \mathbf{x}$  corresponding to a unit (of length 1) vector  $\mathbf{x}$  often is identified with that vector. In many instances, this is a great help and, if administered properly, is consistent and fine (at least for all practical purposes).

The standard (Cartesian) basis in  $n$ -dimensional complex space  $\mathbb{C}^n$  is the set of (usually “straight”) vectors  $\mathbf{e}_i, i = 1, \dots, n$ , represented by  $n$ -tuples, defined by the condition that the  $i$ ’th coordinate of the  $j$ ’th basis vector  $\mathbf{e}_j$  is given by  $\delta_{ij}$ , where  $\delta_{ij}$  is the Kronecker delta function

$$\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j, \\ 1 & \text{for } i = j. \end{cases} \quad (4.9)$$

Thus,

$$\begin{aligned} \mathbf{e}_1 &= (1, 0, \dots, 0), \\ \mathbf{e}_2 &= (0, 1, \dots, 0), \\ &\vdots \\ \mathbf{e}_n &= (0, 0, \dots, 1). \end{aligned} \quad (4.10)$$

In terms of these standard base vectors, every vector  $\mathbf{x}$  can be written as a linear combination

$$\mathbf{x} = \sum_{i=1}^n x_i \mathbf{e}_i = (x_1, x_2, \dots, x_n), \quad (4.11)$$

or, in “dot product notation,” that is, “column times row” and “row times column;” the dot is usually omitted (the superscript “ $T$ ” stands for transposition),

$$\mathbf{x} = (\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n) \cdot (x_1, x_2, \dots, x_n)^T = (\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad (4.12)$$

of the product of the coordinates  $x_i$  with respect to that standard basis. Here the equality sign “=” really means “coded with respect to that standard basis.”

In what follows, we shall often identify the column vector

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$



containing the coordinates of the vector  $\mathbf{x}$  with the vector  $\mathbf{x}$ , but we always need to keep in mind that the tuples of coordinates are defined only with respect to a particular basis  $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ ; otherwise these numbers lack any meaning whatsoever.

Indeed, with respect to some arbitrary basis  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  of some  $n$ -dimensional vector space  $\mathfrak{V}$  with the base vectors  $\mathbf{f}_i$ ,  $1 \leq i \leq n$ , every vector  $\mathbf{x}$  in  $\mathfrak{V}$  can be written as a unique linear combination

$$\mathbf{x} = \sum_{i=1}^n x_i \mathbf{f}_i = (x_1, x_2, \dots, x_n) \quad (4.13)$$

of the product of the coordinates  $x_i$  with respect to the basis  $\mathfrak{B}$ .

The uniqueness of the coordinates is proven indirectly by *reductio ad absurdum*: Suppose there is another decomposition  $\mathbf{x} = \sum_{i=1}^n y_i \mathbf{f}_i = (y_1, y_2, \dots, y_n)$ ; then by subtraction,  $0 = \sum_{i=1}^n (x_i - y_i) \mathbf{f}_i = (0, 0, \dots, 0)$ . Since the basis vectors  $\mathbf{f}_i$  are linearly independent, this can only be valid if all coefficients in the summation vanish; thus  $x_i - y_i = 0$  for all  $1 \leq i \leq n$ ; hence finally  $x_i = y_i$  for all  $1 \leq i \leq n$ . This is in contradiction with our assumption that the coordinates  $x_i$  and  $y_i$  (or at least some of them) are different. Hence the only consistent alternative is the assumption that, with respect to a given basis, the coordinates are uniquely determined.

A set  $\mathfrak{B} = \{\mathbf{a}_1, \dots, \mathbf{a}_n\}$  of vectors of the inner product space  $\mathfrak{V}$  is *orthonormal* if, for all  $\mathbf{a}_i \in \mathfrak{B}$  and  $\mathbf{a}_j \in \mathfrak{B}$ , it follows that

$$\langle \mathbf{a}_i | \mathbf{a}_j \rangle = \delta_{ij}. \quad (4.14)$$

Any such set is called *complete* if it is not a subset of any larger orthonormal set of vectors of  $\mathfrak{V}$ . Any complete set is a basis. If, instead of Eq. (4.14),  $\langle \mathbf{a}_i | \mathbf{a}_j \rangle = \alpha_i \delta_{ij}$  with nonzero factors  $\alpha_i$ , the set is called *orthogonal*.

#### 4.7 Finding orthogonal bases from nonorthogonal ones

A *Gram-Schmidt process* is a systematic method for orthonormalising a set of vectors in a space equipped with a *scalar product*, or by a synonym preferred in mathematics, *inner product*. The Gram-Schmidt process takes a finite, linearly independent set of base vectors and generates an orthonormal basis that spans the same (sub)space as the original set.

The general method is to start out with the original basis, say,

$\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \dots, \mathbf{x}_n\}$ , and generate a new orthogonal basis

The scalar or inner product  $\langle \mathbf{x} | \mathbf{y} \rangle$  of two vectors  $\mathbf{x}$  and  $\mathbf{y}$  is defined on page 21. In Euclidean space such as  $\mathbb{R}^n$ , one often identifies the “dot product”  $\mathbf{x} \cdot \mathbf{y} = x_1 y_1 + \dots + x_n y_n$  of two vectors  $\mathbf{x}$  and  $\mathbf{y}$  with their scalar or inner product.

$\{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \dots, \mathbf{y}_n\}$  by

$$\begin{aligned} \mathbf{y}_1 &= \mathbf{x}_1, \\ \mathbf{y}_2 &= \mathbf{x}_2 - P_{\mathbf{y}_1}(\mathbf{x}_2), \\ \mathbf{y}_3 &= \mathbf{x}_3 - P_{\mathbf{y}_1}(\mathbf{x}_3) - P_{\mathbf{y}_2}(\mathbf{x}_3), \\ &\vdots \\ \mathbf{y}_n &= \mathbf{x}_n - \sum_{i=1}^{n-1} P_{\mathbf{y}_i}(\mathbf{x}_n), \end{aligned} \quad (4.15)$$

where

$$P_{\mathbf{y}}(\mathbf{x}) = \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \mathbf{y}, \text{ and } P_{\mathbf{y}}^{\perp}(\mathbf{x}) = \mathbf{x} - \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \mathbf{y} \quad (4.16)$$

are the orthogonal projections of  $\mathbf{x}$  onto  $\mathbf{y}$  and  $\mathbf{y}^{\perp}$ , respectively (the latter is mentioned for the sake of completeness and is not required here). Note that these orthogonal projections are idempotent and mutually orthogonal; that is,

$$\begin{aligned} P_{\mathbf{y}}^2(\mathbf{x}) &= P_{\mathbf{y}}(P_{\mathbf{y}}(\mathbf{x})) = \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \frac{\langle \mathbf{y} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \mathbf{y} = P_{\mathbf{y}}(\mathbf{x}), \\ (P_{\mathbf{y}}^{\perp})^2(\mathbf{x}) &= P_{\mathbf{y}}^{\perp}(P_{\mathbf{y}}^{\perp}(\mathbf{x})) = \mathbf{x} - \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \mathbf{y} - \left( \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} - \frac{\langle \mathbf{x} | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle^2} \right) \mathbf{y} = P_{\mathbf{y}}^{\perp}(\mathbf{x}), \\ P_{\mathbf{y}}(P_{\mathbf{y}}^{\perp}(\mathbf{x})) &= P_{\mathbf{y}}^{\perp}(P_{\mathbf{y}}(\mathbf{x})) = \frac{\langle \mathbf{x} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle} \mathbf{y} - \frac{\langle \mathbf{x} | \mathbf{y} \rangle \langle \mathbf{y} | \mathbf{y} \rangle}{\langle \mathbf{y} | \mathbf{y} \rangle^2} \mathbf{y} = 0. \end{aligned} \quad (4.17)$$

For a more general discussion of projections, see also page 41.

Subsequently, in order to obtain an orthonormal basis, one can divide every basis vector by its length.

The idea of the proof is as follows (see also Greub<sup>7</sup>, section 7.9). In order to generate an orthogonal basis from a nonorthogonal one, the first vector of the old basis is identified with the first vector of the new basis; that is  $\mathbf{y}_1 = \mathbf{x}_1$ . Then, as depicted in Fig. 4.2, the second vector of the new basis is obtained by taking the second vector of the old basis and subtracting its projection on the first vector of the new basis.

More precisely, take the Ansatz

$$\mathbf{y}_2 = \mathbf{x}_2 + \lambda \mathbf{y}_1, \quad (4.18)$$

thereby determining the arbitrary scalar  $\lambda$  such that  $\mathbf{y}_1$  and  $\mathbf{y}_2$  are orthogonal; that is,  $\langle \mathbf{y}_1 | \mathbf{y}_2 \rangle = 0$ . This yields

$$\langle \mathbf{y}_2 | \mathbf{y}_1 \rangle = \langle \mathbf{x}_2 | \mathbf{y}_1 \rangle + \lambda \langle \mathbf{y}_1 | \mathbf{y}_1 \rangle = 0, \quad (4.19)$$

and thus, since  $\mathbf{y}_1 \neq 0$ ,

$$\lambda = -\frac{\langle \mathbf{x}_2 | \mathbf{y}_1 \rangle}{\langle \mathbf{y}_1 | \mathbf{y}_1 \rangle}. \quad (4.20)$$

To obtain the third vector  $\mathbf{y}_3$  of the new basis, take the Ansatz

$$\mathbf{y}_3 = \mathbf{x}_3 + \mu \mathbf{y}_1 + \nu \mathbf{y}_2, \quad (4.21)$$

<sup>7</sup> Werner Greub. *Linear Algebra*, volume 23 of *Graduate Texts in Mathematics*. Springer, New York, Heidelberg, fourth edition, 1975

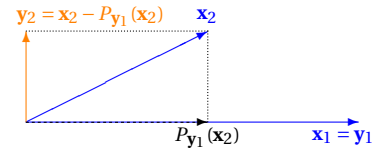


Figure 4.2: Gram-Schmidt construction for two nonorthogonal vectors  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , yielding two orthogonal vectors  $\mathbf{y}_1$  and  $\mathbf{y}_2$ .

and require that it is orthogonal to the two previous orthogonal basis vectors  $\mathbf{y}_1$  and  $\mathbf{y}_2$ ; that is  $\langle \mathbf{y}_1 | \mathbf{y}_3 \rangle = \langle \mathbf{y}_2 | \mathbf{y}_3 \rangle = 0$ . We already know that  $\langle \mathbf{y}_1 | \mathbf{y}_2 \rangle = 0$ . Consider the scalar products of  $\mathbf{y}_1$  and  $\mathbf{y}_2$  with the *Ansatz* for  $\mathbf{y}_3$  in Eq. (4.21); that is,

$$\begin{aligned}\langle \mathbf{y}_3 | \mathbf{y}_1 \rangle &= \langle \mathbf{y}_3 | \mathbf{x}_1 \rangle + \mu \langle \mathbf{y}_1 | \mathbf{y}_1 \rangle + \nu \langle \mathbf{y}_2 | \mathbf{y}_1 \rangle \\ 0 &= \langle \mathbf{y}_3 | \mathbf{x}_1 \rangle + \mu \langle \mathbf{y}_1 | \mathbf{y}_1 \rangle + \nu \cdot 0,\end{aligned}\tag{4.22}$$

and

$$\begin{aligned}\langle \mathbf{y}_3 | \mathbf{y}_2 \rangle &= \langle \mathbf{y}_3 | \mathbf{x}_2 \rangle + \mu \langle \mathbf{y}_1 | \mathbf{y}_2 \rangle + \nu \langle \mathbf{y}_2 | \mathbf{y}_2 \rangle \\ 0 &= \langle \mathbf{y}_3 | \mathbf{x}_2 \rangle + \mu \cdot 0 + \nu \langle \mathbf{y}_2 | \mathbf{y}_2 \rangle.\end{aligned}\tag{4.23}$$

As a result,

$$\mu = -\frac{\langle \mathbf{x}_3 | \mathbf{y}_1 \rangle}{\langle \mathbf{y}_1 | \mathbf{y}_1 \rangle}, \quad \nu = -\frac{\langle \mathbf{x}_3 | \mathbf{y}_2 \rangle}{\langle \mathbf{y}_2 | \mathbf{y}_2 \rangle}.\tag{4.24}$$

A generalization of this construction for all the other new base vectors  $\mathbf{y}_3, \dots, \mathbf{y}_n$ , and thus a proof by complete induction, proceeds by a generalized construction.

Consider, as an example, the standard Euclidean scalar product denoted by “ $\cdot$ ” and the basis  $\{(0, 1), (1, 1)\}$ . Then two orthogonal bases are obtained obtained by taking

(i) either the basis vector  $(0, 1)$  and

$$(1, 1) - \frac{(1, 1) \cdot (0, 1)}{(0, 1) \cdot (0, 1)} (0, 1) = (1, 0),$$

(ii) or the basis vector  $(1, 1)$  and

$$(0, 1) - \frac{(0, 1) \cdot (1, 1)}{(1, 1) \cdot (1, 1)} (1, 1) = \frac{1}{2}(-1, 1).$$

## 4.8 Dual space

Every vector space  $\mathfrak{V}$  has a corresponding *dual vector space* (or just *dual space*) consisting of all linear functionals on  $\mathfrak{V}$ .

A *linear functional* on a vector space  $\mathfrak{V}$  is a scalar-valued linear function  $\mathbf{y}$  defined for every vector  $\mathbf{x} \in \mathfrak{V}$ , with the linear property that

$$\mathbf{y}(\alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2) = \alpha_1 \mathbf{y}(\mathbf{x}_1) + \alpha_2 \mathbf{y}(\mathbf{x}_2).\tag{4.25}$$

For example, let  $\mathbf{x} = (x_1, \dots, x_n)$ , and take  $\mathbf{y}(\mathbf{x}) = x_1$ .

For another example, let again  $\mathbf{x} = (x_1, \dots, x_n)$ , and let  $\alpha_1, \dots, \alpha_n \in \mathbb{C}$  be scalars; and take  $\mathbf{y}(\mathbf{x}) = \alpha_1 x_1 + \dots + \alpha_n x_n$ .

We adopt a square bracket notation “[ $\cdot, \cdot$ ]” for the functional

$$\mathbf{y}(\mathbf{x}) = [\mathbf{x}, \mathbf{y}].\tag{4.26}$$

For proofs and additional information see §13–15 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Note that the usual arithmetic operations of addition and multiplication, that is,

$$(a\mathbf{y} + b\mathbf{z})(\mathbf{x}) = a\mathbf{y}(\mathbf{x}) + b\mathbf{z}(\mathbf{x}), \quad (4.27)$$

together with the “zero functional” (mapping every argument to zero) induce a kind of linear vector space, the “vectors” being identified with the linear functionals. This vector space will be called *dual space*  $\mathfrak{V}^*$ .

As a result, this “bracket” functional is *bilinear* in its two arguments; that is,

$$[\alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2, \mathbf{y}] = \alpha_1 [\mathbf{x}_1, \mathbf{y}] + \alpha_2 [\mathbf{x}_2, \mathbf{y}], \quad (4.28)$$

and

$$[\mathbf{x}, \alpha_1 \mathbf{y}_1 + \alpha_2 \mathbf{y}_2] = \alpha_1 [\mathbf{x}, \mathbf{y}_1] + \alpha_2 [\mathbf{x}, \mathbf{y}_2]. \quad (4.29)$$

Because of linearity, we can completely characterize an arbitrary linear functional  $\mathbf{y} \in \mathfrak{V}^*$  by its values of the vectors of some basis of  $\mathfrak{V}$ : If we know the functional value on the basis vectors in  $\mathfrak{B}$ , we know the functional on all elements of the vector space  $\mathfrak{V}$ . If  $\mathfrak{V}$  is an  $n$ -dimensional vector space, and if  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  is a basis of  $\mathfrak{V}$ , and if  $\{\alpha_1, \dots, \alpha_n\}$  is any set of  $n$  scalars, then there is a unique linear functional  $\mathbf{y}$  on  $\mathfrak{V}$  such that  $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$  for all  $0 \leq i \leq n$ .

A constructive proof of this theorem can be given as follows: Because every  $\mathbf{x} \in \mathfrak{V}$  can be written as a linear combination  $\mathbf{x} = x_1 \mathbf{f}_1 + \dots + x_n \mathbf{f}_n$  of the basis vectors of  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  in one and only one (unique) way, we obtain for any arbitrary linear functional  $\mathbf{y} \in \mathfrak{V}^*$  a unique decomposition in terms of the basis vectors of  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$ ; that is,

$$[\mathbf{x}, \mathbf{y}] = x_1 [\mathbf{f}_1, \mathbf{y}] + \dots + x_n [\mathbf{f}_n, \mathbf{y}]. \quad (4.30)$$

By identifying  $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$  we obtain

$$[\mathbf{x}, \mathbf{y}] = x_1 \alpha_1 + \dots + x_n \alpha_n. \quad (4.31)$$

Conversely, if we *define*  $\mathbf{y}$  by  $[\mathbf{x}, \mathbf{y}] = x_1 \alpha_1 + \dots + x_n \alpha_n$ , then  $\mathbf{y}$  can be interpreted as a linear functional in  $\mathfrak{V}^*$  with  $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$ .

If we introduce a *dual basis* by requiring that  $[\mathbf{f}_i, \mathbf{f}_j^*] = \delta_{ij}$  (cf. Eq. 4.32 below), then the coefficients  $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$ ,  $1 \leq i \leq n$ , can be interpreted as the *coordinates* of the linear functional  $\mathbf{y}$  with respect to the dual basis  $\mathfrak{B}^*$ , such that  $\mathbf{y} = (\alpha_1, \alpha_2, \dots, \alpha_n)^T$ .

Likewise, as will be shown in (4.38),  $x_i = [\mathbf{x}, \mathbf{f}_i^*]$ ; that is, the vector coordinates can be represented by the functionals of the elements of the dual basis.

Let us explicitly construct an example of a linear functional  $\varphi(\mathbf{x}) \equiv [\mathbf{x}, \varphi]$  that is defined on all vectors  $\mathbf{x} = \alpha \mathbf{e}_1 + \beta \mathbf{e}_2$  of a two-dimensional vector space with the basis  $\{\mathbf{e}_1, \mathbf{e}_2\}$  by enumerating its “performance on the basis

The square bracket can be identified with the scalar dot product  $[\mathbf{x}, \mathbf{y}] = \langle \mathbf{x} | \mathbf{y} \rangle$  only for Euclidean vector spaces  $\mathbb{R}^n$ , since for complex spaces this would no longer be positive definite. That is, for Euclidean vector spaces  $\mathbb{R}^n$  the inner or scalar product is bilinear.

vectors"  $\mathbf{e}_1 = (1, 0)$  and  $\mathbf{e}_2 = (0, 1)$ ; more explicitly, say, for an example's sake,  $\varphi(\mathbf{e}_1) \equiv [\mathbf{e}_1, \varphi] = 2$  and  $\varphi(\mathbf{e}_2) \equiv [\mathbf{e}_2, \varphi] = 3$ . Therefore, for example,  $\varphi((5, 7)) \equiv [(5, 7), \varphi] = 5[\mathbf{e}_1, \varphi] + 7[\mathbf{e}_2, \varphi] = 10 + 21 = 31$ .

#### 4.8.1 Dual basis

We now can define a *dual basis*, or, used synonymously, a *reciprocal basis*.

If  $\mathfrak{V}$  is an  $n$ -dimensional vector space, and if  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  is a basis of  $\mathfrak{V}$ , then there is a unique *dual basis*  $\mathfrak{B}^* = \{\mathbf{f}_1^*, \dots, \mathbf{f}_n^*\}$  in the dual vector space  $\mathfrak{V}^*$  defined by

$$[\mathbf{f}_i, \mathbf{f}_j^*] = \delta_{ij}, \quad (4.32)$$

where  $\delta_{ij}$  is the Kronecker delta function. The dual space  $\mathfrak{V}^*$  spanned by the dual basis  $\mathfrak{B}^*$  is  $n$ -dimensional.

More generally, if  $g$  is the *metric tensor*, the dual basis is defined by

$$g(\mathbf{f}_i, \mathbf{f}_j^*) = \delta_{ij}. \quad (4.33)$$

or, in a different notation in which  $\mathbf{f}_j^* = \mathbf{f}^j$ ,

$$g(\mathbf{f}_i, \mathbf{f}^j) = \delta_i^j. \quad (4.34)$$

In terms of the inner product, the representation of the metric  $g$  as outlined and characterized on page 89 with respect to a particular basis.

$\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  may be defined by  $g_{ij} = g(\mathbf{f}_i, \mathbf{f}_j) = \langle \mathbf{f}_i | \mathbf{f}_j \rangle$ . Note however, that the coordinates  $g_{ij}$  of the metric  $g$  need not necessarily be positive definite. For example, special relativity uses the “pseudo-Euclidean” metric  $g = \text{diag}(+1, +1, +1, -1)$  (or just  $g = \text{diag}(+, +, +, -)$ ), where “diag” stands for the *diagonal matrix* with the arguments in the diagonal.

In a real Euclidean vector space  $\mathbb{R}^n$  with the dot product as the scalar product, the dual basis of an orthogonal basis is also orthogonal, and contains vectors with the same directions, although with *reciprocal length* (thereby explaining the wording “reciprocal basis”). Moreover, for an orthonormal basis, the basis vectors are uniquely identifiable by  $\mathbf{e}_i \longrightarrow \mathbf{e}_i^* = \mathbf{e}_i^T$ . This identification can only be made for orthonormal bases; it is *not* true for nonorthonormal bases.

A “reverse construction” of the elements  $\mathbf{f}_j^*$  of the dual basis  $\mathfrak{B}^*$  – thereby using the definition “ $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$  for all  $1 \leq i \leq n$ ” for any element  $\mathbf{y}$  in  $\mathfrak{V}^*$  introduced earlier – can be given as follows: for every  $1 \leq j \leq n$ , we can *define* a vector  $\mathbf{f}_j^*$  in the dual basis  $\mathfrak{B}^*$  by the *requirement*  $[\mathbf{f}_i, \mathbf{f}_j^*] = \delta_{ij}$ . That is, in words: the dual basis element, when applied to the elements of the original  $n$ -dimensional basis, yields one if and only if it corresponds to the respective equally indexed basis element; for all the other  $n - 1$  basis elements it yields zero.

What remains to be proven is the conjecture that  $\mathfrak{B}^* = \{\mathbf{f}_1^*, \dots, \mathbf{f}_n^*\}$  is a basis of  $\mathfrak{V}^*$ ; that is, that the vectors in  $\mathfrak{B}^*$  are linear independent, and that they span  $\mathfrak{V}^*$ .

The metric tensor  $g_{ij}$  represents a *bilinear functional*  $g(\mathbf{x}, \mathbf{y}) = x^i y^j g_{ij}$  that is *symmetric*; that is,  $g(\mathbf{x}, \mathbf{y}) = g(\mathbf{y}, \mathbf{x})$  and *non-degenerate*; that is, for any nonzero vector  $\mathbf{x} \in \mathfrak{V}$ ,  $\mathbf{x} \neq 0$ , there is some vector  $\mathbf{y} \in \mathfrak{V}$ , so that  $g(\mathbf{x}, \mathbf{y}) \neq 0$ .  $g$  also satisfies the triangle inequality  $\|\mathbf{x} - \mathbf{z}\| \leq \|\mathbf{x} - \mathbf{y}\| + \|\mathbf{y} - \mathbf{z}\|$ .

First observe that  $\mathfrak{B}^*$  is a set of linear independent vectors, for if  $\alpha_1 \mathbf{f}_1^* + \cdots + \alpha_n \mathbf{f}_n^* = 0$ , then also

$$[\mathbf{x}, \alpha_1 \mathbf{f}_1^* + \cdots + \alpha_n \mathbf{f}_n^*] = \alpha_1 [\mathbf{x}, \mathbf{f}_1^*] + \cdots + \alpha_n [\mathbf{x}, \mathbf{f}_n^*] = 0 \quad (4.35)$$

for arbitrary  $\mathbf{x} \in \mathfrak{V}$ . In particular, by identifying  $\mathbf{x}$  with  $\mathbf{f}_i \in \mathfrak{B}$ , for  $1 \leq i \leq n$ ,

$$\alpha_1 [\mathbf{f}_i, \mathbf{f}_1^*] + \cdots + \alpha_n [\mathbf{f}_i, \mathbf{f}_n^*] = \alpha_j [\mathbf{f}_i, \mathbf{f}_j^*] = \alpha_j \delta_{ij} = \alpha_i = 0. \quad (4.36)$$

Second, every  $\mathbf{y} \in \mathfrak{V}^*$  is a linear combination of elements in  $\mathfrak{B}^* = \{\mathbf{f}_1^*, \dots, \mathbf{f}_n^*\}$ , because by starting from  $[\mathbf{f}_i, \mathbf{y}] = \alpha_i$ , with  $\mathbf{x} = x_1 \mathbf{f}_1 + \cdots + x_n \mathbf{f}_n$  we obtain

$$[\mathbf{x}, \mathbf{y}] = x_1 [\mathbf{f}_1, \mathbf{y}] + \cdots + x_n [\mathbf{f}_n, \mathbf{y}] = x_1 \alpha_1 + \cdots + x_n \alpha_n. \quad (4.37)$$

Note that, for arbitrary  $\mathbf{x} \in \mathfrak{V}$ ,

$$[\mathbf{x}, \mathbf{f}_i^*] = x_1 [\mathbf{f}_1, \mathbf{f}_i^*] + \cdots + x_n [\mathbf{f}_n, \mathbf{f}_i^*] = x_j [\mathbf{f}_j, \mathbf{f}_i^*] = x_j \delta_{ji} = x_i, \quad (4.38)$$

and by substituting  $[\mathbf{x}, \mathbf{f}_i]$  for  $x_i$  in Eq. (4.37) we obtain

$$\begin{aligned} [\mathbf{x}, \mathbf{y}] &= x_1 \alpha_1 + \cdots + x_n \alpha_n \\ &= [\mathbf{x}, \mathbf{f}_1] \alpha_1 + \cdots + [\mathbf{x}, \mathbf{f}_n] \alpha_n \\ &= [\mathbf{x}, \alpha_1 \mathbf{f}_1 + \cdots + \alpha_n \mathbf{f}_n], \end{aligned} \quad (4.39)$$

and therefore  $\mathbf{y} = \alpha_1 \mathbf{f}_1 + \cdots + \alpha_n \mathbf{f}_n = \alpha_i \mathbf{f}_i$ .

How can one determine the dual basis from a given, not necessarily orthogonal, basis? Suppose for the rest of this section that the metric is identical to the Euclidean metric  $\det(+, +, +)$  representable as the usual “dot product.” The tuples of *row vectors* of the basis  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  can be arranged into a matrix

$$\mathbf{B} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{1,1} & \cdots & \mathbf{f}_{1,n} \\ \mathbf{f}_{2,1} & \cdots & \mathbf{f}_{2,n} \\ \vdots & \vdots & \vdots \\ \mathbf{f}_{n,1} & \cdots & \mathbf{f}_{n,n} \end{pmatrix}. \quad (4.40)$$

Then take the *inverse matrix*  $\mathbf{B}^{-1}$ , and interpret the *column vectors* of

$$\begin{aligned} \mathbf{B}^* &= \mathbf{B}^{-1} \\ &= (\mathbf{f}_1^*, \dots, \mathbf{f}_n^*) \\ &= \begin{pmatrix} \mathbf{f}_{1,1}^* & \cdots & \mathbf{f}_{n,1}^* \\ \mathbf{f}_{1,2}^* & \cdots & \mathbf{f}_{n,2}^* \\ \vdots & \vdots & \vdots \\ \mathbf{f}_{1,n}^* & \cdots & \mathbf{f}_{n,n}^* \end{pmatrix} \end{aligned} \quad (4.41)$$

as the tuples of elements of the dual basis of  $\mathfrak{B}^*$ .

For orthogonal but not orthonormal bases, the term *reciprocal* basis can be easily explained from the fact that the norm (or length) of each vector in the *reciprocal basis* is just the *inverse* of the length of the original vector.

For a direct proof, consider  $\mathbf{B} \cdot \mathbf{B}^{-1} = \mathbb{I}_n$ .

(i) For example, if

$$\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\} = \{(1, 0, \dots, 0), (0, 1, \dots, 0), \dots, (0, 0, \dots, 1)\}$$

is the standard basis in  $n$ -dimensional vector space containing unit vectors of norm (or length) one, then (the superscript “ $T$ ” indicates transposition)

$$\begin{aligned} \mathfrak{B}^* &= \{\mathbf{e}_1^*, \mathbf{e}_2^*, \dots, \mathbf{e}_n^*\} \\ &= \{(1, 0, \dots, 0)^T, (0, 1, \dots, 0)^T, \dots, (0, 0, \dots, 1)^T\} \\ &= \left\{ \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \right\} \end{aligned} \quad (4.42)$$

has elements with identical components, but those tuples are the transposed tuples.

(ii) If

$$\mathfrak{X} = \{\alpha_1 \mathbf{e}_1, \alpha_2 \mathbf{e}_2, \dots, \alpha_n \mathbf{e}_n\} = \{(\alpha_1, 0, \dots, 0), (0, \alpha_2, \dots, 0), \dots, (0, 0, \dots, \alpha_n)\},$$

$\alpha_1, \alpha_2, \dots, \alpha_n \in \mathbb{R}$ , is a “dilated” basis in  $n$ -dimensional vector space containing vectors of norm (or length)  $\alpha_i$ , then

$$\begin{aligned} \mathfrak{X}^* &= \left\{ \frac{1}{\alpha_1} \mathbf{e}_1^*, \frac{1}{\alpha_2} \mathbf{e}_2^*, \dots, \frac{1}{\alpha_n} \mathbf{e}_n^* \right\} \\ &= \left\{ \left( \frac{1}{\alpha_1}, 0, \dots, 0 \right)^T, \left( 0, \frac{1}{\alpha_2}, \dots, 0 \right)^T, \dots, \left( 0, 0, \dots, \frac{1}{\alpha_n} \right)^T \right\} \\ &= \left\{ \frac{1}{\alpha_1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \frac{1}{\alpha_2} \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, \frac{1}{\alpha_n} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \right\} \end{aligned} \quad (4.43)$$

has elements with identical components of inverse length  $\frac{1}{\alpha_i}$ , and again those tuples are the transposed tuples.

(iii) Consider the nonorthogonal basis  $\mathfrak{B} = \{(1, 2), (3, 4)\}$ . The associated row matrix is

$$\mathbf{B} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}.$$

The inverse matrix is

$$\mathbf{B}^{-1} = \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix},$$

and the associated dual basis is obtained from the columns of  $\mathbf{B}^{-1}$  by

$$\mathfrak{B}^* = \left\{ \begin{pmatrix} -2 \\ \frac{3}{2} \end{pmatrix}, \begin{pmatrix} 1 \\ -\frac{1}{2} \end{pmatrix} \right\} = \left\{ \frac{1}{2} \begin{pmatrix} -4 \\ 3 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 2 \\ -1 \end{pmatrix} \right\}. \quad (4.44)$$

#### 4.8.2 Dual coordinates

With respect to a given basis, the components of a vector are often written as tuples of ordered (“ $x_i$  is written before  $x_{i+1}$ ” – not “ $x_i < x_{i+1}$ ”) scalars as *column vectors*

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad (4.45)$$

whereas the components of vectors in dual spaces are often written in terms of tuples of ordered scalars as *row vectors*

$$\mathbf{x}^* = (x_1^*, x_2^*, \dots, x_n^*). \quad (4.46)$$

The coordinates  $(x_1, x_2, \dots, x_n)^T = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$  are called *covariant*, whereas the

coordinates  $(x_1^*, x_2^*, \dots, x_n^*)$  are called *contravariant*. Alternatively, one can denote covariant coordinates by subscripts, and contravariant coordinates by superscripts; that is (see also Havlicek<sup>8</sup>, Section 11.4),

$$x_i = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \text{ and } x^i = (x_1^*, x_2^*, \dots, x_n^*). \quad (4.47)$$

Note again that the covariant and contravariant components  $x_i$  and  $x^i$  are not absolute, but always defined *with respect to* a particular (dual) basis.

Note that the *Einstein summation convention* requires that, when an index variable appears twice in a single term, one has to sum over all of the possible index values. This saves us from drawing the sum sign “ $\sum_i$ ” for the index  $i$ ; for instance  $x_i y_i = \sum_i x_i y_i$ .

In the particular context of covariant and contravariant components – made necessary by nonorthogonal bases whose associated dual bases are *not* identical – the summation always is between some superscript and some subscript; e.g.,  $x_i y^i$ .

Note again that for orthonormal basis,  $x^i = x_i$ .

#### 4.8.3 Representation of a functional by inner product

The following representation theorem, often called *Riesz representation theorem* (sometimes also called the *Fréchet-Riesz theorem*), is about the connection between any functional in a vector space and its inner product; it is stated without proof: To any linear functional  $\mathbf{z}$  on a finite-dimensional

<sup>8</sup> Hans Havlicek. *Lineare Algebra für Technische Mathematiker*. Heldermann Verlag, Lemgo, second edition, 2008

For proofs and additional information see §67 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974



inner product space  $\mathfrak{V}$  there corresponds a unique vector  $\mathbf{y} \in \mathfrak{V}$ , such that

$$\mathbf{z}(\mathbf{x}) = [\mathbf{x}, \mathbf{z}] = \langle \mathbf{x} | \mathbf{y} \rangle \quad (4.48)$$

for all  $\mathbf{x} \in \mathfrak{V}$ .

Note that in real or complex vector space  $\mathbb{R}^n$  or  $\mathbb{C}^n$ , and with the dot product,  $\mathbf{y}^\dagger = \mathbf{z}$ .

Note also that every inner product  $\langle \mathbf{x} | \mathbf{y} \rangle = \phi_y(x)$  defines a linear functional  $\phi_y(x)$  for all  $\mathbf{x} \in \mathfrak{V}$ .

In quantum mechanics, this representation of a functional by the inner product suggests the (unique) existence of the bra vector  $\langle \psi | \in \mathfrak{V}^*$  associated with every ket vector  $|\psi\rangle \in \mathfrak{V}$ .

It also suggests a “natural” duality between propositions and states – that is, between (i) dichotomic (yes/no, or 1/0) observables represented by projections  $\mathbf{E}_x = |\mathbf{x}\rangle\langle\mathbf{x}|$  and their associated linear subspaces spanned by unit vectors  $|\mathbf{x}\rangle$  on the one hand, and (ii) pure states, which are also represented by projections  $\rho_\psi = |\psi\rangle\langle\psi|$  and their associated subspaces spanned by unit vectors  $|\psi\rangle$  on the other hand – *via* the scalar product “ $\langle \cdot | \cdot \rangle$ .” In particular<sup>9</sup>,

$$\psi(\mathbf{x}) \equiv [\mathbf{x}, \psi] = \langle \mathbf{x} | \psi \rangle \quad (4.49)$$

represents the *probability amplitude*. By the *Born rule* for pure states, the absolute square  $|\langle \mathbf{x} | \psi \rangle|^2$  of this probability amplitude is identified with the probability of the occurrence of the proposition  $\mathbf{E}_x$ , given the state  $|\psi\rangle$ .

More general, due to linearity and the spectral theorem (cf. Section 4.28.1 on page 67), the statistical expectation for a Hermitean (normal) operator  $\mathbf{A} = \sum_{i=0}^k \lambda_i \mathbf{E}_i$  and a quantized system prepared in pure state (cf. Sec. 4.12)  $\rho_\psi = |\psi\rangle\langle\psi|$  for some unit vector  $|\psi\rangle$  is given by the *Born rule*

$$\begin{aligned} \langle \mathbf{A} \rangle_\psi &= \text{Tr}(\rho_\psi \mathbf{A}) \\ &= \text{Tr} \left[ \rho_\psi \left( \sum_{i=0}^k \lambda_i \mathbf{E}_i \right) \right] = \text{Tr} \left( \sum_{i=0}^k \lambda_i \rho_\psi \mathbf{E}_i \right) \\ &= \text{Tr} \left( \sum_{i=0}^k \lambda_i (|\psi\rangle\langle\psi|) (|\mathbf{x}_i\rangle\langle\mathbf{x}_i|) \right) \\ &= \text{Tr} \left( \sum_{i=0}^k \lambda_i |\psi\rangle\langle\psi| \mathbf{x}_i \langle\mathbf{x}_i| \right) \\ &= \sum_{j=0}^k \langle \mathbf{x}_j | \left( \sum_{i=0}^k \lambda_i |\psi\rangle\langle\psi| \mathbf{x}_i \langle\mathbf{x}_i| \right) | \mathbf{x}_j \rangle \\ &= \sum_{j=0}^k \sum_{i=0}^k \lambda_i \langle \mathbf{x}_j | \psi \rangle \langle \psi | \mathbf{x}_i \rangle \underbrace{\langle \mathbf{x}_i | \mathbf{x}_j \rangle}_{\delta_{ij}} \\ &= \sum_{i=0}^k \lambda_i \langle \mathbf{x}_i | \psi \rangle \langle \psi | \mathbf{x}_i \rangle \\ &= \sum_{i=0}^k \lambda_i |\langle \mathbf{x}_i | \psi \rangle|^2, \end{aligned} \quad (4.50)$$

<sup>9</sup> Jan Hamhalter. *Quantum Measure Theory. Fundamental Theories of Physics, Vol. 134.* Kluwer Academic Publishers, Dordrecht, Boston, London, 2003. ISBN 1-4020-1714-6

where  $\text{Tr}$  stands for the trace (cf. Section 4.18 on page 54), and we have used the spectral decomposition  $\mathbf{A} = \sum_{i=0}^k \lambda_i \mathbf{E}_i$  (cf. Section 4.28.1 on page 67).

#### 4.8.4 Double dual space

In the following, we strictly limit the discussion to finite dimensional vector spaces.

Because to every vector space  $\mathfrak{V}$  there exists a dual vector space  $\mathfrak{V}^*$  “spanned” by all linear functionals on  $\mathfrak{V}$ , there exists also a dual vector space  $(\mathfrak{V}^*)^* = \mathfrak{V}^{**}$  to the dual vector space  $\mathfrak{V}^*$  “spanned” by all linear functionals on  $\mathfrak{V}^*$ . We state without proof that  $\mathfrak{V}^{**}$  is closely related to, and can be *canonically identified* with  $\mathfrak{V}$  via the *canonical bijection*

$$\begin{aligned} \mathfrak{V} &\rightarrow \mathfrak{V}^{**} : \mathbf{x} \mapsto \langle \cdot | \mathbf{x} \rangle, \text{ with} \\ \langle \cdot | \mathbf{x} \rangle : \mathfrak{V}^* &\rightarrow \mathbb{R} \text{ or } \mathbb{C} : \mathbf{a}^* \mapsto \langle \mathbf{a}^* | \mathbf{x} \rangle; \end{aligned} \quad (4.51)$$

indeed, more generally,

$$\begin{aligned} \mathfrak{V} &\equiv \mathfrak{V}^{**}, \\ \mathfrak{V}^* &\equiv \mathfrak{V}^{***}, \\ \mathfrak{V}^{**} &\equiv \mathfrak{V}^{****} \equiv \mathfrak{V}, \\ \mathfrak{V}^{***} &\equiv \mathfrak{V}^{*****} \equiv \mathfrak{V}^*, \\ &\vdots \end{aligned} \quad (4.52)$$

#### 4.9 Direct sum

Let  $\mathfrak{U}$  and  $\mathfrak{V}$  be vector spaces (over the same field, say  $\mathbb{C}$ ). Their *direct sum* is a vector space  $\mathfrak{W} = \mathfrak{U} \oplus \mathfrak{V}$  consisting of all ordered pairs  $(\mathbf{x}, \mathbf{y})$ , with  $\mathbf{x} \in \mathfrak{U}$  in  $\mathbf{y} \in \mathfrak{V}$ , and with the linear operations defined by

$$(\alpha \mathbf{x}_1 + \beta \mathbf{x}_2, \alpha \mathbf{y}_1 + \beta \mathbf{y}_2) = \alpha (\mathbf{x}_1, \mathbf{y}_1) + \beta (\mathbf{x}_2, \mathbf{y}_2). \quad (4.53)$$

We state without proof that the dimension of the direct sum is the sum of the dimensions of its summands.

We also state without proof that, if  $\mathfrak{U}$  and  $\mathfrak{V}$  are subspaces of a vector space  $\mathfrak{W}$ , then the following three conditions are equivalent:

- (i)  $\mathfrak{W} = \mathfrak{U} \oplus \mathfrak{V}$ ;
- (ii)  $\mathfrak{U} \cap \mathfrak{V} = \mathbf{o}$  and  $\mathfrak{U} + \mathfrak{V} = \mathfrak{W}$ , that is,  $\mathfrak{W}$  is spanned by  $\mathfrak{U}$  and  $\mathfrak{V}$  (i.e.,  $\mathfrak{U}$  and  $\mathfrak{V}$  are complements of each other);
- (iii) every vector  $\mathbf{z} \in \mathfrak{W}$  can be written as  $\mathbf{z} = \mathbf{x} + \mathbf{y}$ , with  $\mathbf{x} \in \mathfrak{U}$  and  $\mathbf{y} \in \mathfrak{V}$ , in one and only one way.

<https://www.dpmms.cam.ac.uk/~wtg10/meta.doubledual.html>

For proofs and additional information see §18 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

For proofs and additional information see §19 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

For proofs and additional information see §18 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Very often the direct sum will be used to “compose” a vector space by the direct sum of its subspaces. Note that there is no “natural” way of composition. A different way of putting two vector spaces together is by the *tensor product*.

## 4.10 Tensor product

### 4.10.1 Sloppy definition

For the moment, suffice it to say that the *tensor product*  $\mathfrak{V} \otimes \mathfrak{U}$  of two linear vector spaces  $\mathfrak{V}$  and  $\mathfrak{U}$  should be such that, to every  $\mathbf{x} \in \mathfrak{V}$  and every  $\mathbf{y} \in \mathfrak{U}$  there corresponds a tensor product  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y} \in \mathfrak{V} \otimes \mathfrak{U}$  which is bilinear in both factors.

A generalization to more than one factors is straightforward.

### 4.10.2 Definition

A more rigorous definition is as follows: The *tensor product*  $\mathfrak{V} \otimes \mathfrak{U}$  of two vector spaces  $\mathfrak{V}$  and  $\mathfrak{U}$  (over the same field, say  $\mathbb{C}$ ) is the dual vector space of all bilinear forms on  $\mathfrak{V} \oplus \mathfrak{U}$ .

For each pair of vectors  $\mathbf{x} \in \mathfrak{V}$  and  $\mathbf{y} \in \mathfrak{U}$  the tensor product  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$  is the element of  $\mathfrak{V} \otimes \mathfrak{U}$  such that  $\mathbf{z}(\mathbf{w}) = \mathbf{w}(\mathbf{x}, \mathbf{y})$  for every bilinear form  $\mathbf{w}$  on  $\mathfrak{V} \oplus \mathfrak{U}$ .

Alternatively we could define the *tensor product* as the linear superpositions of products  $\mathbf{e}_i \otimes \mathbf{f}_j$  of all basis vectors  $\mathbf{e}_i \in \mathfrak{V}$ , with  $1 \leq i \leq n$ , and  $\mathbf{f}_j \in \mathfrak{U}$ , with  $1 \leq j \leq m$  as follows. First we note without proof that if  $\mathfrak{A} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  and  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_m\}$  are bases of  $n$ - and  $m$ - dimensional vector spaces  $\mathfrak{V}$  and  $\mathfrak{U}$ , respectively, then the set of vectors  $\mathbf{e}_i \otimes \mathbf{f}_j$  with  $i = 1, \dots, n$  and  $j = 1, \dots, m$  is a basis of the tensor product  $\mathfrak{V} \otimes \mathfrak{U}$ . Then an arbitrary tensor product can be written as the linear superposition of all its basis vectors  $\mathbf{e}_i \otimes \mathbf{f}_j$  with  $\mathbf{e}_i \in \mathfrak{V}$ , with  $1 \leq i \leq n$ , and  $\mathbf{f}_j \in \mathfrak{U}$ , with  $1 \leq j \leq m$ ; that is,

$$\mathbf{z} = \sum_{i,j} c_{ij} \mathbf{e}_i \otimes \mathbf{f}_j. \quad (4.54)$$

We state without proof that the dimension of  $\mathfrak{V} \otimes \mathfrak{U}$  of an  $n$ -dimensional vector space  $\mathfrak{V}$  and an  $m$ -dimensional vector space  $\mathfrak{U}$  is multiplicative, that is, the dimension of  $\mathfrak{V} \otimes \mathfrak{U}$  is  $nm$ . Informally, this is evident from the number of basis pairs  $\mathbf{e}_i \otimes \mathbf{f}_j$ .

### 4.10.3 Representation

A product of vectors  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$  has three equivalent notations or representations:

- (i) as the scalar coordinates  $x_i y_j$  with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded;

For proofs and additional information see §24 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

- (ii) as the quasi-matrix  $z_{ij} = x_i y_j$ , whose components  $z_{ij}$  are defined with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded;
- (iii) as a quasi-vector or “flattened matrix” defined by the Kronecker product  $\mathbf{z} = (x_1 \mathbf{y}, x_2 \mathbf{y}, \dots, x_n \mathbf{y}) = (x_1 y_1, x_1 y_2, \dots, x_n y_n)$ . Again, the scalar coordinates  $x_i y_j$  are defined with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded.

In all three cases, the pairs  $x_i y_j$  are properly represented by distinct mathematical entities.

Take, for example,  $\mathbf{x} = (2, 3)$  and  $\mathbf{y} = (5, 7, 11)$ . Then  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$  can be represented by (i) the four scalars  $x_1 y_1 = 10$ ,  $x_1 y_2 = 14$ ,  $x_1 y_3 = 22$ ,  $x_2 y_1 = 15$ ,  $x_2 y_2 = 21$ ,  $x_2 y_3 = 33$ , or by (ii) a  $2 \times 3$  matrix  $\begin{pmatrix} 10 & 14 & 22 \\ 15 & 21 & 33 \end{pmatrix}$ , or by (iii) a 4-tuple  $(10, 14, 22, 15, 21, 33)$ .

Note, however, that this kind of quasi-matrix or quasi-vector representation of vector products can be misleading insofar as it (wrongly) suggests that all vectors in the tensor product space are accessible (representable) as quasi-vectors – they are, however, accessible by *linear superpositions* (4.54) of such quasi-vectors. For instance, take the arbitrary form of a (quasi-)vector in  $\mathbb{C}^4$ , which can be parameterized by

$$(\alpha_1, \alpha_2, \alpha_3, \alpha_4), \text{ with } \alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}, \quad (4.55)$$

and compare (4.55) with the general form of a tensor product of two quasi-vectors in  $\mathbb{C}^2$

$$(a_1, a_2) \otimes (b_1, b_2) \equiv (a_1 b_1, a_1 b_2, a_2 b_1, a_2 b_2), \text{ with } a_1, a_2, b_1, b_2 \in \mathbb{C}. \quad (4.56)$$

A comparison of the coordinates in (4.55) and (4.56) yields

$$\begin{aligned} \alpha_1 &= a_1 b_1, \\ \alpha_2 &= a_1 b_2, \\ \alpha_3 &= a_2 b_1, \\ \alpha_4 &= a_2 b_2. \end{aligned} \quad (4.57)$$

By taking the quotient of the two top and the two bottom equations and equating these quotients, one obtains

$$\begin{aligned} \frac{\alpha_1}{\alpha_2} &= \frac{b_1}{b_2} = \frac{\alpha_3}{\alpha_4}, \text{ and thus} \\ \alpha_1 \alpha_4 &= \alpha_2 \alpha_3, \end{aligned} \quad (4.58)$$

which amounts to a condition for the four coordinates  $\alpha_1, \alpha_2, \alpha_3, \alpha_4$  in order for this four-dimensional vector to be decomposable into a tensor product of two two-dimensional quasi-vectors. In quantum mechanics,

In quantum mechanics this amounts to the fact that not all pure two-particle states can be written in terms of (tensor) products of single-particle states; see also Section 1.5 of

David N. Mermin. *Quantum Computer Science*. Cambridge University Press, Cambridge, 2007. ISBN 9780521876582. URL <http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html>

pure states which are not decomposable into a single tensor product are called *entangled*.

A typical example of an entangled state is the *Bell state*,  $|\Psi^-\rangle$  or, more generally, states in the Bell basis

$$\begin{aligned} |\Psi^-\rangle &= \frac{1}{\sqrt{2}} (|0\rangle|1\rangle - |1\rangle|0\rangle), \\ |\Psi^+\rangle &= \frac{1}{\sqrt{2}} (|0\rangle|1\rangle + |1\rangle|0\rangle), \\ |\Phi^-\rangle &= \frac{1}{\sqrt{2}} (|0\rangle|0\rangle - |1\rangle|1\rangle), \\ |\Phi^+\rangle &= \frac{1}{\sqrt{2}} (|0\rangle|0\rangle + |1\rangle|1\rangle), \end{aligned} \quad (4.59)$$

or just

$$\begin{aligned} |\Psi^-\rangle &= \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle), \\ |\Psi^+\rangle &= \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle), \\ |\Phi^-\rangle &= \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle), \\ |\Phi^+\rangle &= \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle). \end{aligned} \quad (4.60)$$

For instance, in the case of  $|\Psi^-\rangle$  a comparison of coefficient yields

$$\begin{aligned} \alpha_1 &= a_1 b_1 = 0, \\ \alpha_2 &= a_1 b_2 = \frac{1}{\sqrt{2}}, \\ \alpha_3 &= a_2 b_1 = -\frac{1}{\sqrt{2}}, \\ \alpha_4 &= a_2 b_2 = 0; \end{aligned} \quad (4.61)$$

and thus

$$\alpha_1 \alpha_4 = 0 \neq \alpha_2 \alpha_3 = \frac{1}{2}.$$

This shows that  $|\Psi^-\rangle$  cannot be considered as a two particle state product. Indeed, the state can only be characterized by considering the *joint properties* of the two particles – in the case of  $|\Psi^-\rangle$  they are associated with the statements<sup>10</sup>: “the quantum numbers (in this case “0” and “1”) of the two particles are always different.”

## 4.11 Linear transformation

### 4.11.1 Definition

A *linear transformation*, or, used synonymously, a *linear operator*,  $\mathbf{A}$  on a vector space  $\mathfrak{V}$  is a correspondence that assigns every vector  $\mathbf{x} \in \mathfrak{V}$  a vector

<sup>10</sup> Anton Zeilinger. A foundational principle for quantum mechanics. *Foundations of Physics*, 29(4):631–643, 1999. DOI: 10.1023/A:1018820410908. URL <http://dx.doi.org/10.1023/A:1018820410908>

For proofs and additional information see §32–34 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

$\mathbf{A}\mathbf{x} \in \mathfrak{V}$ , in a linear way; such that

$$\mathbf{A}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha\mathbf{A}(\mathbf{x}) + \beta\mathbf{A}(\mathbf{y}) = \alpha\mathbf{A}\mathbf{x} + \beta\mathbf{A}\mathbf{y}, \quad (4.62)$$

identically for all vectors  $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$  and all scalars  $\alpha, \beta$ .

#### 4.11.2 Operations

The *sum*  $\mathbf{S} = \mathbf{A} + \mathbf{B}$  of two linear transformations  $\mathbf{A}$  and  $\mathbf{B}$  is defined by  $\mathbf{S}\mathbf{x} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{x}$  for every  $\mathbf{x} \in \mathfrak{V}$ .

The *product*  $\mathbf{P} = \mathbf{A}\mathbf{B}$  of two linear transformations  $\mathbf{A}$  and  $\mathbf{B}$  is defined by  $\mathbf{P}\mathbf{x} = \mathbf{A}(\mathbf{B}\mathbf{x})$  for every  $\mathbf{x} \in \mathfrak{V}$ .

The notation  $\mathbf{A}^n \mathbf{A}^m = \mathbf{A}^{n+m}$  and  $(\mathbf{A}^n)^m = \mathbf{A}^{nm}$ , with  $\mathbf{A}^1 = \mathbf{A}$  and  $\mathbf{A}^0 = \mathbf{1}$  turns out to be useful.

With the exception of commutativity, all formal algebraic properties of numerical addition and multiplication, are valid for transformations; that is  $\mathbf{A}\mathbf{0} = \mathbf{0}\mathbf{A} = \mathbf{0}$ ,  $\mathbf{A}\mathbf{1} = \mathbf{1}\mathbf{A} = \mathbf{A}$ ,  $\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{C}$ ,  $(\mathbf{A} + \mathbf{B})\mathbf{C} = \mathbf{A}\mathbf{C} + \mathbf{B}\mathbf{C}$ , and  $\mathbf{A}(\mathbf{B}\mathbf{C}) = (\mathbf{A}\mathbf{B})\mathbf{C}$ . In *matrix notation*,  $\mathbf{1} = \mathbb{1}$ , and the entries of  $\mathbf{0}$  are 0 everywhere.

The *inverse operator*  $\mathbf{A}^{-1}$  of  $\mathbf{A}$  is defined by  $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbb{1}$ .

The *commutator* of two matrices  $\mathbf{A}$  and  $\mathbf{B}$  is defined by

$$[\mathbf{A}, \mathbf{B}] = \mathbf{A}\mathbf{B} - \mathbf{B}\mathbf{A}. \quad (4.63)$$

The *polynomial* can be directly adopted from ordinary arithmetic; that is, any finite polynomial  $p$  of degree  $n$  of an operator (transformation)  $\mathbf{A}$  can be written as

$$p(\mathbf{A}) = \alpha_0 \mathbf{1} + \alpha_1 \mathbf{A}^1 + \alpha_2 \mathbf{A}^2 + \cdots + \alpha_n \mathbf{A}^n = \sum_{i=0}^n \alpha_i \mathbf{A}^i. \quad (4.64)$$

The Baker-Hausdorff formula

$$e^{i\mathbf{A}} \mathbf{B} e^{-i\mathbf{A}} = \mathbf{B} + i[\mathbf{A}, \mathbf{B}] + \frac{i^2}{2!} [\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \cdots \quad (4.65)$$

for two arbitrary noncommutative linear operators  $\mathbf{A}$  and  $\mathbf{B}$  is mentioned without proof (cf. Messiah, *Quantum Mechanics*, Vol. 1<sup>11</sup>).

If  $[\mathbf{A}, \mathbf{B}]$  commutes with  $\mathbf{A}$  and  $\mathbf{B}$ , then

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A} + \mathbf{B} + \frac{1}{2}[\mathbf{A}, \mathbf{B}]}. \quad (4.66)$$

If  $\mathbf{A}$  commutes with  $\mathbf{B}$ , then

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A} + \mathbf{B}}. \quad (4.67)$$

#### 4.11.3 Linear transformations as matrices

Let  $\mathfrak{V}$  be an  $n$ -dimensional vector space; let  $\mathfrak{B} = \{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  be any basis of  $\mathfrak{V}$ , and let  $\mathbf{A}$  be a linear transformation on  $\mathfrak{V}$ .

The commutator should not be confused with the bilinear functional introduced for dual spaces.

<sup>11</sup> A. Messiah. *Quantum Mechanics*, volume I. North-Holland, Amsterdam, 1962

Because every vector is a linear combination of the basis vectors  $\mathbf{f}_i$ , every linear transformation can be defined by “its performance on the basis vectors;” that is, by the particular mapping of all  $n$  basis vectors into the transformed vectors, which in turn can be represented as linear combination of the  $n$  basis vectors.

Therefore it is possible to define some  $n \times n$  matrix with  $n^2$  coefficients or coordinates  $\alpha_{ij}$  such that

$$\mathbf{A}\mathbf{f}_j = \sum_i \alpha_{ij} \mathbf{f}_i \quad (4.68)$$

for all  $j = 1, \dots, n$ . Again, note that this definition of a *transformation matrix* is “tied to” a basis.

For *orthonormal bases* there is an even closer connection – representable as scalar product – between a matrix defined by an  $n$ -by- $n$  square array and the representation in terms of the elements of the bases; that is,

$$\begin{aligned} \mathbf{A} &\equiv \langle i|A|j\rangle = \langle \mathbf{f}_i|A|\mathbf{f}_j\rangle = \langle \mathbf{f}_i|\mathbf{A}\mathbf{f}_j\rangle \\ &= \langle \mathbf{f}_i|\sum_l \alpha_{lj} \mathbf{f}_l\rangle = \sum_l \alpha_{lj} \langle \mathbf{f}_i|\mathbf{f}_l\rangle = \sum_l \alpha_{lj} \delta_{il} = \alpha_{ij} \\ &\equiv \begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ \alpha_{n1} & \alpha_{n2} & \cdots & \alpha_{nn} \end{pmatrix}. \end{aligned} \quad (4.69)$$

In terms of this matrix notation, it is quite easy to present an example for which the commutator  $[\mathbf{A}, \mathbf{B}]$  does not vanish; that is  $\mathbf{A}$  and  $\mathbf{B}$  do not commute.

Take, for the sake of an example, the *Pauli spin matrices* which are proportional to the angular momentum operators along the  $x, y, z$ -axis <sup>12</sup>:

<sup>12</sup> Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

$$\begin{aligned} \sigma_1 &= \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma_2 &= \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \sigma_3 &= \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (4.70)$$

Together with unity, i.e.,  $\mathbb{1}_2 = \text{diag}(1, 1)$ , they form a complete basis of all  $(4 \times 4)$  matrices. Now take, for instance, the commutator

$$\begin{aligned} [\sigma_1, \sigma_3] &= \sigma_1 \sigma_3 - \sigma_3 \sigma_1 \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= 2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \neq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}. \end{aligned} \quad (4.71)$$

### 4.12 Projection or projection operator

The more I learned about quantum mechanics the more I realized the importance of projection operators for its conceptualization <sup>13</sup>:

- (i) Projections represent (pure) states.
- (ii) Mixed states, should they ontologically exist, can be composed from projections by summing over projectors.
- (iii) Projectors serve as the most elementary observables – they correspond to yes-no propositions.
- (iv) In Section 4.28.1 we will learn that every observable can be (de-)composed into weighted (spectral) sums of projections.
- (v) Furthermore, from dimension three onwards, Gleason's theorem (cf. Section 4.33.1) allows quantum probability theory to be based upon maximal (in terms of co-measurability) “quasi-classical” blocks of projectors.
- (vi) Such maximal blocks of projectors can be bundled together to show (cf. Section 4.33.2) that the corresponding algebraic structure has no two-valued measure (interpretable as truth assignment), and therefore cannot be “embedded” into a “larger” classical (Boolean) algebra.

#### 4.12.1 Definition

If  $\mathfrak{V}$  is the direct sum of some subspaces  $\mathfrak{M}$  and  $\mathfrak{N}$  so that every  $\mathbf{z} \in \mathfrak{V}$  can be uniquely written in the form  $\mathbf{z} = \mathbf{x} + \mathbf{y}$ , with  $\mathbf{x} \in \mathfrak{M}$  and with  $\mathbf{y} \in \mathfrak{N}$ , then the *projection*, or, used synonymously, *projection* on  $\mathfrak{M}$  along  $\mathfrak{N}$  is the transformation  $\mathbf{E}$  defined by  $\mathbf{E}\mathbf{z} = \mathbf{x}$ . Conversely,  $\mathbf{F}\mathbf{z} = \mathbf{y}$  is the projection on  $\mathfrak{N}$  along  $\mathfrak{M}$ .

A (nonzero) linear transformation  $\mathbf{E}$  is a projection if and only if it is idempotent; that is,  $\mathbf{E}\mathbf{E} = \mathbf{E} \neq 0$ .

For a proof note that, if  $\mathbf{E}$  is the projection on  $\mathfrak{M}$  along  $\mathfrak{N}$ , and if  $\mathbf{z} = \mathbf{x} + \mathbf{y}$ , with  $\mathbf{x} \in \mathfrak{M}$  and with  $\mathbf{y} \in \mathfrak{N}$ , the decomposition of  $\mathbf{x}$  yields  $\mathbf{x} + 0$ , so that  $\mathbf{E}^2\mathbf{z} = \mathbf{E}\mathbf{E}\mathbf{z} = \mathbf{E}\mathbf{x} = \mathbf{x} = \mathbf{E}\mathbf{z}$ . The converse – idempotence “ $\mathbf{E}\mathbf{E} = \mathbf{E}$ ” implies that  $\mathbf{E}$  is a projection – is more difficult to prove. For this proof we refer to the literature; e.g., Halmos <sup>14</sup>.

We also mention without proof that a linear transformation  $\mathbf{E}$  is a projection if and only if  $\mathbf{1} - \mathbf{E}$  is a projection. Note that  $(\mathbf{1} - \mathbf{E})^2 = \mathbf{1} - \mathbf{E} - \mathbf{E} + \mathbf{E}^2 = \mathbf{1} - \mathbf{E}$ ; furthermore,  $\mathbf{E}(\mathbf{1} - \mathbf{E}) = (\mathbf{1} - \mathbf{E})\mathbf{E} = \mathbf{E} - \mathbf{E}^2 = 0$ .

Furthermore, if  $\mathbf{E}$  is the projection on  $\mathfrak{M}$  along  $\mathfrak{N}$ , then  $\mathbf{1} - \mathbf{E}$  is the projection on  $\mathfrak{N}$  along  $\mathfrak{M}$ .

For proofs and additional information see §41 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

<sup>13</sup> John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932. English translation in Ref. ; John von Neumann. *Mathematical Foundations of Quantum Mechanics*. Princeton University Press, Princeton, NJ, 1955; and Garrett Birkhoff and John von Neumann. The logic of quantum mechanics. *Annals of Mathematics*, 37(4): 823–843, 1936. DOI: 10.2307/1968621. URL <http://dx.doi.org/10.2307/1968621>

John von Neumann. *Mathematical Foundations of Quantum Mechanics*. Princeton University Press, Princeton, NJ, 1955

<sup>14</sup> Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974



### 4.12.2 Construction of projections from unit vectors

How can we construct projections from unit vectors, or systems of orthogonal projections from some vector in some orthonormal basis with the standard dot product?

Let  $\mathbf{x}$  be the coordinates of a unit vector; that is  $\|\mathbf{x}\| = 1$ . Transposition is indicated by the superscript “ $T$ ” in real vector space. In complex vector space the transposition has to be substituted for the *conjugate transpose* (also denoted as *Hermitian conjugate* or *Hermitian adjoint*), “ $\dagger$ ,” standing for transposition and complex conjugation of the coordinates. More explicitly,

$$(x_1, \dots, x_n)^T = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \quad (4.72)$$

$$\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}^T = (x_1, \dots, x_n), \quad (4.73)$$

and

$$(x_1, \dots, x_n)^\dagger = \begin{pmatrix} \overline{x_1} \\ \vdots \\ \overline{x_n} \end{pmatrix}, \quad (4.74)$$

$$\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}^\dagger = (\overline{x_1}, \dots, \overline{x_n}). \quad (4.75)$$

Note that, just as

$$(\mathbf{x}^T)^T = \mathbf{x}, \quad (4.76)$$

so is

$$(\mathbf{x}^\dagger)^\dagger = \mathbf{x}. \quad (4.77)$$

In real vector space, the *dyadic product*, or *tensor product*, or *outer*

*product* (also in Dirac's bra and ket notation),

$$\begin{aligned}
 \mathbf{E}_{\mathbf{x}} &= \mathbf{x} \otimes \mathbf{x}^T = |\mathbf{x}\rangle\langle\mathbf{x}| \\
 &= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \\
 &= \begin{pmatrix} x_1(x_1, x_2, \dots, x_n) \\ x_2(x_1, x_2, \dots, x_n) \\ \vdots \\ x_n(x_1, x_2, \dots, x_n) \end{pmatrix} \\
 &= \begin{pmatrix} x_1 x_1 & x_1 x_2 & \cdots & x_1 x_n \\ x_2 x_1 & x_2 x_2 & \cdots & x_2 x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n x_1 & x_n x_2 & \cdots & x_n x_n \end{pmatrix}
 \end{aligned} \tag{4.78}$$

is the projection associated with  $\mathbf{x}$ .

If the vector  $\mathbf{x}$  is not normalized, then the associated projection is

$$\mathbf{E}_{\mathbf{x}} = \frac{\mathbf{x} \otimes \mathbf{x}^T}{\langle \mathbf{x} | \mathbf{x} \rangle} = \frac{|\mathbf{x}\rangle\langle\mathbf{x}|}{\langle \mathbf{x} | \mathbf{x} \rangle} \tag{4.79}$$

This construction is related to  $P_{\mathbf{x}}$  on page 27 by  $P_{\mathbf{x}}(\mathbf{y}) = \mathbf{E}_{\mathbf{x}}\mathbf{y}$ .

For a proof, consider only normalized vectors  $\mathbf{x}$ , and let  $\mathbf{E}_{\mathbf{x}} = \mathbf{x} \otimes \mathbf{x}^T$ , then

$$\mathbf{E}_{\mathbf{x}}\mathbf{E}_{\mathbf{x}} = (|\mathbf{x}\rangle\langle\mathbf{x}|)(|\mathbf{x}\rangle\langle\mathbf{x}|) = |\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{x}\rangle\langle\mathbf{x}| = |\mathbf{x}\rangle \cdot 1 \cdot \langle\mathbf{x}| = \mathbf{E}_{\mathbf{x}}.$$

More explicitly, by writing out the coordinate tuples, the equivalent proof is

$$\begin{aligned}
 \mathbf{E}_{\mathbf{x}}\mathbf{E}_{\mathbf{x}} &= (\mathbf{x} \otimes \mathbf{x}^T) \cdot (\mathbf{x} \otimes \mathbf{x}^T) \\
 &= \left( \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \right) \left( \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \right) \\
 &= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) \\
 &= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \cdot 1 \cdot (x_1, x_2, \dots, x_n) = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (x_1, x_2, \dots, x_n) = \mathbf{E}_{\mathbf{x}}.
 \end{aligned} \tag{4.80}$$

For two examples, let  $\mathbf{x} = (1, 0)^T$  and  $\mathbf{y} = (1, -1)^T$ ; then

$$\mathbf{E}_{\mathbf{x}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 0) = \begin{pmatrix} 1(1, 0) \\ 0(1, 0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

and

$$\mathbf{E}_{\mathbf{y}} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} (1, -1) = \frac{1}{2} \begin{pmatrix} 1(1, -1) \\ -1(1, -1) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Note also that

$$\mathbf{E}_{\mathbf{x}} \mathbf{y} = \langle \mathbf{x} | \mathbf{y} \rangle \mathbf{x}, \quad (4.81)$$

which can be directly proven by insertion.

### 4.13 Change of basis

Let  $\mathfrak{V}$  be an  $n$ -dimensional vector space and let  $\mathfrak{X} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  and  $\mathfrak{Y} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  be two bases of  $\mathfrak{V}$ .

Take an arbitrary vector  $\mathbf{z} \in \mathfrak{V}$ . In terms of the two bases  $\mathfrak{X}$  and  $\mathfrak{Y}$ ,  $\mathbf{z}$  can be written as

$$\mathbf{z} = \sum_{i=1}^n x^i \mathbf{e}_i = \sum_{i=1}^n y^i \mathbf{f}_i, \quad (4.82)$$

where  $x^i$  and  $y^i$  stand for the coordinates of the vector  $\mathbf{z}$  with respect to the bases  $\mathfrak{X}$  and  $\mathfrak{Y}$ , respectively.

The following questions arise:

- (i) What is the relation between the “corresponding” basis vectors  $\mathbf{e}_i$  and  $\mathbf{f}_j$ ?
- (ii) What is the relation between the coordinates  $x^i$  (with respect to the basis  $\mathfrak{X}$ ) and  $y^j$  (with respect to the basis  $\mathfrak{Y}$ ) of the vector  $\mathbf{z}$  in Eq. (4.82)?
- (iii) Suppose one fixes the coordinates, say,  $\{v_1, \dots, v_n\}$ , what is the relation between the vectors  $\mathbf{v} = \sum_{i=1}^n v^i \mathbf{e}_i$  and  $\mathbf{w} = \sum_{i=1}^n v^i \mathbf{f}_i$ ?

As an *Ansatz* for answering question (i), recall that, just like any other vector in  $\mathfrak{V}$ , the new basis vectors  $\mathbf{f}_i$  contained in the new basis  $\mathfrak{Y}$  can be (uniquely) written as a *linear combination* (in quantum physics called *linear superposition*) of the basis vectors  $\mathbf{e}_i$  contained in the old basis  $\mathfrak{X}$ . This can be defined *via* a linear transformation  $\mathbf{A}$  between the corresponding vectors of the bases  $\mathfrak{X}$  and  $\mathfrak{Y}$  by

$$\mathbf{f}_i = (\mathbf{A}\mathbf{e})_i, \quad (4.83)$$

for all  $i = 1, \dots, n$ . More specifically, let  $a_i^j$  be the matrix of the linear transformation  $\mathbf{A}$  in the basis  $\mathfrak{X} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$ , and let us rewrite (4.83) as a matrix equation

$$\mathbf{f}_i = \sum_{j=1}^n a_i^j \mathbf{e}_j. \quad (4.84)$$

For proofs and additional information see §46 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

If  $\mathbf{A}$  stands for the matrix whose components (with respect to  $\mathfrak{X}$ ) are  $a_i^j$ , and  $\mathbf{A}^T$  stands for the transpose of  $\mathbf{A}$  whose components (with respect to  $\mathfrak{X}$ ) are  $a_i^j$ , then

$$\begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{pmatrix} = \mathbf{A} \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \vdots \\ \mathbf{e}_n \end{pmatrix}. \quad (4.85)$$

That is, very explicitly,

$$\begin{aligned} \mathbf{f}_1 &= (\mathbf{A}\mathbf{e})_1 = a_1^1 \mathbf{e}_1 + a_1^2 \mathbf{e}_2 + \cdots + a_1^n \mathbf{e}_n = \sum_{i=1}^n a_1^i \mathbf{e}_i, \\ \mathbf{f}_2 &= (\mathbf{A}\mathbf{e})_2 = a_2^1 \mathbf{e}_1 + a_2^2 \mathbf{e}_2 + \cdots + a_2^n \mathbf{e}_n = \sum_{i=1}^n a_2^i \mathbf{e}_i, \\ &\vdots \\ \mathbf{f}_n &= (\mathbf{A}\mathbf{e})_n = a_n^1 \mathbf{e}_1 + a_n^2 \mathbf{e}_2 + \cdots + a_n^n \mathbf{e}_n = \sum_{i=1}^n a_n^i \mathbf{e}_i. \end{aligned} \quad (4.86)$$

This implies

$$\sum_{i=1}^n v^i \mathbf{f}_i = \sum_{i=1}^n v^i (\mathbf{A}\mathbf{e})_i = \mathbf{A} \left( \sum_{i=1}^n v^i \mathbf{e}_i \right). \quad (4.87)$$

- Note that the  $n$  equalities (4.86) really represent  $n^2$  linear equations for the  $n^2$  unknowns  $a_i^j$ ,  $1 \leq i, j \leq n$ , since every pair of basis vectors  $\{\mathbf{f}_i, \mathbf{e}_i\}$ ,  $1 \leq i \leq n$  has  $n$  components or coefficients.
- If one knows how the basis vectors  $\{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  of  $\mathfrak{X}$  transform, then one knows (by linearity) how all other vectors  $\mathbf{v} = \sum_{i=1}^n v^i \mathbf{e}_i$  (represented in this basis) transform; namely  $\mathbf{A}(\mathbf{v}) = \sum_{i=1}^n v^i (\mathbf{A}\mathbf{e})_i$ .
- Finally note that, if  $\mathfrak{X}$  is an orthonormal basis, then the basis transformation has a diagonal form

$$\mathbf{A} = \sum_{i=1}^n \mathbf{f}_i^\dagger \mathbf{e}_i = \sum_{i=1}^n |\mathbf{f}_i\rangle \langle \mathbf{e}_i| \quad (4.88)$$

because all the off-diagonal components  $a_{ij}$ ,  $i \neq j$  of  $\mathbf{A}$  explicitly written down in Eqs.(4.86) vanish. This can be easily checked by applying  $\mathbf{A}$  to the elements  $\mathbf{e}_i$  of the basis  $\mathfrak{X}$ . See also Section 4.24.3 on page 60 for a representation of unitary transformations in terms of basis changes. In quantum mechanics, the temporal evolution is represented by nothing but a change of orthonormal bases in Hilbert space.

Having settled question (i) by the *Ansatz* (4.83), we turn to question (ii) next. Since

$$\mathbf{z} = \sum_{j=1}^n y^j \mathbf{f}_j = \sum_{j=1}^n y^j (\mathbf{A}\mathbf{e})_j = \sum_{j=1}^n y^j \sum_{i=1}^n a_j^i \mathbf{e}_i = \sum_{i=1}^n \left( \sum_{j=1}^n a_j^i y^j \right) \mathbf{e}_i; \quad (4.89)$$

we obtain by comparison of the coefficients in Eq. (4.82),

$$x^i = \sum_{j=1}^n a_j^i y^j. \quad (4.90)$$

That is, in terms of the “old” coordinates  $x^i$ , the “new” coordinates are

$$\sum_{i=1}^n (a^{-1})_i^l x^i = \sum_{i=1}^n (a^{-1})_i^l \sum_{j=1}^n a_j^i y^j = \sum_{i=1}^n \sum_{j=1}^n (a^{-1})_i^l a_j^i y^j = \sum_{i=1}^n \sum_{j=1}^n a_j^i (a^{-1})_i^l y^j = \sum_{j=1}^n \delta_j^l y^j = y^l. \quad (4.91)$$

If we prefer to represent the vector coordinates of  $\mathbf{x}$  and  $\mathbf{y}$  as  $n$ -tuples, then Eqs. (4.90) and (4.91) have an interpretation as matrix multiplication; that is,

$$\mathbf{x} = \mathbf{A}^T \mathbf{y}, \text{ and } \mathbf{y} = (\mathbf{A}^{-1})^T \mathbf{x}. \quad (4.92)$$

Finally, let us answer question (iii) by substituting the *Ansatz*  $\mathbf{f}_i = \mathbf{A} \mathbf{e}_i$  defined in Eq. (4.83), while considering

$$\mathbf{w} = \sum_{i=1}^n v^i \mathbf{f}_i = \sum_{i=1}^n v^i \mathbf{A} \mathbf{e}_i = \mathbf{A} \sum_{i=1}^n v^i \mathbf{e}_i = \mathbf{A} \left( \sum_{i=1}^n v^i \mathbf{e}_i \right) = \mathbf{A} \mathbf{v}. \quad (4.93)$$

For the sake of an example,

1. consider a change of basis in the plane  $\mathbb{R}^2$  by rotation of an angle  $\varphi = \frac{\pi}{4}$  around the origin, depicted in Fig. 4.3. According to Eq. (4.83), we have

$$\begin{aligned} \mathbf{f}_1 &= a_1^1 \mathbf{e}_1 + a_2^1 \mathbf{e}_2, \\ \mathbf{f}_2 &= a_1^2 \mathbf{e}_1 + a_2^2 \mathbf{e}_2, \end{aligned} \quad (4.94)$$

which amounts to four linear equations in the four unknowns  $a_1^1$ ,  $a_1^2$ ,  $a_2^1$ , and  $a_2^2$ . By inserting the basis vectors  $\mathbf{x}_1$ ,  $\mathbf{x}_2$ ,  $\mathbf{y}_1$ , and  $\mathbf{y}_2$  one obtains for the rotation matrix with respect to the basis  $\mathfrak{X}$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1, 1 \\ -1, 1 \end{pmatrix} = \begin{pmatrix} a_1^1 & a_2^1 \\ a_1^2 & a_2^2 \end{pmatrix} \begin{pmatrix} 1, 0 \\ 0, 1 \end{pmatrix}, \quad (4.95)$$

the first pair of equations yielding  $a_1^1 = a_2^1 = \frac{1}{\sqrt{2}}$ , the second pair of equations yielding  $a_1^2 = -\frac{1}{\sqrt{2}}$  and  $a_2^2 = \frac{1}{\sqrt{2}}$ . Thus,

$$\mathbf{A} = \begin{pmatrix} a_1^1 & a_1^2 \\ a_2^1 & a_2^2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \quad (4.96)$$

As both coordinate systems  $\mathfrak{X} = \{\mathbf{e}_1, \mathbf{e}_2\}$  and  $\mathfrak{Y} = \{\mathbf{f}_1, \mathbf{f}_2\}$  are orthogonal, we might have just computed the diagonal form (4.88)

$$\begin{aligned} \mathbf{A} &= \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ 1 \end{pmatrix} (1, 0) + \begin{pmatrix} -1 \\ 1 \end{pmatrix} (0, 1) \right] \\ &= \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1(1, 0) \\ 1(1, 0) \end{pmatrix} + \begin{pmatrix} -1(0, 1) \\ 1(0, 1) \end{pmatrix} \right] \\ &= \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix} \right] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \end{aligned} \quad (4.97)$$

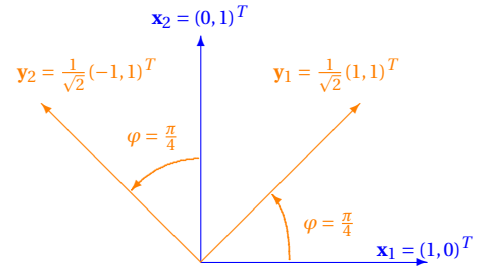


Figure 4.3: Basis change by rotation of  $\varphi = \frac{\pi}{4}$  around the origin.

Likewise, the rotation matrix with respect to the basis  $\mathfrak{V}$  is

$$\mathbf{A}' = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1, 1) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} (-1, 1) \right] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \quad (4.98)$$

2. By a similar calculation, taking into account the definition for the sine and cosine functions, one obtains the transformation matrix  $\mathbf{A}(\varphi)$  associated with an arbitrary angle  $\varphi$ ,

$$\mathbf{A} = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix}. \quad (4.99)$$

The coordinates transform as

$$\mathbf{A}^{-1} = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix}. \quad (4.100)$$

3. Consider the more general rotation depicted in Fig. 4.4. Again, by inserting the basis vectors  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{f}_1$ , and  $\mathbf{f}_2$ , one obtains

$$\frac{1}{2} \begin{pmatrix} \sqrt{3}, 1 \\ 1, \sqrt{3} \end{pmatrix} = \begin{pmatrix} a_1^1 & a_2^1 \\ a_1^2 & a_2^2 \end{pmatrix} \begin{pmatrix} 1, 0 \\ 0, 1 \end{pmatrix}, \quad (4.101)$$

yielding  $a_1^1 = a_2^2 = \frac{\sqrt{3}}{2}$ , the second pair of equations yielding  $a_1^2 = a_2^1 = \frac{1}{2}$ .

Thus,

$$\mathbf{A} = \begin{pmatrix} a & b \\ b & a \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sqrt{3} & 1 \\ 1 & \sqrt{3} \end{pmatrix}. \quad (4.102)$$

The coordinates transform according to the inverse transformation, which in this case can be represented by

$$\mathbf{A}^{-1} = \frac{1}{a^2 - b^2} \begin{pmatrix} a & -b \\ -b & a \end{pmatrix} = \begin{pmatrix} \sqrt{3} & -1 \\ -1 & \sqrt{3} \end{pmatrix}. \quad (4.103)$$

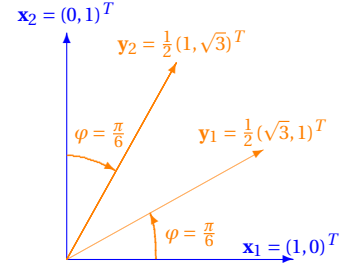


Figure 4.4: More general basis change by rotation.

#### 4.14 Mutually unbiased bases

Two orthonormal bases  $\mathfrak{B} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  and  $\mathfrak{B}' = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  are said to be *mutually unbiased* if their scalar or inner products are

$$|\langle \mathbf{e}_i | \mathbf{f}_j \rangle|^2 = \frac{1}{n} \quad (4.104)$$

for all  $1 \leq i, j \leq n$ . Note without proof – that is, you do not have to be concerned that you need to understand this from what has been said so far – that “the elements of two or more mutually unbiased bases are mutually maximally apart.”

In physics, one seeks maximal sets of orthogonal bases who are maximally apart<sup>15</sup>. Such maximal sets of bases are used in quantum infor-

<sup>15</sup> W. K. Wootters and B. D. Fields. Optimal state-determination by mutually unbiased measurements. *Annals of Physics*, 191:363–381, 1989. DOI: 10.1016/0003-4916(89)90322-9. URL [http://dx.doi.org/10.1016/0003-4916\(89\)90322-9](http://dx.doi.org/10.1016/0003-4916(89)90322-9); and Thomas Durt, Berthold-Georg Englert, Ingemar Bengtsson, and Karol Zyczkowski. On mutually unbiased bases. *International Journal of Quantum Information*, 8:535–640, 2010. DOI: 10.1142/S0219749810000502.

mation theory to assure maximal performance of certain protocols used in quantum cryptography, or for the production of quantum random sequences by beam splitters. They are essential for the practical exploitations of quantum complementary properties and resources.

Schwinger presented an algorithm (see <sup>16</sup> for a proof) to construct a new mutually unbiased basis  $\mathfrak{B}$  from an existing orthogonal one. The proof idea is to create a new basis “inbetween” the old basis vectors. by the following construction steps:

- (i) take the existing orthogonal basis and permute all of its elements by “shift-permuting” its elements; that is, by changing the basis vectors according to their enumeration  $i \rightarrow i + 1$  for  $i = 1, \dots, n - 1$ , and  $n \rightarrow 1$ ; or any other nontrivial (i.e., do not consider identity for any basis element) permutation;
- (ii) consider the (unitary) transformation (cf. Sections 4.13 and 4.24.3) corresponding to the basis change from the old basis to the new, “permuted” basis;
- (iii) finally, consider the (orthonormal) *eigenvectors* of this (unitary; cf. page 59) transformation associated with the basis change. These eigenvectors are the elements of a new bases  $\mathfrak{B}'$ . Together with  $\mathfrak{B}$  these two bases – that is,  $\mathfrak{B}$  and  $\mathfrak{B}'$  – are mutually unbiased.

Consider, for example, the real plane  $\mathbb{R}^2$ , and the basis

$$\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2\} \equiv \{(1, 0), (0, 1)\}.$$

The shift-permutation [step (i)] brings  $\mathfrak{B}$  to a new, “shift-permuted” basis  $\mathfrak{S}$ ; that is,

$$\{\mathbf{e}_1, \mathbf{e}_2\} \mapsto \mathfrak{S} = \{\mathbf{f}_1 = \mathbf{e}_2, \mathbf{f}_2 = \mathbf{e}_1\} \equiv \{(0, 1), (1, 0)\}.$$

The (unitary) basis transformation [step (ii)] between  $\mathfrak{B}$  and  $\mathfrak{S}$  can be constructed by a diagonal sum

$$\begin{aligned} \mathbf{U} &= \mathbf{f}_1^\dagger \mathbf{e}_1 + \mathbf{f}_2^\dagger \mathbf{e}_2 = \mathbf{e}_2^\dagger \mathbf{e}_1 + \mathbf{e}_1^\dagger \mathbf{e}_2 \\ &= |\mathbf{f}_1\rangle\langle\mathbf{e}_1| + |\mathbf{f}_2\rangle\langle\mathbf{e}_2| = |\mathbf{e}_2\rangle\langle\mathbf{e}_1| + |\mathbf{e}_1\rangle\langle\mathbf{e}_2| \\ &\equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1, 0) + \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0, 1) \\ &\equiv \begin{pmatrix} 0(1, 0) \\ 1(1, 0) \end{pmatrix} + \begin{pmatrix} 1(0, 1) \\ 0(0, 1) \end{pmatrix} \\ &\equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \end{aligned} \tag{4.105}$$

The set of eigenvectors [step (iii)] of this (unitary) basis transformation  $\mathbf{U}$

<sup>16</sup> Julian Schwinger. Unitary operators bases. *Proceedings of the National Academy of Sciences (PNAS)*, 46:570–579, 1960. DOI: 10.1073/pnas.46.4.570. URL <http://dx.doi.org/10.1073/pnas.46.4.570>

For a *Mathematica(R)* program, see <http://tph.tuwien.ac.at/~svozil/publ/2012-schwinger.m>

forms a new basis

$$\begin{aligned}
 \mathfrak{B}' &= \left\{ \frac{1}{\sqrt{2}}(\mathbf{f}_1 - \mathbf{e}_1), \frac{1}{\sqrt{2}}(\mathbf{f}_2 + \mathbf{e}_2) \right\} \\
 &= \left\{ \frac{1}{\sqrt{2}}(|\mathbf{f}_1\rangle - |\mathbf{e}_1\rangle), \frac{1}{\sqrt{2}}(|\mathbf{f}_2\rangle + |\mathbf{e}_2\rangle) \right\} \\
 &= \left\{ \frac{1}{\sqrt{2}}(|\mathbf{e}_2\rangle - |\mathbf{e}_1\rangle), \frac{1}{\sqrt{2}}(|\mathbf{e}_1\rangle + |\mathbf{e}_2\rangle) \right\} \\
 &\equiv \left\{ \frac{1}{\sqrt{2}}(-1, 1), \frac{1}{\sqrt{2}}(1, 1) \right\}.
 \end{aligned} \tag{4.106}$$

For a proof of mutually unbiasedness, just form the four inner products of one vector in  $\mathfrak{B}$  times one vector in  $\mathfrak{B}'$ , respectively.

In three-dimensional complex vector space  $\mathbb{C}^3$ , a similar construction from the Cartesian standard basis  $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} \equiv \{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$  yields

$$\begin{aligned}
 \mathfrak{B}' &\equiv \frac{1}{\sqrt{3}} \{ (1, 1, 1), \\
 &\quad \left( \frac{1}{2} [\sqrt{3}i - 1], \frac{1}{2} [-\sqrt{3}i - 1], 1 \right), \\
 &\quad \left( \frac{1}{2} [-\sqrt{3}i - 1], \frac{1}{2} [\sqrt{3}i - 1], 1 \right) \}.
 \end{aligned} \tag{4.107}$$

Nobody knows how to systematically derive and construct a *complete* or *maximal* set of mutually unbiased bases; nor is it clear in general, that is, for arbitrary dimensions, *how many* bases there are in such sets.

#### 4.15 Representation of unity in terms of base vectors

Unity  $\mathbb{I}_n$  in an  $n$ -dimensional vector space  $\mathfrak{V}$  can be represented in terms of the sum over all outer (by another naming tensor or dyadic) products of all vectors of an arbitrary orthonormal basis  $\mathfrak{B} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\} \equiv \{|\mathbf{e}_1\rangle, \dots, |\mathbf{e}_n\rangle\}$ ; that is,

$$\mathbb{I}_n = \sum_{i=1}^n |\mathbf{e}_i\rangle\langle\mathbf{e}_i| \equiv \sum_{i=1}^n \mathbf{e}_i \mathbf{e}_i^\dagger. \tag{4.108}$$

For a proof, consider an arbitrary vector  $|\mathbf{x}\rangle \in \mathfrak{V}$ . Then,

$$\mathbb{I}_n |\mathbf{x}\rangle = \left( \sum_{i=1}^n |\mathbf{e}_i\rangle\langle\mathbf{e}_i| \right) |\mathbf{x}\rangle = \sum_{i=1}^n |\mathbf{e}_i\rangle\langle\mathbf{e}_i|\mathbf{x}\rangle = \sum_{i=1}^n |\mathbf{e}_i\rangle x_i = |\mathbf{x}\rangle. \tag{4.109}$$

Consider, for example, the basis  $\mathfrak{B} = \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle\} \equiv \{(1, 0)^T, (0, 1)^T\}$ . Then the two-dimensional unity  $\mathbb{I}_2$  can be written as

$$\begin{aligned}
 \mathbb{I}_2 &= |\mathbf{e}_1\rangle\langle\mathbf{e}_1| + |\mathbf{e}_2\rangle\langle\mathbf{e}_2| \\
 &= (1, 0)^T (1, 0) + (0, 1)^T (0, 1) = \begin{pmatrix} 1(1, 0) \\ 0(1, 0) \end{pmatrix} + \begin{pmatrix} 0(0, 1) \\ 1(0, 1) \end{pmatrix} \\
 &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.
 \end{aligned} \tag{4.110}$$



Consider, for another example, the basis  $\mathfrak{B}' \equiv \{\frac{1}{\sqrt{2}}(-1, 1)^T, \frac{1}{\sqrt{2}}(1, 1)^T\}$ . Then the two-dimensional unity  $\mathbb{I}_2$  can be written as

$$\begin{aligned}\mathbb{I}_2 &= \frac{1}{\sqrt{2}}(-1, 1)^T \frac{1}{\sqrt{2}}(-1, 1) + \frac{1}{\sqrt{2}}(1, 1)^T \frac{1}{\sqrt{2}}(1, 1) = \frac{1}{2} \begin{pmatrix} -1(-1, 1) \\ 1(-1, 1) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1(1, 1) \\ 1(1, 1) \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.\end{aligned}\tag{4.111}$$

#### 4.16 Rank

The (column or row) *rank*,  $\rho(\mathbf{A})$ , or  $\text{rk}(\mathbf{A})$ , of a linear transformation  $\mathbf{A}$  in an  $n$ -dimensional vector space  $\mathfrak{V}$  is the maximum number of linearly independent (column or, equivalently, row) vectors of the associated  $n$ -by- $n$  square matrix  $A$ , represented by its entries  $a_{ij}$ .

This definition can be generalized to arbitrary  $m$ -by- $n$  matrices  $A$ , represented by its entries  $a_{ij}$ . Then, the row and column ranks of  $A$  are identical; that is,

$$\text{row rk}(A) = \text{column rk}(A) = \text{rk}(A).\tag{4.112}$$

For a proof, consider Mackiw's argument<sup>17</sup>. First we show that  $\text{row rk}(A) \leq \text{column rk}(A)$  for any real (a generalization to complex vector space requires some adjustments)  $m$ -by- $n$  matrix  $A$ . Let the vectors  $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_r\}$  with  $\mathbf{e}_i \in \mathbb{R}^n$ ,  $1 \leq i \leq r$ , be a basis spanning the *row space* of  $A$ ; that is, all vectors that can be obtained by a linear combination of the  $m$  row vectors

$$\begin{pmatrix} (a_{11}, a_{12}, \dots, a_{1n}) \\ (a_{21}, a_{22}, \dots, a_{2n}) \\ \vdots \\ (a_{m1}, a_{m2}, \dots, a_{mn}) \end{pmatrix}$$

of  $A$  can also be obtained as a linear combination of  $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_r$ . Note that  $r \leq m$ .

Now form the *column vectors*  $A\mathbf{e}_i^T$  for  $1 \leq i \leq r$ , that is,  $A\mathbf{e}_1^T, A\mathbf{e}_2^T, \dots, A\mathbf{e}_r^T$  via the usual rules of matrix multiplication. Let us prove that these resulting column vectors  $A\mathbf{e}_i^T$  are linearly independent.

Suppose they were not (proof by contradiction). Then, for some scalars  $c_1, c_2, \dots, c_r \in \mathbb{R}$ ,

$$c_1 A\mathbf{e}_1^T + c_2 A\mathbf{e}_2^T + \dots + c_r A\mathbf{e}_r^T = A(c_1 \mathbf{e}_1^T + c_2 \mathbf{e}_2^T + \dots + c_r \mathbf{e}_r^T) = \mathbf{0}$$

without all  $c_i$ 's vanishing.

That is,  $\mathbf{v} = c_1 \mathbf{e}_1^T + c_2 \mathbf{e}_2^T + \dots + c_r \mathbf{e}_r^T$ , must be in the *null space* of  $A$  defined by all vectors  $\mathbf{x}$  with  $A\mathbf{x} = \mathbf{0}$ , and  $A(\mathbf{v}) = \mathbf{0}$ . (In this case the inner

<sup>17</sup> George Mackiw. A note on the equality of the column and row rank of a matrix. *Mathematics Magazine*, 68(4):pp. 285–286, 1995. ISSN 0025570X. URL <http://www.jstor.org/stable/2690576>

(Euclidean) product of  $\mathbf{x}$  with all the rows of  $A$  must vanish.) But since the  $\mathbf{e}_i$ 's form also a basis of the row vectors,  $\mathbf{v}^T$  is also some vector in the row space of  $A$ . The linear independence of the basis elements  $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_r$  of the row space of  $A$  guarantees that all the coefficients  $c_i$  have to vanish; that is,  $c_1 = c_2 = \dots = c_r = 0$ .

At the same time, as for every vector  $\mathbf{x} \in \mathbb{R}^n$ ,  $A\mathbf{x}$  is a linear combination of the column vectors

$$\left( \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{pmatrix}, \begin{pmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{pmatrix}, \dots, \begin{pmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{pmatrix} \right),$$

the  $r$  linear independent vectors  $A\mathbf{e}_1^T, A\mathbf{e}_2^T, \dots, A\mathbf{e}_r^T$  are all linear combinations of the column vectors of  $A$ . Thus, they are in the column space of  $A$ . Hence,  $r \leq \text{column rk}(A)$ . And, as  $r = \text{row rk}(A)$ , we obtain  $\text{row rk}(A) \leq \text{column rk}(A)$ .

By considering the transposed matrix  $A^T$ , and by an analogous argument we obtain that  $\text{row rk}(A^T) \leq \text{column rk}(A^T)$ . But  $\text{row rk}(A^T) = \text{column rk}(A)$  and  $\text{column rk}(A^T) = \text{row rk}(A)$ , and thus  $\text{row rk}(A^T) = \text{column rk}(A) \leq \text{column rk}(A^T) = \text{row rk}(A)$ . Finally, by considering both estimates  $\text{row rk}(A) \leq \text{column rk}(A)$  as well as  $\text{column rk}(A) \leq \text{row rk}(A)$ , we obtain that  $\text{row rk}(A) = \text{column rk}(A)$ .

## 4.17 Determinant

### 4.17.1 Definition

In what follows, the *determinant* of a matrix  $A$  will be denoted by  $\det A$  or, equivalently, by  $|A|$ .

Suppose  $A = a_{ij}$  is the  $n$ -by- $n$  square matrix representation of a linear transformation  $\mathbf{A}$  in an  $n$ -dimensional vector space  $\mathfrak{V}$ . We shall define its *determinant* in two equivalent ways.

The *Leibniz formula* defines the determinant of the  $n$ -by- $n$  square matrix  $A = a_{ij}$  by

$$\det A = \sum_{\sigma \in S_n} \text{sgn}(\sigma) \prod_{i=1}^n a_{\sigma(i), i}, \quad (4.113)$$

where “sgn” represents the *sign function* of permutations in the permutation group  $S_n$  on  $n$  elements  $\{1, 2, \dots, n\}$ , which returns  $-1$  and  $+1$  for odd and even permutations, respectively.

An equivalent definition

$$\det A = \varepsilon_{i_1 i_2 \dots i_n} a_{1i_1} a_{2i_2} \dots a_{ni_n}, \quad (4.114)$$

makes use of the totally antisymmetric Levi-Civita symbol (5.88) on page 103, and makes use of the Einstein summation convention.

The second, *Laplace formula* definition of the determinant is recursive and expands the determinant in cofactors. It is also called *Laplace expansion*, or *cofactor expansion*. First, a *minor*  $M_{ij}$  of an  $n$ -by- $n$  square matrix  $A$  is defined to be the determinant of the  $(n-1) \times (n-1)$  submatrix that remains after the entire  $i$ th row and  $j$ th column have been deleted from  $A$ .

A *cofactor*  $A_{ij}$  of an  $n$ -by- $n$  square matrix  $A$  is defined in terms of its associated minor by

$$A_{ij} = (-1)^{i+j} M_{ij}. \quad (4.115)$$

The *determinant* of a square matrix  $A$ , denoted by  $\det A$  or  $|A|$ , is a scalar rekursively defined by

$$\det A = \sum_{j=1}^n a_{ij} A_{ij} = \sum_{i=1}^n a_{ij} A_{ij} \quad (4.116)$$

for any  $i$  (row expansion) or  $j$  (column expansion), with  $i, j = 1, \dots, n$ . For  $1 \times 1$  matrices (i.e., scalars),  $\det A = a_{11}$ .

#### 4.17.2 Properties

The following properties of determinants are mentioned (almost) without proof:

- (i) If  $A$  and  $B$  are square matrices of the same order, then  $\det AB = (\det A)(\det B)$ .
- (ii) If either two rows or two columns are exchanged, then the determinant is multiplied by a factor “ $-1$ .”
- (iii) The determinant of the transposed matrix is equal to the determinant of the original matrix; that is,  $\det(A^T) = \det A$ .
- (iv) The determinant  $\det A$  of a matrix  $A$  is nonzero if and only if  $A$  is invertible. In particular, if  $A$  is not invertible,  $\det A = 0$ . If  $A$  has an inverse matrix  $A^{-1}$ , then  $\det(A^{-1}) = (\det A)^{-1}$ .

This is a very important property which we shall use in Eq. (4.156) on page 63 for the determination of nontrivial eigenvalues  $\lambda$  (including the associated eigenvectors) of a matrix  $A$  by solving the secular equation  $\det(A - \lambda \mathbb{I}) = 0$ .

- (v) Multiplication of any row or column with a factor  $\alpha$  results in a determinant which is  $\alpha$  times the original determinant. Consequently, multiplication of an  $n \times n$  matrix with a scalar  $\alpha$  results in a determinant which is  $\alpha^n$  times the original determinant.
- (vi) The determinant of a unit matrix is one; that is,  $\det \mathbb{I}_n = 1$ . Likewise, the determinat of a diagonal matrix is just the product of the diagonal entries; that is,  $\det[\text{diag}(\lambda_1, \dots, \lambda_n)] = \lambda_1 \cdots \lambda_n$ .

- (vii) The determinant is not changed if a multiple of an existing row is added to another row.

This can be easily demonstrated by considering the Leibniz formula: suppose a multiple  $\alpha$  of the  $j$ 'th column is added to the  $k$ 'th column since

$$\begin{aligned} & \varepsilon_{i_1 i_2 \dots i_j \dots i_k \dots i_n} a_{1i_1} a_{2i_2} \dots a_{ji_j} \dots (a_{ki_k} + \alpha a_{ji_k}) \dots a_{ni_n} \\ &= \varepsilon_{i_1 i_2 \dots i_j \dots i_k \dots i_n} a_{1i_1} a_{2i_2} \dots a_{ji_j} \dots a_{ki_k} \dots a_{ni_n} + \\ & \quad \alpha \varepsilon_{i_1 i_2 \dots i_j \dots i_k \dots i_n} a_{1i_1} a_{2i_2} \dots a_{ji_j} \dots a_{ji_k} \dots a_{ni_n}. \end{aligned} \quad (4.117)$$

The second summation term vanishes, since  $a_{ji_j} a_{ji_k} = a_{ji_k} a_{ji_j}$  is totally symmetric in the indices  $i_j$  and  $i_k$ , and the Levi-Civita symbol  $\varepsilon_{i_1 i_2 \dots i_j \dots i_k \dots i_n}$ .

- (viii) The absolute value of the determinant of a square matrix  $A = (\mathbf{e}_1, \dots, \mathbf{e}_n)$  formed by (not necessarily orthogonal) row (or column) vectors of a basis  $\mathfrak{B} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  is equal to the *volume* of the parallelepiped  $\{\mathbf{x} \mid \mathbf{x} = \sum_{i=1}^n t_i \mathbf{e}_i, 0 \leq t_i \leq 1, 0 \leq i \leq n\}$  formed by those vectors.

This can be demonstrated by supposing that the square matrix  $A$  consists of all the  $n$  row (column) vectors of an orthogonal basis of dimension  $n$ . Then  $AA^T = A^T A$  is a diagonal matrix which just contains the square of the length of all the basis vectors forming a perpendicular parallelepiped which is just an  $n$  dimensional box. Therefore the volume is just the positive square root of  $\det(AA^T) = (\det A)(\det A^T) = (\det A)(\det A) = (\det A)^2$ .

For any nonorthogonal basis all we need to employ is a Gram-Schmidt process to obtain a (perpendicular) box of equal volume to the original parallelepiped formed by the nonorthogonal basis vectors – any volume that is cut is compensated by adding the same amount to the new volume. Note that the Gram-Schmidt process operates by adding (subtracting) the projections of already existing orthogonalized vectors from the old basis vectors (to render these sums orthogonal to the existing vectors of the new orthogonal basis); a process which does not change the determinant.

This result can be used for changing the differential volume element in integrals *via* the Jacobian matrix  $J$  (5.20), as

$$dx'_1 dx'_2 \dots dx'_n = |\det J| dx_1 dx_2 \dots dx_n = \sqrt{\left[ \det \left( \frac{dx'_i}{dx_j} \right) \right]^2} dx_1 dx_2 \dots dx_n. \quad (4.118)$$

- (ix) The *sign* of a determinant of a matrix formed by the row (column) vectors of a basis indicates the orientation of that basis.

see, for instance, Section 4.3 of Strang's account

Gilbert Strang. *Introduction to linear algebra*. Wellesley-Cambridge Press, Wellesley, MA, USA, fourth edition, 2009. ISBN 0-9802327-1-6. URL <http://math.mit.edu/linearalgebra/>

## 4.18 Trace

### 4.18.1 Definition

The *trace* of an  $n$ -by- $n$  square matrix  $A = a_{ij}$ , denoted by  $\text{Tr} A$ , is a scalar defined to be the sum of the elements on the main diagonal (the diagonal from the upper left to the lower right) of  $A$ ; that is (also in Dirac's bra and ket notation),

$$\text{Tr} A = a_{11} + a_{22} + \cdots + a_{nn} = \sum_{i=1}^n a_{ii} = \sum_{i=1}^n \langle i | A | i \rangle. \quad (4.119)$$

The German word for trace is *Spur*.

In quantum mechanics, traces can be realized *via* an orthonormal basis  $\mathfrak{B} = \{\mathbf{e}_1, \dots, \mathbf{e}_n\}$  by “sandwiching” an operator  $\mathbf{A}$  between all basis elements – thereby effectively taking the diagonal components of  $\mathbf{A}$  with respect to the basis  $\mathfrak{B}$  – and summing over all these scalar components; that is,

$$\text{Tr} \mathbf{A} = \sum_{i=1}^n \langle \mathbf{e}_i | \mathbf{A} | \mathbf{e}_i \rangle = \sum_{i=1}^n \langle \mathbf{e}_i | \mathbf{A} \mathbf{e}_i \rangle. \quad (4.120)$$

### 4.18.2 Properties

The following properties of traces are mentioned without proof:

- (i)  $\text{Tr}(A + B) = \text{Tr} A + \text{Tr} B$ ;
- (ii)  $\text{Tr}(\alpha A) = \alpha \text{Tr} A$ , with  $\alpha \in \mathbb{C}$ ;
- (iii)  $\text{Tr}(AB) = \text{Tr}(BA)$ , hence the trace of the commutator vanishes; that is,  $\text{Tr}([A, B]) = 0$ ;
- (iv)  $\text{Tr} A = \text{Tr} A^T$ ;
- (v)  $\text{Tr}(A \otimes B) = (\text{Tr} A)(\text{Tr} B)$ ;
- (vi) the trace is the sum of the eigenvalues of a *normal operator* (cf. page 66);
- (vii)  $\det(e^A) = e^{\text{Tr} A}$ ;
- (viii) the trace is the derivative of the determinant at the identity;
- (ix) the complex conjugate of the trace of an operator is equal to the trace of its adjoint (cf. page 56); that is  $\overline{(\text{Tr} A)} = \text{Tr}(A^\dagger)$ ;
- (x) the trace is invariant under rotations of the basis as well as under cyclic permutations.
- (xi) the trace of an  $n \times n$  matrix  $A$  for which  $AA = \alpha A$  for some  $\alpha \in \mathbb{R}$  is  $\text{Tr} A = \alpha \text{rank}(A)$ , where rank is the rank of  $A$  defined on page 50. Consequently, the trace of an idempotent (with  $\alpha = 1$ ) operator – that is, a projection – is equal to its rank; and, in particular, the trace of a one-dimensional projection is one.

A *trace class* operator is a compact operator for which a trace is finite and independent of the choice of basis.

#### 4.18.3 Partial trace

The quantum mechanics of multi-particle (multipartite) systems allows for configurations – actually rather processes – that can be informally described as “beam dump experiments;” in which we start out with entangled states (such as the Bell states on page 38) which carry information about *joint properties of the constituent quanta* and *choose to disregard* one quantum state entirely; that is, we pretend not to care of the (possible) outcomes of a measurement on this particle. In this case, we have to *trace out* that particle; and as a result we obtain a *reduced state* without this particle we do not care about.

For an example’s sake, consider the Bell state  $|\Psi^-\rangle$  defined in Eq. (4.59). Suppose we do not care about the state of the first particle, then we may ask what kind of reduced state results from this pretension. Then the partial trace is just the trace over the first particle; that is, with subscripts referring to the particle number,

$$\begin{aligned}
 & \text{Tr}_1 |\Psi^-\rangle\langle\Psi^-| \\
 &= \sum_{i_1=0}^1 \langle i_1|\Psi^-\rangle\langle\Psi^-|i_1\rangle \\
 &= \langle 0_1|\Psi^-\rangle\langle\Psi^-|0_1\rangle + \langle 1_1|\Psi^-\rangle\langle\Psi^-|1_1\rangle \\
 &= \langle 0_1|\frac{1}{\sqrt{2}}(|0_1 1_2\rangle - |1_1 0_2\rangle)\frac{1}{\sqrt{2}}(\langle 0_1 1_2| - \langle 1_1 0_2|)|0_1\rangle \\
 &\quad + \langle 1_1|\frac{1}{\sqrt{2}}(|0_1 1_2\rangle - |1_1 0_2\rangle)\frac{1}{\sqrt{2}}(\langle 0_1 1_2| - \langle 1_1 0_2|)|1_1\rangle \\
 &= \frac{1}{2}(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|).
 \end{aligned} \tag{4.121}$$

The resulting state is a *mixed state* defined by the property that its trace is equal to one, but the trace of its square is smaller than one; in this case the trace is  $\frac{1}{2}$ , because

$$\begin{aligned}
 & \text{Tr}_2 \frac{1}{2}(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|) \\
 &= \frac{1}{2}\langle 0_2|(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|)|0_2\rangle + \frac{1}{2}\langle 1_2|(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|)|1_2\rangle \\
 &= \frac{1}{2} + \frac{1}{2} = 1;
 \end{aligned} \tag{4.122}$$

but

$$\begin{aligned}
 & \text{Tr}_2 \left[ \frac{1}{2}(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|) \frac{1}{2}(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|) \right] \\
 &= \text{Tr}_2 \frac{1}{4}(|1_2\rangle\langle 1_2| + |0_2\rangle\langle 0_2|) = \frac{1}{2}.
 \end{aligned} \tag{4.123}$$

The same is true for all elements of the Bell basis. Be careful here to make the experiment in such a way that in no way you could know the state of the first particle. You may actually think about this as a measurement of the state of the first particle by a degenerate observable with only a single, nondiscriminating measurement outcome.

This *mixed state* is a 50:50 mixture of the pure particle states  $|0_2\rangle$  and  $|1_2\rangle$ , respectively. Note that this is different from a coherent superposition  $|0_2\rangle + |1_2\rangle$  of the pure particle states  $|0_2\rangle$  and  $|1_2\rangle$ , respectively – also formalizing a 50:50 mixture with respect to measurements of property 0 *versus* 1, respectively.

## 4.19 Adjoint

### 4.19.1 Definition

Let  $\mathfrak{V}$  be a vector space and let  $\mathbf{y}$  be any element of its dual space  $\mathfrak{V}^*$ . For any linear transformation  $\mathbf{A}$ , consider the bilinear functional  $\mathbf{y}'(\mathbf{x}) = [\mathbf{x}, \mathbf{y}'] = [\mathbf{Ax}, \mathbf{y}]$ . Let the *adjoint* transformation  $\mathbf{A}^\dagger$  be defined by

$$[\mathbf{x}, \mathbf{A}^* \mathbf{y}] = [\mathbf{Ax}, \mathbf{y}]. \quad (4.124)$$

In real inner product spaces,

$$[\mathbf{x}, \mathbf{A}^T \mathbf{y}] = [\mathbf{Ax}, \mathbf{y}]. \quad (4.125)$$

In complex inner product spaces,

$$[\mathbf{x}, \mathbf{A}^\dagger \mathbf{y}] = [\mathbf{Ax}, \mathbf{y}]. \quad (4.126)$$

Here  $[\cdot, \cdot]$  is the bilinear functional, not the commutator.

### 4.19.2 Properties

We mention without proof that the adjoint operator is a linear operator. Furthermore,  $\mathbf{0}^\dagger = \mathbf{0}$ ,  $\mathbf{1}^\dagger = \mathbf{1}$ ,  $(\mathbf{A} + \mathbf{B})^\dagger = \mathbf{A}^\dagger + \mathbf{B}^\dagger$ ,  $(\alpha \mathbf{A})^\dagger = \alpha \mathbf{A}^\dagger$ ,  $(\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger$ , and  $(\mathbf{A}^{-1})^\dagger = (\mathbf{A}^\dagger)^{-1}$ ; as well as (in finite dimensional spaces)

$$\mathbf{A}^{\dagger\dagger} = \mathbf{A}. \quad (4.127)$$

### 4.19.3 Adjoint matrix notation

In matrix notation and in complex vector space with the dot product, note that there is a correspondence with the inner product (cf. page 33) so that, for all  $\mathbf{z} \in \mathfrak{V}$  and for all  $\mathbf{x} \in \mathfrak{V}$ , there exist a unique  $\mathbf{y} \in \mathfrak{V}$  with

$$\begin{aligned} [\mathbf{Ax}, \mathbf{z}] &= \langle \mathbf{Ax} | \mathbf{y} \rangle = \overline{\langle \mathbf{y} | \mathbf{Ax} \rangle} \\ &= \overline{(\overline{y_i}) \overline{A_{ij}} \overline{x_j}} = y_i \overline{A_{ij}} \overline{x_j} = y_i \overline{A_{ji}}^T \overline{x_j} = \overline{x} \overline{A}^T y, \end{aligned} \quad (4.128)$$

and another unique vector  $\mathbf{y}'$  obtained from  $\mathbf{y}$  by some linear operator  $\mathbf{A}^\dagger$  such that  $\mathbf{y}' = \mathbf{A}^\dagger \mathbf{y}$  with

$$\begin{aligned} [\mathbf{x}, \mathbf{A}^\dagger \mathbf{z}] &= \langle \mathbf{x} | \mathbf{y}' \rangle = \langle \mathbf{x} | \mathbf{A}^\dagger \mathbf{y} \rangle \\ &= \overline{x_i} A_{ij}^\dagger y_j = \overline{x} A^\dagger y; \end{aligned} \quad (4.129)$$

and therefore

$$A^\dagger = (\overline{A})^T = \overline{A}^T, \text{ or } A_{ij}^\dagger = \overline{A_{ji}}. \quad (4.130)$$

In words: in matrix notation, the adjoint transformation is just the transpose of the complex conjugate of the original matrix.

#### 4.20 Self-adjoint transformation

The following definition yields some analogy to real numbers as compared to complex numbers (“a complex number  $z$  is real if  $\bar{z} = z$ ”), expressed in terms of operators on a complex vector space.

An operator  $\mathbf{A}$  on a linear vector space  $\mathfrak{V}$  is called *self-adjoint*, if

$$\mathbf{A}^* = \mathbf{A} \quad (4.131)$$

and if the domains of  $\mathbf{A}$  and  $\mathbf{A}^*$  – that is, the set of vectors on which they are well defined – coincide.

In finite dimensional *real* inner product spaces, self-adjoint operators are called *symmetric*, since they are symmetric with respect to transpositions; that is,

$$\mathbf{A}^* = \mathbf{A}^T = \mathbf{A}. \quad (4.132)$$

In finite dimensional *complex* inner product spaces, self-adjoint operators are called *Hermitian*, since they are identical with respect to Hermitian conjugation (transposition of the matrix and complex conjugation of its entries); that is,

$$\mathbf{A}^* = \mathbf{A}^\dagger = \mathbf{A}. \quad (4.133)$$

In what follows, we shall consider only the latter case and identify self-adjoint operators with Hermitian ones. In terms of matrices, a matrix  $A$  corresponding to an operator  $\mathbf{A}$  in some fixed basis is self-adjoint if

$$A^\dagger \equiv (\overline{A_{ij}})^T = \overline{A_{ji}} = A_{ij} \equiv A. \quad (4.134)$$

That is, suppose  $A_{ij}$  is the matrix representation corresponding to a linear transformation  $\mathbf{A}$  in some basis  $\mathfrak{B}$ , then the *Hermitian* matrix  $\mathbf{A}^* = \mathbf{A}^\dagger$  to the dual basis  $\mathfrak{B}^*$  is  $(\overline{A_{ij}})^T$ .

For the sake of an example, consider again the *Pauli spin matrices*

$$\begin{aligned} \sigma_1 = \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma_2 = \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \sigma_3 = \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (4.135)$$

which, together with unity, i.e.,  $\mathbb{1}_2 = \text{diag}(1, 1)$ , are all self-adjoint.

The following operators are not self-adjoint:

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix}, \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}. \quad (4.136)$$

For infinite dimensions, a distinction must be made between self-adjoint operators and Hermitian ones; see, for instance,

Dietrich Grau. *Übungsaufgaben zur Quantentheorie*. Karl Thiemeig, Karl Hanser, München, 1975, 1993, 2005. URL <http://www.dietrich-grau.at>; François Gieres. Mathematical surprises and Dirac's formalism in quantum mechanics. *Reports on Progress in Physics*, 63(12):1893–1931, 2000. DOI: <http://dx.doi.org/10.1088/0034-4885/63/12/201>. URL [10.1088/0034-4885/63/12/201](https://doi.org/10.1088/0034-4885/63/12/201); and Guy Bonneau, Jacques Faraut, and Galliano Valent. Self-adjoint extensions of operators and the teaching of quantum mechanics. *American Journal of Physics*, 69(3):322–331, 2001. DOI: [10.1119/1.1328351](https://doi.org/10.1119/1.1328351). URL <http://dx.doi.org/10.1119/1.1328351>



Note that the coherent real-valued superposition of a self-adjoint transformations (such as the sum or difference of correlations in the Clauser-Horne-Shimony-Holt expression<sup>18</sup>) is a self-adjoint transformation.

For a direct proof, suppose that  $\alpha_i \in \mathbb{R}$  for all  $1 \leq i \leq n$  are  $n$  real-valued coefficients and  $\mathbf{A}_1, \dots, \mathbf{A}_n$  are  $n$  self-adjoint operators. Then  $\mathbf{B} = \sum_{i=1}^n \alpha_i \mathbf{A}_i$  is self-adjoint, since

$$\mathbf{B}^* = \sum_{i=1}^n \overline{\alpha_i} \mathbf{A}_i^* = \sum_{i=1}^n \alpha_i \mathbf{A}_i = \mathbf{B}. \quad (4.137)$$

#### 4.21 Positive transformation

A linear transformation  $\mathbf{A}$  on an inner product space  $\mathfrak{V}$  is *positive*, that is in symbols  $\mathbf{A} \geq 0$ , if it is self-adjoint, and if  $\langle \mathbf{A}\mathbf{x} | \mathbf{x} \rangle \geq 0$  for all  $\mathbf{x} \in \mathfrak{V}$ . If  $\langle \mathbf{A}\mathbf{x} | \mathbf{x} \rangle = 0$  implies  $\mathbf{x} = 0$ ,  $\mathbf{A}$  is called *strictly positive*.

#### 4.22 Permutation

Permutation (matrices) are the “classical analogues”<sup>19</sup> of unitary transformations (matrices) which will be introduced later on page 59. The permutation matrices are defined by the requirement that they only contain a single nonvanishing entry “1” per row and column; all the other row and column entries vanish “0.” For example, the matrices  $\mathbb{I}_n = \text{diag}(\underbrace{1, \dots, 1}_{n \text{ times}})$ , or

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \text{ or } \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

are permutation matrices.

Note that from the definition and from matrix multiplication follows that, if  $P$  is a permutation matrix, then  $PP^T = P^T P = \mathbb{I}_n$ . That is,  $P^T$  represents the inverse element of  $P$ . As  $P$  is real-valued, it is a *normal operator* (cf. page 66).

Note further that any permutation matrix can be interpreted in terms of row and column vectors. The set of all these row and column vectors constitute the Cartesian standard basis of  $n$ -dimensional vector space, with permuted elements.

Note also that, if  $P$  and  $Q$  are permutation matrices, so is  $PQ$  and  $QP$ . The set of all  $n!$  permutation ( $n \times n$ )–matrices corresponding to permutations of  $n$  elements of  $\{1, 2, \dots, n\}$  form the *symmetric group*  $S_n$ , with  $\mathbb{I}_n$  being the identity element.

<sup>18</sup> Stefan Filipp and Karl Svozil. Generalizing Tsirelson's bound on Bell inequalities using a min-max principle. *Physical Review Letters*, 93:130407, 2004. DOI: 10.1103/PhysRevLett.93.130407. URL <http://dx.doi.org/10.1103/PhysRevLett.93.130407>

<sup>19</sup> David N. Mermin. Lecture notes on quantum computation. 2002-2008. URL <http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html>; and David N. Mermin. *Quantum Computer Science*. Cambridge University Press, Cambridge, 2007. ISBN 9780521876582. URL <http://people.ccmr.cornell.edu/~mermin/qcomp/CS483.html>

### 4.23 Orthonormal (orthogonal) transformations

An *orthonormal* or *orthogonal transformation*  $\mathbf{R}$  is a linear transformation whose corresponding square matrix  $R$  has real-valued entries and mutually orthogonal, normalized row (or, equivalently, column) vectors. As a consequence,

$$RR^T = R^T R = \mathbb{I}, \text{ or } R^{-1} = R^T. \quad (4.138)$$

If  $\det R = 1$ ,  $\mathbf{R}$  corresponds to a *rotation*. If  $\det R = -1$ ,  $\mathbf{R}$  corresponds to a rotation and a *reflection*. A reflection is an isometry (a distance preserving map) with a hyperplane as set of fixed points.

Orthonormal transformations  $\mathbf{R}$  are “real valued cases” of the more general unitary transformations discussed next. They preserve a symmetric inner product; that is,  $\langle \mathbf{R}\mathbf{x} | \mathbf{R}\mathbf{y} \rangle = \langle \mathbf{x} | \mathbf{y} \rangle$  for all  $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$

As a two-dimensional example of rotations in the plane  $\mathbb{R}^2$ , take the rotation matrix in Eq. (4.99) representing a rotation of the basis by an angle  $\varphi$ .

Permutation matrices represent orthonormal transformations.

### 4.24 Unitary transformations and isometries

#### 4.24.1 Definition

Note that a complex number  $z$  has absolute value one if  $\bar{z} = 1/z$ , or  $z\bar{z} = 1$ . In analogy to this “modulus one” behavior, consider *unitary transformations*, or, used synonymously, *(one-to-one) isometries*  $\mathbf{U}$  for which

$$\mathbf{U}^* = \mathbf{U}^\dagger = \mathbf{U}^{-1}, \text{ or } \mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbb{I}. \quad (4.139)$$

Alternatively, we mention without proof that the following conditions are equivalent:

- (i)  $\langle \mathbf{U}\mathbf{x} | \mathbf{U}\mathbf{y} \rangle = \langle \mathbf{x} | \mathbf{y} \rangle$  for all  $\mathbf{x}, \mathbf{y} \in \mathfrak{V}$ ;
- (ii)  $\|\mathbf{U}\mathbf{x}\| = \|\mathbf{x}\|$  for all  $\mathbf{x} \in \mathfrak{V}$ ;

Unitary transformations can also be defined via *permutations preserving the scalar product*. That is, functions such as  $f : x \mapsto x' = \alpha x$  with  $\alpha \neq e^{i\varphi}$ ,  $\varphi \in \mathbb{R}$ , do not correspond to a unitary transformation in a one-dimensional Hilbert space, as the scalar product  $f : \langle x|y \rangle \mapsto \langle x'|y' \rangle = |\alpha|^2 \langle x|y \rangle$  is not preserved; whereas if  $\alpha$  is a modulus of one; that is, with  $\alpha = e^{i\varphi}$ ,  $\varphi \in \mathbb{R}$ ,  $|\alpha|^2 = 1$ , and the scalar product is preserved. Thus,  $u : x \mapsto x' = e^{i\varphi} x$ ,  $\varphi \in \mathbb{R}$ , represents a unitary transformation.

#### 4.24.2 Characterization of change of orthonormal basis

Let  $\mathfrak{B} = \{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  be an orthonormal basis of an  $n$ -dimensional inner product space  $\mathfrak{V}$ . If  $\mathbf{U}$  is an isometry, then  $\mathbf{U}\mathfrak{B} = \{\mathbf{U}\mathbf{f}_1, \mathbf{U}\mathbf{f}_2, \dots, \mathbf{U}\mathbf{f}_n\}$  is also an orthonormal basis of  $\mathfrak{V}$ . (The converse is also true.)

For proofs and additional information see §73 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

#### 4.24.3 Characterization in terms of orthonormal basis

A complex matrix  $\mathbf{U}$  is unitary if and only if its row (or column) vectors form an orthonormal basis.

This can be readily verified<sup>20</sup> by writing  $\mathbf{U}$  in terms of two orthonormal bases  $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$   $\mathfrak{B}' = \{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  as

$$\mathbf{U}_{ef} = \sum_{i=1}^n \mathbf{e}_i^\dagger \mathbf{f}_i = \sum_{i=1}^n |\mathbf{e}_i\rangle \langle \mathbf{f}_i|. \quad (4.140)$$

Together with  $\mathbf{U}_{fe} = \sum_{i=1}^n \mathbf{f}_i^\dagger \mathbf{e}_i = \sum_{i=1}^n |\mathbf{f}_i\rangle \langle \mathbf{e}_i|$  we form

$$\begin{aligned} & \mathbf{e}_k \mathbf{U}_{ef} \\ &= \mathbf{e}_k \sum_{i=1}^n \mathbf{e}_i^\dagger \mathbf{f}_i \\ &= \sum_{i=1}^n (\mathbf{e}_k \mathbf{e}_i^\dagger) \mathbf{f}_i \\ &= \sum_{i=1}^n \delta_{ki} \mathbf{f}_i \\ &= \mathbf{f}_k. \end{aligned} \quad (4.141)$$

In a similar way we find that

$$\begin{aligned} \mathbf{U}_{ef} \mathbf{f}_k^\dagger &= \mathbf{e}_k^\dagger, \\ \mathbf{f}_k \mathbf{U}_{fe} &= \mathbf{e}_k, \\ \mathbf{U}_{fe} \mathbf{e}_k^\dagger &= \mathbf{f}_k^\dagger. \end{aligned} \quad (4.142)$$

Moreover,

$$\begin{aligned} & \mathbf{U}_{ef} \mathbf{U}_{fe} \\ &= \sum_{i=1}^n \sum_{j=1}^n (|\mathbf{e}_i\rangle \langle \mathbf{f}_i|) (|\mathbf{f}_j\rangle \langle \mathbf{e}_j|) \\ &= \sum_{i=1}^n \sum_{j=1}^n |\mathbf{e}_i\rangle \delta_{ij} \langle \mathbf{e}_j| \\ &= \sum_{i=1}^n |\mathbf{e}_i\rangle \langle \mathbf{e}_i| \\ &= \mathbb{I}. \end{aligned} \quad (4.143)$$

In a similar way we obtain  $\mathbf{U}_{fe} \mathbf{U}_{ef} = \mathbb{I}$ . Since

$$\mathbf{U}_{ef}^\dagger = \sum_{i=1}^n \mathbf{f}_i^\dagger (\mathbf{e}_i^\dagger)^\dagger = \sum_{i=1}^n \mathbf{f}_i^\dagger \mathbf{e}_i = \mathbf{U}_{fe}, \quad (4.144)$$

we obtain that  $\mathbf{U}_{ef}^\dagger = (\mathbf{U}_{ef})^{-1}$  and  $\mathbf{U}_{fe}^\dagger = (\mathbf{U}_{fe})^{-1}$ .

Note also that the *composition* holds; that is,  $\mathbf{U}_{ef} \mathbf{U}_{fg} = \mathbf{U}_{eg}$ .

If we identify one of the bases  $\mathfrak{B}$  and  $\mathfrak{B}'$  by the Cartesian standard basis, it becomes clear that, for instance, every unitary operator  $\mathbf{U}$  can be written

<sup>20</sup> Julian Schwinger. Unitary operators bases. *Proceedings of the National Academy of Sciences (PNAS)*, 46:570–579, 1960. DOI: 10.1073/pnas.46.4.570. URL <http://dx.doi.org/10.1073/pnas.46.4.570>

in terms of an orthonormal basis  $\mathfrak{B} = \{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  by “stacking” the vectors of that orthonormal basis “on top of each other;” that is

$$\mathbf{U} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{pmatrix}. \quad (4.145)$$

Thereby the vectors of the orthonormal basis  $\mathfrak{B}$  serve as the rows of  $\mathbf{U}$ .

Also, every unitary operator  $\mathbf{U}$  can be written in terms of an orthonormal basis  $\mathfrak{B} = \{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  by “pasting” the (transposed) vectors of that orthonormal basis “one after another;” that is

$$\mathbf{U} = (\mathbf{f}_1^T, \mathbf{f}_2^T, \dots, \mathbf{f}_n^T). \quad (4.146)$$

Thereby the (transposed) vectors of the orthonormal basis  $\mathfrak{B}$  serve as the columns of  $\mathbf{U}$ .

Note also that any permutation of vectors in  $\mathfrak{B}$  would also yield unitary matrices.

#### 4.25 Perpendicular projections

*Perpendicular projections* are associated with a *direct sum decomposition* of the vector space  $\mathfrak{V}$ ; that is,

$$\mathfrak{M} \oplus \mathfrak{M}^\perp = \mathfrak{V}. \quad (4.147)$$

Let  $\mathbf{E} = P_{\mathfrak{M}}$  denote the projection on  $\mathfrak{M}$  along  $\mathfrak{M}^\perp$ . The following propositions are stated without proof.

A linear transformation  $\mathbf{E}$  is a perpendicular projection if and only if  $\mathbf{E} = \mathbf{E}^2 = \mathbf{E}^*$ .

Perpendicular projections are *positive* linear transformations, with  $\|\mathbf{E}\mathbf{x}\| \leq \|\mathbf{x}\|$  for all  $\mathbf{x} \in \mathfrak{V}$ . Conversely, if a linear transformation  $\mathbf{E}$  is idempotent; that is,  $\mathbf{E}^2 = \mathbf{E}$ , and  $\|\mathbf{E}\mathbf{x}\| \leq \|\mathbf{x}\|$  for all  $\mathbf{x} \in \mathfrak{V}$ , then  $\mathbf{E}$  is self-adjoint; that is,  $\mathbf{E} = \mathbf{E}^*$ .

Recall that for *real* inner product spaces, the self-adjoint operator can be identified with a *symmetric* operator  $\mathbf{E} = \mathbf{E}^T$ , whereas for *complex* inner product spaces, the self-adjoint operator can be identified with a *Hermitean* operator  $\mathbf{E} = \mathbf{E}^\dagger$ .

If  $\mathbf{E}_1, \mathbf{E}_2, \dots, \mathbf{E}_n$  are (perpendicular) projections, then a necessary and sufficient condition that  $\mathbf{E} = \mathbf{E}_1 + \mathbf{E}_2 + \dots + \mathbf{E}_n$  be a (perpendicular) projection is that  $\mathbf{E}_i \mathbf{E}_j = \delta_{ij} \mathbf{E}_i = \delta_{ij} \mathbf{E}_j$ ; and, in particular,  $\mathbf{E}_i \mathbf{E}_j = 0$  whenever  $i \neq j$ ; that is, that all  $\mathbf{E}_i$  are pairwise orthogonal.

For a start, consider just two projections  $\mathbf{E}_1$  and  $\mathbf{E}_2$ . Then we can assert that  $\mathbf{E}_1 + \mathbf{E}_2$  is a projection if and only if  $\mathbf{E}_1 \mathbf{E}_2 = \mathbf{E}_2 \mathbf{E}_1 = 0$ .

For a quantum mechanical application, see

M. Reck, Anton Zeilinger, H. J. Bernstein, and P. Bertani. Experimental realization of any discrete unitary operator. *Physical Review Letters*, 73:58–61, 1994. DOI: 10.1103/PhysRevLett.73.58. URL <http://dx.doi.org/10.1103/PhysRevLett.73.58>

For proofs and additional information see §5.11.3, Theorem 5.1.5 and subsequent Corollary in

Satish D. Joglekar. *Mathematical Physics: The Basics*. CRC Press, Boca Raton, Florida, 2007

For proofs and additional information see §42, §75 & §76 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Because, for  $\mathbf{E}_1 + \mathbf{E}_2$  to be a projection, it must be idempotent; that is,

$$(\mathbf{E}_1 + \mathbf{E}_2)^2 = (\mathbf{E}_1 + \mathbf{E}_2)(\mathbf{E}_1 + \mathbf{E}_2) = \mathbf{E}_1^2 + \mathbf{E}_1\mathbf{E}_2 + \mathbf{E}_2\mathbf{E}_1 + \mathbf{E}_2^2 = \mathbf{E}_1 + \mathbf{E}_2. \quad (4.148)$$

As a consequence, the cross-product terms in (4.148) must vanish; that is,

$$\mathbf{E}_1\mathbf{E}_2 + \mathbf{E}_2\mathbf{E}_1 = 0. \quad (4.149)$$

Multiplication of (4.149) with  $\mathbf{E}_1$  from the left and from the right yields

$$\begin{aligned} \mathbf{E}_1\mathbf{E}_1\mathbf{E}_2 + \mathbf{E}_1\mathbf{E}_2\mathbf{E}_1 &= 0, \\ \mathbf{E}_1\mathbf{E}_2 + \mathbf{E}_1\mathbf{E}_2\mathbf{E}_1 &= 0; \text{ and} \\ \mathbf{E}_1\mathbf{E}_2\mathbf{E}_1 + \mathbf{E}_2\mathbf{E}_1\mathbf{E}_1 &= 0, \\ \mathbf{E}_1\mathbf{E}_2\mathbf{E}_1 + \mathbf{E}_2\mathbf{E}_1 &= 0. \end{aligned} \quad (4.150)$$

Subtraction of the resulting pair of equations yields

$$\mathbf{E}_1\mathbf{E}_2 - \mathbf{E}_2\mathbf{E}_1 = [\mathbf{E}_1, \mathbf{E}_2] = 0, \quad (4.151)$$

or

$$\mathbf{E}_1\mathbf{E}_2 = \mathbf{E}_2\mathbf{E}_1. \quad (4.152)$$

Hence, in order for the cross-product terms in Eqs. (4.148) and (4.149) to vanish, we must have

$$\mathbf{E}_1\mathbf{E}_2 = \mathbf{E}_2\mathbf{E}_1 = 0. \quad (4.153)$$

Proving the reverse statement is straightforward, since (4.153) implies (4.148).

A generalisation by induction to more than two projections is straightforward, since, for instance,  $(\mathbf{E}_1 + \mathbf{E}_2)\mathbf{E}_3 = 0$  implies  $\mathbf{E}_1\mathbf{E}_3 + \mathbf{E}_2\mathbf{E}_3 = 0$ .

Multiplication with  $\mathbf{E}_1$  from the left yields  $\mathbf{E}_1\mathbf{E}_1\mathbf{E}_3 + \mathbf{E}_1\mathbf{E}_2\mathbf{E}_3 = \mathbf{E}_1\mathbf{E}_3 = 0$ .

## 4.26 Proper value or eigenvalue

### 4.26.1 Definition

A scalar  $\lambda$  is a *proper value* or *eigenvalue*, and a nonzero vector  $\mathbf{x}$  is a *proper vector* or *eigenvector* of a linear transformation  $\mathbf{A}$  if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} = \lambda\mathbb{I}\mathbf{x}. \quad (4.154)$$

In an  $n$ -dimensional vector space  $\mathfrak{V}$  The set of the set of eigenvalues and the set of the associated eigenvectors  $\{\{\lambda_1, \dots, \lambda_k\}, \{\mathbf{x}_1, \dots, \mathbf{x}_n\}\}$  of a linear transformation  $\mathbf{A}$  form an *eigensystem* of  $\mathbf{A}$ .

### 4.26.2 Determination

Since the eigenvalues and eigenvectors are those scalars  $\lambda$  vectors  $\mathbf{x}$  for which  $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ , this equation can be rewritten with a zero vector on the

For proofs and additional information see §54 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

right side of the equation; that is ( $\mathbb{I} = \text{diag}(1, \dots, 1)$  stands for the identity matrix),

$$(\mathbf{A} - \lambda \mathbb{I})\mathbf{x} = \mathbf{0}. \quad (4.155)$$

Suppose that  $\mathbf{A} - \lambda \mathbb{I}$  is invertible. Then we could formally write  $\mathbf{x} = (\mathbf{A} - \lambda \mathbb{I})^{-1}\mathbf{0}$ ; hence  $\mathbf{x}$  must be the zero vector.

We are not interested in this trivial solution of Eq. (4.155). Therefore, suppose that, contrary to the previous assumption,  $\mathbf{A} - \lambda \mathbb{I}$  is *not* invertible. We have mentioned earlier (without proof) that this implies that its determinant vanishes; that is,

$$\det(\mathbf{A} - \lambda \mathbb{I}) = |\mathbf{A} - \lambda \mathbb{I}| = 0. \quad (4.156)$$

This determinant is often called the *secular determinant*; and the corresponding equation after expansion of the determinant is called the *secular equation* or *characteristic equation*. Once the eigenvalues, that is, the roots (i.e., the solutions) of this equation are determined, the eigenvectors can be obtained one-by-one by inserting these eigenvalues one-by-one into Eq. (4.155).

For the sake of an example, consider the matrix

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad (4.157)$$

The secular equation is

$$\begin{vmatrix} 1-\lambda & 0 & 1 \\ 0 & 1-\lambda & 0 \\ 1 & 0 & 1-\lambda \end{vmatrix} = 0,$$

yielding the characteristic equation  $(1-\lambda)^3 - (1-\lambda) = (1-\lambda)[(1-\lambda)^2 - 1] = (1-\lambda)[\lambda^2 - 2\lambda] = -\lambda(1-\lambda)(2-\lambda) = 0$ , and therefore three eigenvalues  $\lambda_1 = 0$ ,  $\lambda_2 = 1$ , and  $\lambda_3 = 2$  which are the roots of  $\lambda(1-\lambda)(2-\lambda) = 0$ .

Next let us determine the eigenvectors of  $A$ , based on the eigenvalues.

Insertion  $\lambda_1 = 0$  into Eq. (4.155) yields

$$\left[ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4.158)$$

therefore  $x_1 + x_3 = 0$  and  $x_2 = 0$ . We are free to choose any (nonzero)

$x_1 = -x_3$ , but if we are interested in normalized eigenvectors, we obtain

$\mathbf{x}_1 = (1/\sqrt{2})(1, 0, -1)^T$ .

Insertion  $\lambda_2 = 1$  into Eq. (4.155) yields

$$\left[ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4.159)$$

therefore  $x_1 = x_3 = 0$  and  $x_2$  is arbitrary. We are again free to choose any (nonzero)  $x_2$ , but if we are interested in normalized eigenvectors, we obtain  $\mathbf{x}_2 = (0, 1, 0)^T$ .

Insertion  $\lambda_3 = 2$  into Eq. (4.155) yields

$$\left[ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4.160)$$

therefore  $-x_1 + x_3 = 0$  and  $x_2 = 0$ . We are free to choose any (nonzero)  $x_1 = x_3$ , but if we are once more interested in normalized eigenvectors, we obtain  $\mathbf{x}_3 = (1/\sqrt{2})(1, 0, 1)^T$ .

Note that the eigenvectors are mutually orthogonal. We can construct the corresponding orthogonal projections by the outer (dyadic or tensor) product of the eigenvectors; that is,

$$\begin{aligned} \mathbf{E}_1 &= \mathbf{x}_1 \otimes \mathbf{x}_1^T = \frac{1}{2} (1, 0, -1)^T (1, 0, -1) = \frac{1}{2} \begin{pmatrix} 1(1, 0, -1) \\ 0(1, 0, -1) \\ -1(1, 0, -1) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \\ \mathbf{E}_2 &= \mathbf{x}_2 \otimes \mathbf{x}_2^T = (0, 1, 0)^T (0, 1, 0) = \begin{pmatrix} 0(0, 1, 0) \\ 1(0, 1, 0) \\ 0(0, 1, 0) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \mathbf{E}_3 &= \mathbf{x}_3 \otimes \mathbf{x}_3^T = \frac{1}{2} (1, 0, 1)^T (1, 0, 1) = \frac{1}{2} \begin{pmatrix} 1(1, 0, 1) \\ 0(1, 0, 1) \\ 1(1, 0, 1) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \end{aligned} \quad (4.161)$$

Note also that  $A$  can be written as the sum of the products of the eigenvalues with the associated projections; that is (here,  $\mathbf{E}$  stands for the corresponding matrix),  $A = 0\mathbf{E}_1 + 1\mathbf{E}_2 + 2\mathbf{E}_3$ . Also, the projections are mutually orthogonal – that is,  $\mathbf{E}_1\mathbf{E}_2 = \mathbf{E}_1\mathbf{E}_3 = \mathbf{E}_2\mathbf{E}_3 = 0$  – and add up to unity; that is,  $\mathbf{E}_1 + \mathbf{E}_2 + \mathbf{E}_3 = \mathbb{I}$ .

If the eigenvalues obtained are not distinct and thus some eigenvalues are *degenerate*, the associated eigenvectors traditionally – that is, by convention and not necessity – are chosen to be *mutually orthogonal*. A more formal motivation will come from the spectral theorem below.

For the sake of an example, consider the matrix

$$B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad (4.162)$$

The secular equation yields

$$\begin{vmatrix} 1-\lambda & 0 & 1 \\ 0 & 2-\lambda & 0 \\ 1 & 0 & 1-\lambda \end{vmatrix} = 0,$$

which yields the characteristic equation  $(2 - \lambda)(1 - \lambda)^2 + [-(2 - \lambda)] = (2 - \lambda)[(1 - \lambda)^2 - 1] = -\lambda(2 - \lambda)^2 = 0$ , and therefore just two eigenvalues  $\lambda_1 = 0$ , and  $\lambda_2 = 2$  which are the roots of  $\lambda(2 - \lambda)^2 = 0$ .

Let us now determine the eigenvectors of  $B$ , based on the eigenvalues. Insertion  $\lambda_1 = 0$  into Eq. (4.155) yields

$$\left[ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4.163)$$

therefore  $x_1 + x_3 = 0$  and  $x_2 = 0$ . Again we are free to choose any (nonzero)  $x_1 = -x_3$ , but if we are interested in normalized eigenvectors, we obtain  $\mathbf{x}_1 = (1/\sqrt{2})(1, 0, -1)^T$ .

Insertion  $\lambda_2 = 2$  into Eq. (4.155) yields

$$\left[ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \right] \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4.164)$$

therefore  $x_1 = x_3$ ;  $x_2$  is arbitrary. We are again free to choose any values of  $x_1, x_3$  and  $x_2$  as long as  $x_1 = x_3$  as well as  $x_2$  are satisfied. Take, for the sake of choice, the orthogonal normalized eigenvectors  $\mathbf{x}_{2,1} = (0, 1, 0)^T$  and  $\mathbf{x}_{2,2} = (1/\sqrt{2})(1, 0, 1)^T$ , which are also orthogonal to  $\mathbf{x}_1 = (1/\sqrt{2})(1, 0, -1)^T$ .

Note again that we can find the corresponding orthogonal projections by the outer (dyadic or tensor) product of the eigenvectors; that is, by

$$\begin{aligned} \mathbf{E}_1 &= \mathbf{x}_1 \otimes \mathbf{x}_1^T = \frac{1}{2}(1, 0, -1)^T(1, 0, -1) = \frac{1}{2} \begin{pmatrix} 1(1, 0, -1) \\ 0(1, 0, -1) \\ -1(1, 0, -1) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \\ \mathbf{E}_{2,1} &= \mathbf{x}_{2,1} \otimes \mathbf{x}_{2,1}^T = (0, 1, 0)^T(0, 1, 0) = \begin{pmatrix} 0(0, 1, 0) \\ 1(0, 1, 0) \\ 0(0, 1, 0) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \mathbf{E}_{2,2} &= \mathbf{x}_{2,2} \otimes \mathbf{x}_{2,2}^T = \frac{1}{2}(1, 0, 1)^T(1, 0, 1) = \frac{1}{2} \begin{pmatrix} 1(1, 0, 1) \\ 0(1, 0, 1) \\ 1(1, 0, 1) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \end{aligned} \quad (4.165)$$

Note also that  $B$  can be written as the sum of the products of the eigenvalues with the associated projections; that is (here,  $\mathbf{E}$  stands for the corresponding matrix),  $B = 0\mathbf{E}_1 + 2(\mathbf{E}_{2,1} + \mathbf{E}_{2,2})$ . Again, the projections are mutually orthogonal – that is,  $\mathbf{E}_1\mathbf{E}_{2,1} = \mathbf{E}_1\mathbf{E}_{2,2} = \mathbf{E}_{2,1}\mathbf{E}_{2,2} = 0$  – and add up to unity; that is,  $\mathbf{E}_1 + \mathbf{E}_{2,1} + \mathbf{E}_{2,2} = \mathbb{I}$ . This leads us to the much more general spectral theorem.

Another, extreme, example would be the unit matrix in  $n$  dimensions; that is,  $\mathbb{I}_n = \text{diag}(\underbrace{1, \dots, 1}_{n \text{ times}})$ , which has an  $n$ -fold degenerate eigenvalue 1



corresponding to a solution to  $(1 - \lambda)^n = 0$ . The corresponding projection operator is  $\mathbb{I}_n$ . [Note that  $(\mathbb{I}_n)^2 = \mathbb{I}_n$  and thus  $\mathbb{I}_n$  is a projection.] If one (somehow arbitrarily but conveniently) chooses a decomposition of unity  $\mathbb{I}_n$  into projections corresponding to the standard basis (any other orthonormal basis would do as well), then

$$\begin{aligned} \mathbb{I}_n &= \text{diag}(1, 0, 0, \dots, 0) + \text{diag}(0, 1, 0, \dots, 0) + \dots + \text{diag}(0, 0, 0, \dots, 1) \\ &= \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} + \\ &+ \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} + \dots + \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \end{aligned} \quad (4.166)$$

where all the matrices in the sum carrying one nonvanishing entry “1” in their diagonal are projections. Note that

$$\begin{aligned} \mathbf{e}_i &= |\mathbf{e}_i\rangle \\ &\equiv (\underbrace{0, \dots, 0}_{i-1 \text{ times}}, 1, \underbrace{0, \dots, 0}_{n-i \text{ times}}) \\ &\equiv \text{diag}(\underbrace{0, \dots, 0}_{i-1 \text{ times}}, 1, \underbrace{0, \dots, 0}_{n-i \text{ times}}) \\ &\equiv \mathbf{E}_i. \end{aligned} \quad (4.167)$$

The following theorems are enumerated without proofs.

If  $\mathbf{A}$  is a self-adjoint transformation on an inner product space, then every proper value (eigenvalue) of  $\mathbf{A}$  is real. If  $\mathbf{A}$  is positive, or strictly positive, then every proper value of  $\mathbf{A}$  is positive, or strictly positive, respectively.

Due to their idempotence  $\mathbf{E}\mathbf{E} = \mathbf{E}$ , projections have eigenvalues 0 or 1.

Every eigenvalue of an isometry has absolute value one.

If  $\mathbf{A}$  is either a self-adjoint transformation or an isometry, then proper vectors of  $\mathbf{A}$  belonging to distinct proper values are orthogonal.

#### 4.27 Normal transformation

A transformation  $\mathbf{A}$  is called *normal* if it commutes with its adjoint; that is,

$$[\mathbf{A}, \mathbf{A}^*] = \mathbf{A}\mathbf{A}^* - \mathbf{A}^*\mathbf{A} = 0. \quad (4.168)$$

It follows from their definition that Hermitian and unitary transformations are normal. That is,  $\mathbf{A}^* = \mathbf{A}^\dagger$ , and for Hermitian operators,  $\mathbf{A} = \mathbf{A}^\dagger$ , and

thus  $[\mathbf{A}, \mathbf{A}^\dagger] = \mathbf{A}\mathbf{A} - \mathbf{A}\mathbf{A} = (\mathbf{A})^2 - (\mathbf{A})^2 = 0$ . For unitary operators,  $\mathbf{A}^\dagger = \mathbf{A}^{-1}$ , and thus  $[\mathbf{A}, \mathbf{A}^\dagger] = \mathbf{A}\mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{A} = \mathbb{I} - \mathbb{I} = 0$ .

We mention without proof that a normal transformation on a finite-dimensional unitary space is (i) Hermitian, (ii) positive, (iii) strictly positive, (iv) unitary, (v) invertible, (vi) idempotent if and only if all its proper values are (i) real, (ii) positive, (iii) strictly positive, (iv) of absolute value one, (v) different from zero, (vi) equal to zero or one.

## 4.28 Spectrum

### 4.28.1 Spectral theorem

Let  $\mathfrak{V}$  be an  $n$ -dimensional linear vector space. The *spectral theorem* states that to every self-adjoint (more general, normal) transformation  $\mathbf{A}$  on an  $n$ -dimensional inner product space there correspond real numbers, the *spectrum*  $\lambda_1, \lambda_2, \dots, \lambda_k$  of all the eigenvalues of  $\mathbf{A}$ , and their associated orthogonal projections  $\mathbf{E}_1, \mathbf{E}_2, \dots, \mathbf{E}_k$  where  $0 < k \leq n$  is a strictly positive integer so that

- (i) the  $\lambda_i$  are pairwise distinct,
- (ii) the  $\mathbf{E}_i$  are pairwise orthogonal and different from  $\mathbf{0}$ ,
- (iii)  $\sum_{i=1}^k \mathbf{E}_i = \mathbb{I}_n$ , and
- (iv)  $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$  is the *spectral form* of  $\mathbf{A}$ .

Rather than proving the spectral theorem in its full generality, we suppose that the spectrum of a Hermitian (self-adjoint) operator  $\mathbf{A}$  is *nondegenerate*; that is, all  $n$  eigenvalues of  $\mathbf{A}$  are pairwise distinct. That is, we are assuming a strong form of (i).

This distinctness of the eigenvalues then translates into mutual orthogonality of all the eigenvectors of  $\mathbf{A}$ . Thereby, the set of  $n$  eigenvectors form an orthogonal basis of the  $n$ -dimensional linear vector space  $\mathfrak{V}$ . The respective normalized eigenvectors can then be represented by perpendicular projections which can be summed up to yield the identity (iii).

More explicitly, suppose, for the sake of a proof by contradiction of the pairwise orthogonality of the eigenvectors (ii), that two different eigenvalues  $\lambda_1$  and  $\lambda_2$  belong to two respective eigenvectors  $\mathbf{x}_1$  and  $\mathbf{x}_2$  which are not orthogonal. But then, because  $\mathbf{A}$  is self-adjoint with real eigenvalues,

$$\begin{aligned} \lambda_1 \langle \mathbf{x}_1 | \mathbf{x}_2 \rangle &= \langle \lambda_1 \mathbf{x}_1 | \mathbf{x}_2 \rangle = \langle \mathbf{A} \mathbf{x}_1 | \mathbf{x}_2 \rangle \\ &= \langle \mathbf{x}_1 | \mathbf{A}^* \mathbf{x}_2 \rangle = \langle \mathbf{x}_1 | \mathbf{A} \mathbf{x}_2 \rangle = \langle \mathbf{x}_1 | \lambda_2 \mathbf{x}_2 \rangle = \lambda_2 \langle \mathbf{x}_1 | \mathbf{x}_2 \rangle, \end{aligned} \quad (4.169)$$

which implies that either  $\lambda_1 = \lambda_2$  – which is in contradiction to our assumption of the distinctness of  $\lambda_1$  and  $\lambda_2$ ; or that  $\langle \mathbf{x}_1 | \mathbf{x}_2 \rangle = 0$  (thus allowing  $\lambda_1 \neq \lambda_2$ ) – which is in contradiction to our assumption that  $\mathbf{x}_1$  and  $\mathbf{x}_2$  are

For proofs and additional information see §78 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

not orthogonal. Hence, for distinct  $\lambda_1$  and  $\lambda_2$ , the associated eigenvectors must be orthogonal, thereby assuring (ii).

Since by our assumption there are  $n$  distinct eigenvalues, this implies that there are  $n$  orthogonal eigenvectors. These  $n$  mutually orthogonal eigenvectors span the entire  $n$ -dimensional linear vector space  $\mathfrak{V}$ ; and hence their union  $\{|\mathbf{x}_i\rangle | i \leq n\}$  forms an orthogonal basis. Consequently, the sum of the associated perpendicular projections  $\mathbf{E}_i = \frac{|\mathbf{x}_i\rangle\langle\mathbf{x}_i|}{\langle\mathbf{x}_i|\mathbf{x}_i\rangle}$  is a decomposition of unity  $\mathbb{I}_n$ , thereby justifying (iii).

In the last step, let us define the  $i$ 'th projection of an arbitrary vector  $\mathbf{x} \in \mathfrak{V}$  by  $\mathbf{x}_i = \mathbf{E}_i \mathbf{x}$ , thereby keeping in mind that the resulting vector  $\mathbf{x}_i$  is an eigenvector of  $\mathbf{A}$  with the associated eigenvalue  $\lambda_i$ ; that is,  $\mathbf{A}\mathbf{x}_i = \lambda_i \mathbf{x}_i$ . Then,

$$\begin{aligned} \mathbf{A}\mathbf{x} &= \mathbf{A}\mathbb{I}_n \mathbf{x} = \mathbf{A} \left( \sum_{i=1}^n \mathbf{E}_i \right) \mathbf{x} = \mathbf{A} \left( \sum_{i=1}^n \mathbf{E}_i \mathbf{x} \right) = \mathbf{A} \left( \sum_{i=1}^n \mathbf{x}_i \right) \\ &= \sum_{i=1}^n \mathbf{A}\mathbf{x}_i = \sum_{i=1}^n \lambda_i \mathbf{x}_i = \sum_{i=1}^n \lambda_i \mathbf{E}_i \mathbf{x} = \left( \sum_{i=1}^n \lambda_i \mathbf{E}_i \right) \mathbf{x}, \end{aligned} \quad (4.170)$$

which is the spectral form of  $\mathbf{A}$ .

#### 4.28.2 Composition of the spectral form

If the spectrum of a Hermitian (or, more general, normal) operator  $\mathbf{A}$  is nondegenerate, that is,  $k = n$ , then the  $i$ th projection can be written as the outer (dyadic or tensor) product  $\mathbf{E}_i = \mathbf{x}_i \otimes \mathbf{x}_i^T$  of the  $i$ th normalized eigenvector  $\mathbf{x}_i$  of  $\mathbf{A}$ . In this case, the set of all normalized eigenvectors  $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  is an orthonormal basis of the vector space  $\mathfrak{V}$ . If the spectrum of  $\mathbf{A}$  is degenerate, then the projection can be chosen to be the orthogonal sum of projections corresponding to orthogonal eigenvectors, associated with the same eigenvalues.

Furthermore, for a Hermitian (or, more general, normal) operator  $\mathbf{A}$ , if  $1 \leq i \leq k$ , then there exist polynomials with real coefficients, such as, for instance,

$$p_i(t) = \prod_{\substack{1 \leq j \leq k \\ j \neq i}} \frac{t - \lambda_j}{\lambda_i - \lambda_j} \quad (4.171)$$

so that  $p_i(\lambda_j) = \delta_{ij}$ ; moreover, for every such polynomial,  $p_i(\mathbf{A}) = \mathbf{E}_i$ .

For a proof, it is not too difficult to show that  $p_i(\lambda_i) = 1$ , since in this case in the product of fractions all numerators are equal to denominators, and  $p_i(\lambda_j) = 0$  for  $j \neq i$ , since some numerator in the product of fractions vanishes.

Now, substituting for  $t$  the spectral form  $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$  of  $\mathbf{A}$ , as well as decomposing unity in terms of the projections  $\mathbf{E}_i$  in the spectral form of  $\mathbf{A}$ ;

that is,  $\mathbb{I}_n = \sum_{i=1}^k \mathbf{E}_i$ , yields

$$p_i(\mathbf{A}) = \prod_{1 \leq j \leq k, j \neq i} \frac{\mathbf{A} - \lambda_j \mathbb{I}_n}{\lambda_i - \lambda_j} = \prod_{1 \leq j \leq k, j \neq i} \frac{\sum_{l=1}^k \lambda_l \mathbf{E}_l - \lambda_j \sum_{l=1}^k \mathbf{E}_l}{\lambda_i - \lambda_j}, \quad (4.172)$$

and, because of the idempotence and pairwise orthogonality of the projections  $\mathbf{E}_l$ ,

$$\begin{aligned} &= \prod_{1 \leq j \leq k, j \neq i} \frac{\sum_{l=1}^k \mathbf{E}_l (\lambda_l - \lambda_j)}{\lambda_i - \lambda_j} \\ &= \sum_{l=1}^k \mathbf{E}_l \prod_{1 \leq j \leq k, j \neq i} \frac{\lambda_l - \lambda_j}{\lambda_i - \lambda_j} = \sum_{l=1}^k \mathbf{E}_l \delta_{li} = \mathbf{E}_i. \end{aligned} \quad (4.173)$$

With the help of the polynomial  $p_i(t)$  defined in Eq. (4.171), which requires knowledge of the eigenvalues, the spectral form of a Hermitian (or, more general, normal) operator  $\mathbf{A}$  can thus be rewritten as

$$\mathbf{A} = \sum_{i=1}^k \lambda_i p_i(\mathbf{A}) = \sum_{i=1}^k \lambda_i \prod_{1 \leq j \leq k, j \neq i} \frac{\mathbf{A} - \lambda_j \mathbb{I}_n}{\lambda_i - \lambda_j}. \quad (4.174)$$

That is, knowledge of all the eigenvalues entails construction of all the projections in the spectral decomposition of a normal transformation.

For the sake of an example, consider again the matrix

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (4.175)$$

and the associated Eigensystem

$$\begin{aligned} &\{ \{ \lambda_1, \lambda_2, \lambda_3 \}, \{ \mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3 \} \} \\ &= \left\{ \{0, 1, 2\}, \left\{ \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \right\} \right\}. \end{aligned} \quad (4.176)$$

The projections associated with the eigenvalues, and, in particular,  $\mathbf{E}_1$ , can be obtained from the set of eigenvalues  $\{0, 1, 2\}$  by

$$\begin{aligned} p_1(A) &= \left( \frac{A - \lambda_2 \mathbb{I}}{\lambda_1 - \lambda_2} \right) \left( \frac{A - \lambda_3 \mathbb{I}}{\lambda_1 - \lambda_3} \right) \\ &= \frac{\left( \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - 1 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right) \left( \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} - 2 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right)}{(0-1)(0-2)} \\ &= \frac{1}{2} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} = \mathbf{E}_1. \end{aligned} \quad (4.177)$$

For the sake of another, degenerate, example consider again the matrix

$$B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad (4.178)$$

Again, the projections  $\mathbf{E}_1, \mathbf{E}_2$  can be obtained from the set of eigenvalues  $\{0, 2\}$  by

$$\begin{aligned} p_1(A) &= \frac{A - \lambda_2 \mathbb{I}}{\lambda_1 - \lambda_2} = \frac{\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - 2 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}{(0 - 2)} = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} = \mathbf{E}_1, \\ p_2(A) &= \frac{A - \lambda_1 \mathbb{I}}{\lambda_2 - \lambda_1} = \frac{\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - 0 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}{(2 - 0)} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \mathbf{E}_2. \end{aligned} \quad (4.179)$$

Note that, in accordance with the spectral theorem,  $\mathbf{E}_1 \mathbf{E}_2 = 0$ ,  $\mathbf{E}_1 + \mathbf{E}_2 = \mathbb{I}$  and  $0 \cdot \mathbf{E}_1 + 2 \cdot \mathbf{E}_2 = B$ .

#### 4.29 Functions of normal transformations

Suppose  $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$  is a normal transformation in its spectral form. If  $f$  is an arbitrary complex-valued function defined at least at the eigenvalues of  $\mathbf{A}$ , then a linear transformation  $f(\mathbf{A})$  can be defined by

$$f(\mathbf{A}) = f\left(\sum_{i=1}^k \lambda_i \mathbf{E}_i\right) = \sum_{i=1}^k f(\lambda_i) \mathbf{E}_i. \quad (4.180)$$

Note that, if  $f$  has a polynomial expansion such as analytic functions, then orthogonality and idempotence of the projections  $\mathbf{E}_i$  in the spectral form guarantees this kind of “linearization.”

For the definition of the “square root” for every positive operator  $\mathbf{A}$ , consider

$$\sqrt{\mathbf{A}} = \sum_{i=1}^k \sqrt{\lambda_i} \mathbf{E}_i. \quad (4.181)$$

With this definition,  $(\sqrt{\mathbf{A}})^2 = \sqrt{\mathbf{A}} \sqrt{\mathbf{A}} = \mathbf{A}$ .

Consider, for instance, the “square root” of the **not** operator

$$\mathbf{not} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (4.182)$$

The denomination “not” for **not** can be motivated by enumerating its performance at the two “classical bit states”  $|0\rangle \equiv (1, 0)^T$  and  $|1\rangle \equiv (0, 1)^T$ :  $\mathbf{not}|0\rangle = |1\rangle$  and  $\mathbf{not}|1\rangle = |0\rangle$ .

To enumerate  $\sqrt{\mathbf{not}}$  we need to find the *spectral form* of **not** first. The eigenvalues of **not** can be obtained by solving the secular equation

$$\det(\mathbf{not} - \lambda \mathbb{I}_2) = \det \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right) = \det \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0. \quad (4.183)$$

$\lambda^2 = 1$  yields the two eigenvalues  $\lambda_1 = 1$  and  $\lambda_1 = -1$ . The associated eigenvectors  $\mathbf{x}_1$  and  $\mathbf{x}_2$  can be derived from either the equations  $\mathbf{not}\mathbf{x}_1 = \mathbf{x}_1$  and  $\mathbf{not}\mathbf{x}_2 = -\mathbf{x}_2$ , or inserting the eigenvalues into the polynomial (4.171).

We choose the former method. Thus, for  $\lambda_1 = 1$ ,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_{1,2} \\ x_{1,2} \end{pmatrix} = \begin{pmatrix} x_{1,2} \\ x_{1,2} \end{pmatrix}, \quad (4.184)$$

which yields  $x_{1,2} = x_{1,2}$ , and thus, by normalizing the eigenvector,  $\mathbf{x}_1 = (1/\sqrt{2})(1, 1)^T$ . The associated projection is

$$\mathbf{E}_1 = \mathbf{x}_1 \mathbf{x}_1^T = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (4.185)$$

Likewise, for  $\lambda_2 = -1$ ,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_{2,2} \\ x_{2,2} \end{pmatrix} = - \begin{pmatrix} x_{2,2} \\ x_{2,2} \end{pmatrix}, \quad (4.186)$$

which yields  $x_{2,2} = -x_{2,2}$ , and thus, by normalizing the eigenvector,  $\mathbf{x}_2 = (1/\sqrt{2})(1, -1)^T$ . The associated projection is

$$\mathbf{E}_2 = \mathbf{x}_2 \mathbf{x}_2^T = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \quad (4.187)$$

Thus we are finally able to calculate  $\sqrt{\mathbf{not}}$  through its spectral form

$$\begin{aligned} \sqrt{\mathbf{not}} &= \sqrt{\lambda_1} \mathbf{E}_1 + \sqrt{\lambda_2} \mathbf{E}_2 \\ &= \sqrt{1} \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \sqrt{-1} \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}. \end{aligned} \quad (4.188)$$

It can be readily verified that  $\sqrt{\mathbf{not}}\sqrt{\mathbf{not}} = \mathbf{not}$ .

## 4.30 Decomposition of operators

### 4.30.1 Standard decomposition

In analogy to the decomposition of every imaginary number  $z = \Re z + i \Im z$  with  $\Re z, \Im z \in \mathbb{R}$ , every arbitrary transformation **A** on a finite-dimensional vector space can be decomposed into two Hermitian operators **B** and **C** such that

$$\begin{aligned} \mathbf{A} &= \mathbf{B} + i\mathbf{C}; \text{ with} \\ \mathbf{B} &= \frac{1}{2}(\mathbf{A} + \mathbf{A}^\dagger), \\ \mathbf{C} &= \frac{1}{2i}(\mathbf{A} - \mathbf{A}^\dagger). \end{aligned} \quad (4.189)$$

For proofs and additional information see §83 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

Proof by insertion; that is,

$$\begin{aligned}
 \mathbf{A} &= \mathbf{B} + i\mathbf{C} \\
 &= \frac{1}{2}(\mathbf{A} + \mathbf{A}^\dagger) + i \left[ \frac{1}{2i}(\mathbf{A} - \mathbf{A}^\dagger) \right], \\
 \mathbf{B}^\dagger &= \left[ \frac{1}{2}(\mathbf{A} + \mathbf{A}^\dagger) \right]^\dagger = \frac{1}{2} \left[ \mathbf{A}^\dagger + (\mathbf{A}^\dagger)^\dagger \right] \\
 &= \frac{1}{2} \left[ \mathbf{A}^\dagger + \mathbf{A} \right] = \mathbf{B}, \\
 \mathbf{C}^\dagger &= \left[ \frac{1}{2i}(\mathbf{A} - \mathbf{A}^\dagger) \right]^\dagger = -\frac{1}{2i} \left[ \mathbf{A}^\dagger - (\mathbf{A}^\dagger)^\dagger \right] \\
 &= -\frac{1}{2i} \left[ \mathbf{A}^\dagger - \mathbf{A} \right] = \mathbf{C}.
 \end{aligned} \tag{4.190}$$

#### 4.30.2 Polar representation

In analogy to the polar representation of every imaginary number  $z = Re^{i\varphi}$  with  $R, \varphi \in \mathbb{R}$ ,  $R > 0$ ,  $0 \leq \varphi < 2\pi$ , every arbitrary transformation  $\mathbf{A}$  on a finite-dimensional inner product space can be decomposed into a unique positive transform  $\mathbf{P}$  and an isometry  $\mathbf{U}$ , such that  $\mathbf{A} = \mathbf{U}\mathbf{P}$ . If  $\mathbf{A}$  is invertible, then  $\mathbf{U}$  is uniquely determined by  $\mathbf{A}$ . A necessary and sufficient condition that  $\mathbf{A}$  is normal is that  $\mathbf{U}\mathbf{P} = \mathbf{P}\mathbf{U}$ .

#### 4.30.3 Decomposition of isometries

Any unitary or orthogonal transformation in finite-dimensional inner product space can be composed from a succession of two-parameter unitary transformations in two-dimensional subspaces, and a multiplication of a single diagonal matrix with elements of modulus one in an algorithmic, constructive and tractable manner. The method is similar to Gaussian elimination and facilitates the parameterization of elements of the unitary group in arbitrary dimensions (e.g., Ref. <sup>21</sup>, Chapter 2).

It has been suggested to implement these group theoretic results by realizing interferometric analogues of any discrete unitary and Hermitian operator in a unified and experimentally feasible way by “generalized beam splitters” <sup>22</sup>.

#### 4.30.4 Singular value decomposition

The *singular value decomposition* (SVD) of an  $(m \times n)$  matrix  $\mathbf{A}$  is a factorization of the form

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}, \tag{4.191}$$

where  $\mathbf{U}$  is a unitary  $(m \times m)$  matrix (i.e. an isometry),  $\mathbf{V}$  is a unitary  $(n \times n)$  matrix, and  $\Sigma$  is a unique  $(m \times n)$  diagonal matrix with nonnegative real

<sup>21</sup> F. D. Murnaghan. *The Unitary and Rotation Groups*. Spartan Books, Washington, D.C., 1962

<sup>22</sup> M. Reck, Anton Zeilinger, H. J. Bernstein, and P. Bertani. Experimental realization of any discrete unitary operator. *Physical Review Letters*, 73:58–61, 1994. DOI: 10.1103/PhysRevLett.73.58. URL <http://dx.doi.org/10.1103/PhysRevLett.73.58>; and M. Reck and Anton Zeilinger. Quantum phase tracing of correlated photons in optical multiports. In F. De Martini, G. Denardo, and Anton Zeilinger, editors, *Quantum Interferometry*, pages 170–177, Singapore, 1994. World Scientific

numbers on the diagonal; that is,

$$\Sigma = \begin{pmatrix} \sigma_1 & & & & & & \\ & \ddots & & & & & \\ & & \sigma_r & & & & \\ - & - & - & - & - & - & \\ & & & & & & \\ \dots & 0 & \dots & & \dots & 0 & \dots \\ & & & & & & \end{pmatrix}. \quad (4.192)$$

The entries  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$  of  $\Sigma$  are called *singular values* of  $\mathbf{A}$ . No proof is presented here.

#### 4.30.5 Schmidt decomposition of the tensor product of two vectors

Let  $\mathfrak{U}$  and  $\mathfrak{V}$  be two linear vector spaces of dimension  $n \geq m$  and  $m$ , respectively. Then, for any vector  $\mathbf{z} \in \mathfrak{U} \otimes \mathfrak{V}$  in the tensor product space, there exist orthonormal basis sets of vectors  $\{\mathbf{u}_1, \dots, \mathbf{u}_n\} \subset \mathfrak{U}$  and  $\{\mathbf{v}_1, \dots, \mathbf{v}_m\} \subset \mathfrak{V}$  such that  $\mathbf{z} = \sum_{i=1}^m \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i$ , where the  $\sigma_i$ s are nonnegative scalars and the set of scalars is uniquely determined by  $\mathbf{z}$ .

Equivalently<sup>23</sup>, suppose that  $|\mathbf{z}\rangle$  is some tensor product contained in the set of all tensor products of vectors  $\mathfrak{U} \otimes \mathfrak{V}$  of two linear vector spaces  $\mathfrak{U}$  and  $\mathfrak{V}$ . Then there exist orthonormal vectors  $|\mathbf{u}_i\rangle \in \mathfrak{U}$  and  $|\mathbf{v}_i\rangle \in \mathfrak{V}$  so that

$$|\mathbf{z}\rangle = \sum_i \sigma_i |\mathbf{u}_i\rangle |\mathbf{v}_i\rangle, \quad (4.193)$$

where the  $\sigma_i$ s are nonnegative scalars; if  $|\mathbf{z}\rangle$  is normalized, then the  $\sigma_i$ s are satisfying  $\sum_i \sigma_i^2 = 1$ ; they are called the *Schmidt coefficients*.

For a proof by reduction to the singular value decomposition, let  $|i\rangle$  and  $|j\rangle$  be any two fixed orthonormal bases of  $\mathfrak{U}$  and  $\mathfrak{V}$ , respectively. Then,  $|\mathbf{z}\rangle$  can be expanded as  $|\mathbf{z}\rangle = \sum_{ij} a_{ij} |i\rangle |j\rangle$ , where the  $a_{ij}$ s can be interpreted as the components of a matrix  $\mathbf{A}$ .  $\mathbf{A}$  can then be subjected to a singular value decomposition  $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}$ , or, written in index form [note that  $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$  is a diagonal matrix],  $a_{ij} = \sum_l u_{il} \sigma_l v_{lj}$ ; and hence  $|\mathbf{z}\rangle = \sum_{ijl} u_{il} \sigma_l v_{lj} |i\rangle |j\rangle$ . Finally, by identifying  $|\mathbf{u}_l\rangle = \sum_i u_{il} |i\rangle$  as well as  $|\mathbf{v}_l\rangle = \sum_j v_{lj} |j\rangle$  one obtains the Schmidt decomposition (4.193). Since  $u_{il}$  and  $v_{lj}$  represent unitary matrices, and because  $|i\rangle$  as well as  $|j\rangle$  are orthonormal, the newly formed vectors  $|\mathbf{u}_l\rangle$  as well as  $|\mathbf{v}_l\rangle$  form orthonormal bases as well. The sum of squares of the  $\sigma_i$ 's is one if  $|\mathbf{z}\rangle$  is a unit vector, because (note that  $\sigma_i$ s are real-valued)  $\langle \mathbf{z} | \mathbf{z} \rangle = 1 = \sum_{lm} \sigma_l \sigma_m \langle \mathbf{u}_l | \mathbf{u}_m \rangle \langle \mathbf{v}_l | \mathbf{v}_m \rangle = \sum_{lm} \sigma_l \sigma_m \delta_{lm} = \sum_l \sigma_l^2$ .

Note that the Schmidt decomposition cannot, in general, be extended for more factors than two. Note also that the Schmidt decomposition needs not be unique<sup>24</sup>; in particular if some of the Schmidt coefficients

<sup>23</sup> M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000

<sup>24</sup> Artur Ekert and Peter L. Knight. Entangled quantum systems and the Schmidt decomposition. *American Journal of Physics*, 63(5):415–423, 1995. doi: 10.1119/1.17904. URL <http://dx.doi.org/10.1119/1.17904>



$\sigma_i$  are equal. For the sake of an example of nonuniqueness of the Schmidt decomposition, take, for instance, the representation of the *Bell state* with the two bases

$$\begin{aligned} \{|\mathbf{e}_1\rangle \equiv (1, 0), |\mathbf{e}_2\rangle \equiv (0, 1)\} \text{ and} \\ \left\{ |\mathbf{f}_1\rangle \equiv \frac{1}{\sqrt{2}}(1, 1), |\mathbf{f}_2\rangle \equiv \frac{1}{\sqrt{2}}(-1, 1) \right\}. \end{aligned} \quad (4.194)$$

as follows:

$$\begin{aligned} |\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|\mathbf{e}_1\rangle|\mathbf{e}_2\rangle - |\mathbf{e}_2\rangle|\mathbf{e}_1\rangle) \\ &\equiv \frac{1}{\sqrt{2}}[(1(0, 1), 0(0, 1)) - (0(1, 0), 1(1, 0))] = \frac{1}{\sqrt{2}}(0, 1, -1, 0); \\ |\Psi^-\rangle &= \frac{1}{\sqrt{2}}(|\mathbf{f}_1\rangle|\mathbf{f}_2\rangle - |\mathbf{f}_2\rangle|\mathbf{f}_1\rangle) \\ &\equiv \frac{1}{2\sqrt{2}}[(1(-1, 1), 1(-1, 1)) - (-1(1, 1), 1(1, 1))] \\ &\equiv \frac{1}{2\sqrt{2}}[(-1, 1, -1, 1) - (-1, -1, 1, 1)] = \frac{1}{\sqrt{2}}(0, 1, -1, 0). \end{aligned} \quad (4.195)$$

### 4.31 Purification

In general, quantum states  $\rho$  satisfy three criteria<sup>25</sup>: (i)  $\text{Tr}(\rho) = 1$ , (ii)  $\rho^\dagger = \rho$ , and (iii)  $\langle \mathbf{x} | \rho | \mathbf{x} \rangle = \langle \mathbf{x} | \rho \mathbf{x} \rangle \geq 0$  for all vectors  $\mathbf{x}$  of some Hilbert space.

With dimension  $n$  it follows immediately from (ii) that  $\rho$  is normal and thus has a spectral decomposition

$$\rho = \sum_{i=1}^n \rho_i |\psi_i\rangle \langle \psi_i| \quad (4.196)$$

into projections  $|\psi_i\rangle \langle \psi_i|$ , with (i) yielding  $\sum_{i=1}^n \rho_i = 1$  (hint: take a trace with the orthonormal basis corresponding to all the  $|\psi_i\rangle$ ); (ii) yielding  $\overline{\rho_i} = \rho_i$ ; and (iii) implying  $\rho_i \geq 0$ , and hence [with (i)]  $0 \leq \rho_i \leq 1$  for all  $1 \leq i \leq n$ .

Quantum mechanics differentiates between “two sorts of states,” namely pure states and one mixed ones:

- (i) Pure states  $\rho_p$  are represented by projections. They can be written as  $\rho_p = |\psi\rangle \langle \psi|$  for some unit vector  $|\psi\rangle$  (discussed in Sec. 4.12), and satisfy  $(\rho_p)^2 = \rho_p$ .
- (ii) General, mixed states  $\rho_m$ , are ones that are no projections and therefore satisfy  $(\rho_m)^2 \neq \rho_m$ . They can be composed from projections by their spectral form (4.196).

The question arises: is it possible to “purify” any mixed state by (maybe somewhat superficially) “enlarging” its Hilbert space, such that the resulting state “living in a larger Hilbert space” is pure? This can indeed be

For additional information see page 110, Sect. 2.5 in

M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2010. 10th Anniversary Edition

<sup>25</sup> L. E. Ballentine. *Quantum Mechanics*. Prentice Hall, Englewood Cliffs, NJ, 1989

achieved by a rather simple procedure: By considering the spectral form (4.196) of a general mixed state  $\rho$ , define a new, “enlarged,” pure state  $|\Psi\rangle\langle\Psi|$ , with

$$|\Psi\rangle = \sum_{i=1}^n \sqrt{\rho_i} |\psi_i\rangle |\psi_i\rangle. \quad (4.197)$$

That  $|\Psi\rangle\langle\Psi|$  is pure can be tediously verified by proving that it is idempotent:

$$\begin{aligned} & (|\Psi\rangle\langle\Psi|)^2 \\ &= \left\{ \left[ \sum_{i=1}^n \sqrt{\rho_i} |\psi_i\rangle |\psi_i\rangle \right] \left[ \sum_{j=1}^n \sqrt{\rho_j} \langle\psi_j| \langle\psi_j| \right] \right\}^2 \\ &= \left[ \sum_{i_1=1}^n \sqrt{\rho_{i_1}} |\psi_{i_1}\rangle |\psi_{i_1}\rangle \right] \left[ \sum_{j_1=1}^n \sqrt{\rho_{j_1}} \langle\psi_{j_1}| \langle\psi_{j_1}| \right] \times \\ & \quad \left[ \sum_{i_2=1}^n \sqrt{\rho_{i_2}} |\psi_{i_2}\rangle |\psi_{i_2}\rangle \right] \left[ \sum_{j_2=1}^n \sqrt{\rho_{j_2}} \langle\psi_{j_2}| \langle\psi_{j_2}| \right] \\ &= \left[ \sum_{i_1=1}^n \sqrt{\rho_{i_1}} |\psi_{i_1}\rangle |\psi_{i_1}\rangle \right] \left[ \sum_{j_1=1}^n \sum_{i_2=1}^n \sqrt{\rho_{j_1}} \sqrt{\rho_{i_2}} (\delta_{i_2 j_1})^2 \right] \left[ \sum_{j_2=1}^n \sqrt{\rho_{j_2}} \langle\psi_{j_2}| \langle\psi_{j_2}| \right] \\ &= \left[ \sum_{i_1=1}^n \sqrt{\rho_{i_1}} |\psi_{i_1}\rangle |\psi_{i_1}\rangle \right] \left[ \sum_{j_2=1}^n \sqrt{\rho_{j_2}} \langle\psi_{j_2}| \langle\psi_{j_2}| \right] \\ &= |\Psi\rangle\langle\Psi|. \end{aligned} \quad (4.198)$$

Note that this construction is not unique – any auxiliary component representing some orthonormal basis would suffice.

The original mixed state  $\rho$  is obtained from the pure state corresponding to the unit vector  $|\Psi\rangle = |\psi\rangle |\psi^a\rangle = |\psi\psi^a\rangle$  – we might say that “the superscript  $a$  stands for auxiliary” – by a partial trace (cf. Sec. 4.18.3) over one of its components, say  $|\psi^a\rangle$ .

For the sake of a proof let us “trace out of the auxiliary components  $|\psi^a\rangle$ ,” that is, take the trace

$$\text{Tr}_a(|\Psi\rangle\langle\Psi|) = \sum_{k=1}^n \langle\psi_k^a|(|\Psi\rangle\langle\Psi|)|\psi_k^a\rangle \quad (4.199)$$

of  $|\Psi\rangle\langle\Psi|$  with respect to one of its components  $|\psi^a\rangle$ :

$$\begin{aligned}
 & \text{Tr}_a(|\Psi\rangle\langle\Psi|) \\
 &= \text{Tr}_a\left(\left[\sum_{i=1}^n \sqrt{\rho_i}|\psi_i\rangle\langle\psi_i^a|\right]\left[\sum_{j=1}^n \sqrt{\rho_j}\langle\psi_j^a|\langle\psi_j|\right]\right) \\
 &= \sum_{k=1}^n \left\langle \psi_k^a \left| \left( \left[\sum_{i=1}^n \sqrt{\rho_i}|\psi_i\rangle\langle\psi_i^a|\right] \left[\sum_{j=1}^n \sqrt{\rho_j}\langle\psi_j^a|\langle\psi_j|\right] \right) \right| \psi_k^a \right\rangle \quad (4.200) \\
 &= \sum_{k=1}^n \sum_{i=1}^n \sum_{j=1}^n \delta_{ki} \delta_{kj} \sqrt{\rho_i} \sqrt{\rho_j} |\psi_i\rangle\langle\psi_j| \\
 &= \sum_{k=1}^n \rho_k |\psi_k\rangle\langle\psi_k| = \boldsymbol{\rho}.
 \end{aligned}$$

#### 4.32 Commutativity

If  $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$  is the spectral form of a self-adjoint transformation  $\mathbf{A}$  on a finite-dimensional inner product space, then a necessary and sufficient condition (“if and only if = iff”) that a linear transformation  $\mathbf{B}$  commutes with  $\mathbf{A}$  is that it commutes with each  $\mathbf{E}_i$ ,  $1 \leq i \leq k$ .

Sufficiency is derived easily: whenever  $\mathbf{B}$  commutes with all the projectors  $\mathbf{E}_i$ ,  $1 \leq i \leq k$  in the spectral composition of  $\mathbf{A}$ , then, by linearity, it commutes with  $\mathbf{A}$ .

Necessity follows from the fact that, if  $\mathbf{B}$  commutes with  $\mathbf{A}$  then it also commutes with every polynomial of  $\mathbf{A}$ ; and hence also with  $p_i(\mathbf{A}) = \mathbf{E}_i$ , as shown in (4.173).

If  $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{E}_i$  and  $\mathbf{B} = \sum_{j=1}^l \mu_j \mathbf{F}_j$  are the spectral forms of a self-adjoint transformations  $\mathbf{A}$  and  $\mathbf{B}$  on a finite-dimensional inner product space, then a necessary and sufficient condition (“if and only if = iff”) that  $\mathbf{A}$  and  $\mathbf{B}$  commute is that the projections  $\mathbf{E}_i$ ,  $1 \leq i \leq k$  and  $\mathbf{F}_j$ ,  $1 \leq j \leq l$  commute with each other; i.e.,  $[\mathbf{E}_i, \mathbf{F}_j] = \mathbf{E}_i \mathbf{F}_j - \mathbf{F}_j \mathbf{E}_i = 0$ .

Again, sufficiency is derived easily: if  $\mathbf{F}_j$ ,  $1 \leq j \leq l$  occurring in the spectral decomposition of  $\mathbf{B}$  commutes with all the projectors  $\mathbf{E}_i$ ,  $1 \leq i \leq k$  in the spectral composition of  $\mathbf{A}$ , then, by linearity,  $\mathbf{B}$  commutes with  $\mathbf{A}$ .

Necessity follows from the fact that, if  $\mathbf{F}_j$ ,  $1 \leq j \leq l$  commutes with  $\mathbf{A}$  then it also commutes with every polynomial of  $\mathbf{A}$ ; and hence also with  $p_i(\mathbf{A}) = \mathbf{E}_i$ , as shown in (4.173). Conversely, if  $\mathbf{E}_i$ ,  $1 \leq i \leq k$  commutes with  $\mathbf{B}$  then it also commutes with every polynomial of  $\mathbf{B}$ ; and hence also with the associated polynomial  $q_j(\mathbf{A}) = \mathbf{E}_j$ , as shown in (4.173).

If  $\mathbf{E}_x = |\mathbf{x}\rangle\langle\mathbf{x}|$  and  $\mathbf{E}_y = |\mathbf{y}\rangle\langle\mathbf{y}|$  are two commuting projections (into one-dimensional subspaces of  $\mathfrak{V}$ ) corresponding to the normalized vectors  $\mathbf{x}$  and  $\mathbf{y}$ , respectively; that is, if  $[\mathbf{E}_x, \mathbf{E}_y] = \mathbf{E}_x \mathbf{E}_y - \mathbf{E}_y \mathbf{E}_x = 0$ , then they are either identical (the vectors are collinear) or orthogonal (the vectors  $\mathbf{x}$  is orthogonal to  $\mathbf{y}$ ).

For proofs and additional information see §79 & §84 in

Paul R. Halmos. *Finite-dimensional Vector Spaces*. Springer, New York, Heidelberg, Berlin, 1974

For a proof, note that if  $\mathbf{E}_x$  and  $\mathbf{E}_y$  commute, then  $\mathbf{E}_x\mathbf{E}_y = \mathbf{E}_y\mathbf{E}_x$ ; and hence  $|\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{y}\rangle\langle\mathbf{y}| = |\mathbf{y}\rangle\langle\mathbf{y}|\mathbf{x}\rangle\langle\mathbf{x}|$ . Thus,  $(\langle\mathbf{x}|\mathbf{y}\rangle)|\mathbf{x}\rangle\langle\mathbf{y}| = (\overline{\langle\mathbf{x}|\mathbf{y}\rangle})|\mathbf{y}\rangle\langle\mathbf{x}|$ , which, applied to arbitrary vectors  $|\nu\rangle \in \mathfrak{V}$ , is only true if either  $\mathbf{x} = \pm\mathbf{y}$ , or if  $\mathbf{x} \perp \mathbf{y}$  (and thus  $\langle\mathbf{x}|\mathbf{y}\rangle = 0$ ).

A set  $\mathbf{M} = \{\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k\}$  of self-adjoint transformations on a finite-dimensional inner product space are mutually commuting if and only if there exists a self-adjoint transformation  $\mathbf{R}$  and a set of real-valued functions  $F = \{f_1, f_2, \dots, f_k\}$  of a real variable so that  $\mathbf{A}_1 = f_1(\mathbf{R})$ ,  $\mathbf{A}_2 = f_2(\mathbf{R})$ , ...,  $\mathbf{A}_k = f_k(\mathbf{R})$ . If such a *maximal operator*  $\mathbf{R}$  exists, then it can be written as a function of all transformations in the set  $\mathbf{M}$ ; that is,  $\mathbf{R} = G(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$ , where  $G$  is a suitable real-valued function of  $n$  variables (cf. Ref. <sup>26</sup>, Satz 8).

The maximal operator  $\mathbf{R}$  can be interpreted as encoding or containing all the information of a collection of commuting operators at once; stated pointedly, rather than consider all the operators in  $\mathbf{M}$  separately, the maximal operator  $\mathbf{R}$  represents  $\mathbf{M}$ ; in a sense, the operators  $\mathbf{A}_i \in \mathbf{M}$  are all just incomplete *aspects* of, or individual “lossy” (i.e., one-to-many) functional views on, the maximal operator  $\mathbf{R}$ .

Let us demonstrate the machinery developed so far by an example. Consider the normal matrices

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 2 & 3 & 0 \\ 3 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \mathbf{C} = \begin{pmatrix} 5 & 7 & 0 \\ 7 & 5 & 0 \\ 0 & 0 & 11 \end{pmatrix},$$

which are mutually commutative; that is,  $[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA} = [\mathbf{A}, \mathbf{C}] = \mathbf{AC} - \mathbf{BC} = [\mathbf{B}, \mathbf{C}] = \mathbf{BC} - \mathbf{CB} = 0$ .

The eigensystems – that is, the set of the set of eigenvalues and the set of the associated eigenvectors – of  $\mathbf{A}$ ,  $\mathbf{B}$  and  $\mathbf{C}$  are

$$\begin{aligned} &\{\{1, -1, 0\}, \{(1, 1, 0)^T, (-1, 1, 0)^T, (0, 0, 1)^T\}, \\ &\{5, -1, 0\}, \{(1, 1, 0)^T, (-1, 1, 0)^T, (0, 0, 1)^T\}, \\ &\{12, -2, 11\}, \{(1, 1, 0)^T, (-1, 1, 0)^T, (0, 0, 1)^T\}. \end{aligned} \quad (4.201)$$

They share a common orthonormal set of eigenvectors

$$\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

which form an orthonormal basis of  $\mathbb{R}^3$  or  $\mathbb{C}^3$ . The associated projections are obtained by the outer (dyadic or tensor) products of these vectors; that

<sup>26</sup> John von Neumann. Über Funktionen von Funktionaloperatoren. *Annals of Mathematics*, 32:191–226, 1931. URL <http://www.jstor.org/stable/1968185>

is,

$$\begin{aligned}\mathbf{E}_1 &= \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \mathbf{E}_2 &= \frac{1}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ \mathbf{E}_3 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.\end{aligned}\tag{4.202}$$

Thus the spectral decompositions of  $\mathbf{A}$ ,  $\mathbf{B}$  and  $\mathbf{C}$  are

$$\begin{aligned}\mathbf{A} &= \mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3, \\ \mathbf{B} &= 5\mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3, \\ \mathbf{C} &= 12\mathbf{E}_1 - 2\mathbf{E}_2 + 11\mathbf{E}_3,\end{aligned}\tag{4.203}$$

respectively.

One way to define the maximal operator  $\mathbf{R}$  for this problem would be

$$\mathbf{R} = \alpha\mathbf{E}_1 + \beta\mathbf{E}_2 + \gamma\mathbf{E}_3,$$

with  $\alpha, \beta, \gamma \in \mathbb{R} - 0$  and  $\alpha \neq \beta \neq \gamma \neq \alpha$ . The functional coordinates  $f_i(\alpha)$ ,  $f_i(\beta)$ , and  $f_i(\gamma)$ ,  $i \in \{\mathbf{A}, \mathbf{B}, \mathbf{C}\}$ , of the three functions  $f_{\mathbf{A}}(\mathbf{R})$ ,  $f_{\mathbf{B}}(\mathbf{R})$ , and  $f_{\mathbf{C}}(\mathbf{R})$  chosen to match the projection coefficients obtained in Eq. (4.203); that is,

$$\begin{aligned}\mathbf{A} &= f_{\mathbf{A}}(\mathbf{R}) = \mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3, \\ \mathbf{B} &= f_{\mathbf{B}}(\mathbf{R}) = 5\mathbf{E}_1 - \mathbf{E}_2 + 0\mathbf{E}_3, \\ \mathbf{C} &= f_{\mathbf{C}}(\mathbf{R}) = 12\mathbf{E}_1 - 2\mathbf{E}_2 + 11\mathbf{E}_3.\end{aligned}\tag{4.204}$$

As a consequence, the functions  $\mathbf{A}$ ,  $\mathbf{B}$ ,  $\mathbf{C}$  need to satisfy the relations

$$\begin{aligned}f_{\mathbf{A}}(\alpha) &= 1, f_{\mathbf{A}}(\beta) = -1, f_{\mathbf{A}}(\gamma) = 0, \\ f_{\mathbf{B}}(\alpha) &= 5, f_{\mathbf{B}}(\beta) = -1, f_{\mathbf{B}}(\gamma) = 0, \\ f_{\mathbf{C}}(\alpha) &= 12, f_{\mathbf{C}}(\beta) = -2, f_{\mathbf{C}}(\gamma) = 11.\end{aligned}\tag{4.205}$$

It is no coincidence that the projections in the spectral forms of  $\mathbf{A}$ ,  $\mathbf{B}$  and  $\mathbf{C}$  are identical. Indeed it can be shown that mutually commuting *normal operators* always share the same eigenvectors; and thus also the same projections.

Let the set  $\mathbf{M} = \{\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k\}$  be mutually commuting normal (or Hermitian, or self-adjoint) transformations on an  $n$ -dimensional inner product space. Then there exists an orthonormal basis  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  such that every  $\mathbf{f}_j \in \mathfrak{B}$  is an eigenvector of each of the  $\mathbf{A}_i \in \mathbf{M}$ . Equivalently, there exist  $n$  orthogonal projections (let the vectors  $\mathbf{f}_j$  be represented by

the coordinates which are column vectors)  $\mathbf{E}_j = \mathbf{f}_j \otimes \mathbf{f}_j^T$  such that every  $\mathbf{E}_j$ ,  $1 \leq j \leq n$  occurs in the spectral form of each of the  $\mathbf{A}_i \in \mathbf{M}$ .

Informally speaking, a “generic” maximal operator  $\mathbf{R}$  on an  $n$ -dimensional Hilbert space  $\mathfrak{H}$  can be interpreted as some orthonormal basis  $\{\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_n\}$  of  $\mathfrak{H}$  – indeed, the  $n$  elements of that basis would have to correspond to the projections occurring in the spectral decomposition of the self-adjoint operators generated by  $\mathbf{R}$ .

Likewise, the “maximal knowledge” about a quantized physical system – in terms of empirical operational quantities – would correspond to such a single maximal operator; or to the orthonormal basis corresponding to the spectral decomposition of it. Thus it might not be unreasonable to speculate that a particular (pure) physical state is best characterized by a particular orthonormal basis.

### 4.33 Measures on closed subspaces

In what follows we shall assume that all (*probability*) *measures* or *states*  $w$  behave quasi-classically on sets of mutually commuting self-adjoint operators, and in particular on orthogonal projections.

Suppose  $\mathbf{E} = \{\mathbf{E}_1, \mathbf{E}_2, \dots, \mathbf{E}_n\}$  is a set of mutually commuting orthogonal projections on a finite-dimensional inner product space  $\mathfrak{H}$ . Then, the probability measure  $w$  should be *additive*; that is,

$$w(\mathbf{E}_1 + \mathbf{E}_2 + \dots + \mathbf{E}_n) = w(\mathbf{E}_1) + w(\mathbf{E}_2) + \dots + w(\mathbf{E}_n). \quad (4.206)$$

Stated differently, we shall assume that, for any two orthogonal projections  $\mathbf{E}, \mathbf{F}$  so that  $\mathbf{E}\mathbf{F} = \mathbf{F}\mathbf{E} = 0$ , their sum  $\mathbf{G} = \mathbf{E} + \mathbf{F}$  has expectation value

$$\langle \mathbf{G} \rangle = \langle \mathbf{E} \rangle + \langle \mathbf{F} \rangle. \quad (4.207)$$

We shall consider only vector spaces of dimension three or greater, since only in these cases two orthonormal bases can be interlinked by a common vector – in two dimensions, distinct orthonormal bases contain distinct basis vectors.

#### 4.33.1 Gleason's theorem

Suppose again the additivity of probabilities of mutually commuting (co-measurable) perpendicular projections. Then, for a Hilbert space of dimension three or greater, the only possible form of the expectation value of an self-adjoint operator  $\mathbf{A}$  has the form<sup>27</sup>

$$\langle \mathbf{A} \rangle = \text{Tr}(\rho \mathbf{A}), \quad (4.208)$$

the trace of the operator product of the density matrix (which is a positive operator of the trace class)  $\rho$  for the system with the matrix representation of  $\mathbf{A}$ .

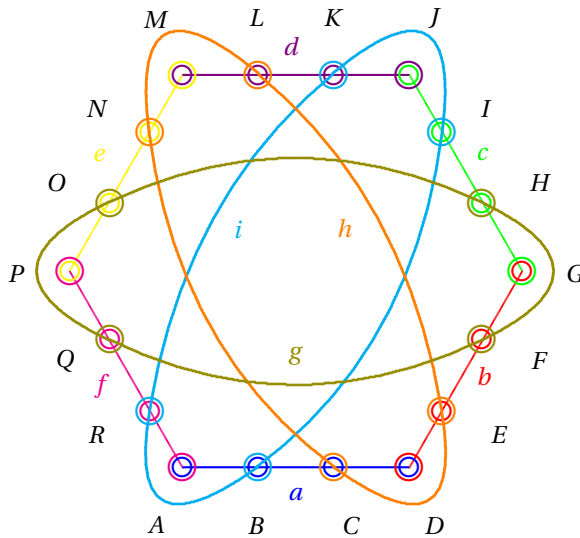
<sup>27</sup> Andrew M. Gleason. Measures on the closed subspaces of a Hilbert space. *Journal of Mathematics and Mechanics (now Indiana University Mathematics Journal)*, 6(4):885–893, 1957. ISSN 0022-2518. DOI: 10.1512/iumj.1957.6.56050. URL <http://dx.doi.org/10.1512/iumj.1957.6.56050>; Anatolij Dvurečenskij. *Gleason's Theorem and Its Applications*. Kluwer Academic Publishers, Dordrecht, 1993; Itamar Pitowsky. Infinite and finite Gleason's theorems and the logic of indeterminacy. *Journal of Mathematical Physics*, 39(1):218–228, 1998. DOI: 10.1063/1.532334. URL <http://dx.doi.org/10.1063/1.532334>; Fred Richman and Douglas Bridges. A constructive proof of Gleason's theorem. *Journal of Functional Analysis*, 162:287–

In particular, if  $\mathbf{A}$  is a projection  $\mathbf{E}$  corresponding to an elementary yes-no proposition “the system has property  $Q$ ,” then  $\langle \mathbf{E} \rangle = \text{Tr}(\rho \mathbf{E})$  corresponds to the probability of that property  $Q$  if the system is in state  $\rho$ .

#### 4.33.2 Kochen-Specker theorem

For a Hilbert space of dimension three or greater, there does not exist any two-valued probability measures interpretable as consistent, overall truth assignment<sup>28</sup>. As a result of the nonexistence of two-valued states, the classical strategy to construct probabilities by a convex combination of all two-valued states fails entirely.

In *Greechie diagram*<sup>29</sup>, points represent basis vectors. If they belong to the same basis, they are connected by smooth curves.



The most compact way of deriving the Kochen-Specker theorem in four dimensions has been given by Cabello<sup>30</sup>. For the sake of demonstration, consider a Greechie (orthogonality) diagram of a finite subset of the continuum of blocks or contexts embeddable in four-dimensional real Hilbert space without a two-valued probability measure. The proof of the Kochen-Specker theorem uses nine tightly interconnected contexts  $a = \{A, B, C, D\}$ ,  $b = \{D, E, F, G\}$ ,  $c = \{G, H, I, J\}$ ,  $d = \{J, K, L, M\}$ ,  $e = \{M, N, O, P\}$ ,  $f = \{P, Q, R, A\}$ ,  $g = \{B, I, K, R\}$ ,  $h = \{C, E, L, N\}$ ,  $i = \{F, H, O, Q\}$  consisting of the 18 projections associated with the one dimensional subspaces spanned by the vectors from the origin  $(0, 0, 0, 0)$  to  $A = (0, 0, 1, -1)$ ,  $B = (1, -1, 0, 0)$ ,  $C = (1, 1, -1, -1)$ ,  $D = (1, 1, 1, 1)$ ,  $E = (1, -1, 1, -1)$ ,  $F = (1, 0, -1, 0)$ ,  $G = (0, 1, 0, -1)$ ,  $H = (1, 0, 1, 0)$ ,  $I = (1, 1, -1, 1)$ ,  $J = (-1, 1, 1, 1)$ ,  $K = (1, 1, 1, -1)$ ,  $L = (1, 0, 0, 1)$ ,  $M = (0, 1, -1, 0)$ ,  $N = (0, 1, 1, 0)$ ,  $O = (0, 0, 0, 1)$ ,  $P = (1, 0, 0, 0)$ ,  $Q = (0, 1, 0, 0)$ ,  $R = (0, 0, 1, 1)$ , respectively. Greechie diagrams represent atoms by points, and contexts by maximal smooth, unbroken curves.

<sup>28</sup> Ernst Specker. Die Logik nicht gleichzeitig entscheidbarer Aussagen. *Dialectica*, 14(2-3):239–246, 1960. DOI: 10.1111/j.1746-8361.1960.tb00422.x. URL <http://dx.doi.org/10.1111/j.1746-8361.1960.tb00422.x>; and Simon Kochen and Ernst P. Specker. The problem of hidden variables in quantum mechanics. *Journal of Mathematics and Mechanics (now Indiana University Mathematics Journal)*, 17(1):59–87, 1967. ISSN 0022-2518. DOI: 10.1512/iumj.1968.17.17004. URL <http://dx.doi.org/10.1512/iumj.1968.17.17004>

<sup>29</sup> J. R. Greechie. Orthomodular lattices admitting no states. *Journal of Combinatorial Theory*, 10:119–132, 1971. DOI: 10.1016/0097-3165(71)90015-X. URL [http://dx.doi.org/10.1016/0097-3165\(71\)90015-X](http://dx.doi.org/10.1016/0097-3165(71)90015-X)

<sup>30</sup> Adán Cabello, José M. Estebaranz, and G. García-Alcaine. Bell-Kochen-Specker theorem: A proof with 18 vectors. *Physics Letters A*, 212(4):183–187, 1996. DOI: 10.1016/0375-9601(96)00134-X. URL [http://dx.doi.org/10.1016/0375-9601\(96\)00134-X](http://dx.doi.org/10.1016/0375-9601(96)00134-X); and Adán Cabello. Kochen-Specker theorem and experimental test on hidden variables. *International Journal of Modern Physics, A* 15(18):2813–2820, 2000. DOI: 10.1142/S0217751X00002020. URL <http://dx.doi.org/10.1142/S0217751X00002020>

In a proof by contradiction, note that, on the one hand, every observable proposition occurs in exactly *two* contexts. Thus, in an enumeration of the four observable propositions of each of the nine contexts, there appears to be an *even* number of true propositions, provided that the value of an observable does not depend on the context (i.e. the assignment is *non-contextual*). Yet, on the other hand, as there is an *odd* number (actually nine) of contexts, there should be an *odd* number (actually nine) of true propositions.







# 5

## Tensors

What follows is a “corollary,” or rather an expansion and extension, of what has been presented in the previous chapter; in particular, with regards to dual vector spaces (page 28), and the tensor product (page 36).

### 5.1 Notation

Let us consider the vector space  $\mathbb{R}^n$  of dimension  $n$ ; a basis  $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$  consisting of  $n$  basis vectors  $\mathbf{e}_i$ , and  $k$  arbitrary vectors  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k \in \mathbb{R}^n$ ; the vector  $\mathbf{x}_i$  having the vector components  $X_1^i, X_2^i, \dots, X_k^i \in \mathbb{R}$ .

Please note again that, just like any tensor (field), the tensor product  $\mathbf{z} = \mathbf{x} \otimes \mathbf{y}$  of two vectors  $\mathbf{x}$  and  $\mathbf{y}$  has three equivalent representations:

- (i) as the scalar coordinates  $X^i Y^j$  with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded; this form is often used in the theory of (general) relativity;
- (ii) as the quasi-matrix  $z^{ij} = X^i Y^j$ , whose components  $z^{ij}$  are defined with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded; this form is often used in classical (as compared to quantum) mechanics and electrodynamics;
- (iii) as a quasi-vector or “flattened matrix” defined by the Kronecker product  $\mathbf{z} = (X^1 \mathbf{y}, X^2 \mathbf{y}, \dots, X^n \mathbf{y}) = (X^1 Y^1, \dots, X^1 Y^n, \dots, X^n Y^1, \dots, X^n Y^n)$ . Again, the scalar coordinates  $X^i Y^j$  are defined with respect to the basis in which the vectors  $\mathbf{x}$  and  $\mathbf{y}$  have been defined and coded. This latter form is often used in (few-partite) quantum mechanics.

In all three cases, the pairs  $X^i Y^j$  are properly represented by distinct mathematical entities.

*Tensor fields* define tensors in every point of  $\mathbb{R}^n$  separately. In general, with respect to a particular basis, the components of a tensor field depend on the coordinates.

We adopt Einstein’s summation convention to sum over equal indices (a pair with a superscript and a subscript). Sometimes, sums are written out

explicitly.

In what follows, the notations “ $x \cdot y$ ”, “ $(x, y)$ ” and “ $\langle x | y \rangle$ ” will be used synonymously for the *scalar product* or *inner product*. Note, however, that the “dot notation  $x \cdot y$ ” may be a little bit misleading; for example, in the case of the “pseudo-Euclidean” metric represented by the matrix  $\text{diag}(+, +, +, \dots, +, -)$ , it is no more the standard Euclidean dot product  $\text{diag}(+, +, +, \dots, +, +)$ .

For a more systematic treatment, see for instance Klingbeil’s or Dirschmid’s introductions<sup>1</sup>.

<sup>1</sup> Ebergard Klingbeil. *Tensorrechnung für Ingenieure*. Bibliographisches Institut, Mannheim, 1966; and Hans Jörg Dirschmid. *Tensoren und Felder*. Springer, Vienna, 1996

## 5.2 Multilinear form

A *multilinear form*

$$\alpha : \mathfrak{V}^k \mapsto \mathbb{R} \text{ or } \mathbb{C} \quad (5.1)$$

is a map from (multiple) arguments  $\mathbf{x}_i$  which are elements of some vector space  $\mathfrak{V}$  into some scalars in  $\mathbb{R}$  or  $\mathbb{C}$ , satisfying

$$\begin{aligned} \alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, A\mathbf{y} + B\mathbf{z}, \dots, \mathbf{x}_k) &= A\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{y}, \dots, \mathbf{x}_k) \\ &\quad + B\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{z}, \dots, \mathbf{x}_k) \end{aligned} \quad (5.2)$$

for every one of its (multi-)arguments.

In what follows we shall concentrate on *real-valued* multilinear forms which map  $k$  vectors in  $\mathbb{R}^n$  into  $\mathbb{R}$ .

## 5.3 Covariant tensors

Let  $\mathbf{x}_i = \sum_{j_i=1}^n X_i^{j_i} \mathbf{e}_{j_i} = X_i^{j_i} \mathbf{e}_{j_i}$  be some vector in (i.e., some element of) an  $n$ -dimensional vector space  $\mathfrak{V}$  labelled by an index  $i$ . A tensor of rank  $k$

$$\alpha : \mathfrak{V}^k \mapsto \mathbb{R} \quad (5.3)$$

is a multilinear form

$$\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k) = \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n X_1^{i_1} X_2^{i_2} \dots X_k^{i_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_k}). \quad (5.4)$$

The

$$A_{i_1 i_2 \dots i_k} \stackrel{\text{def}}{=} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_k}) \quad (5.5)$$

are the *components* or *coordinates* of the tensor  $\alpha$  with respect to the basis  $\mathfrak{B}$ .

Note that a tensor of type (or rank)  $k$  in  $n$ -dimensional vector space has  $n^k$  coordinates.

To prove that tensors are multilinear forms, insert

$$\begin{aligned}
 & \alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, A\mathbf{x}_j^1 + B\mathbf{x}_j^2, \dots, \mathbf{x}_k) \\
 = & \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_k=1}^n X_1^{i_1} X_2^{i_2} \cdots [A(X^1)_j^{i_j} + B(X^2)_j^{i_j}] \cdots X_k^{i_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_j}, \dots, \mathbf{e}_{i_k}) \\
 = & A \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_k=1}^n X_1^{i_1} X_2^{i_2} \cdots (X^1)_j^{i_j} \cdots X_k^{i_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_j}, \dots, \mathbf{e}_{i_k}) \\
 & + B \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_k=1}^n X_1^{i_1} X_2^{i_2} \cdots (X^2)_j^{i_j} \cdots X_k^{i_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_j}, \dots, \mathbf{e}_{i_k}) \\
 = & A\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_j^1, \dots, \mathbf{x}_k) + B\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_j^2, \dots, \mathbf{x}_k)
 \end{aligned}$$

### 5.3.1 Change of Basis

Let  $\mathfrak{B}$  and  $\mathfrak{B}'$  be two arbitrary bases of  $\mathbb{R}^n$ . Then every vector  $\mathbf{e}'_i$  of  $\mathfrak{B}'$  can be represented as linear combination of basis vectors from  $\mathfrak{B}$  [see also Eqs. (4.83) and (4.84)]; that is,

$$\mathbf{e}'_i = \sum_{j=1}^n a_i^j \mathbf{e}_j, \quad i = 1, \dots, n. \quad (5.6)$$

Consider an arbitrary vector  $\mathbf{x} \in \mathbb{R}^n$  with components  $X^i$  with respect to the basis  $\mathfrak{B}$  and  $X'^i$  with respect to the basis  $\mathfrak{B}'$ :

$$\mathbf{x} = \sum_{i=1}^n X^i \mathbf{e}_i = \sum_{i=1}^n X'^i \mathbf{e}'_i. \quad (5.7)$$

Insertion into (5.6) yields

$$\begin{aligned}
 \mathbf{x} &= \sum_{i=1}^n X^i \mathbf{e}_i = \sum_{i=1}^n X'^i \mathbf{e}'_i = \sum_{i=1}^n X'^i \sum_{j=1}^n a_i^j \mathbf{e}_j \\
 &= \sum_{i=1}^n \left[ \sum_{j=1}^n a_i^j X'^i \right] \mathbf{e}_j = \sum_{j=1}^n \left[ \sum_{i=1}^n a_i^j X'^i \right] \mathbf{e}_j = \sum_{j=1}^n \left[ \sum_{i=1}^n a_j^i X'^i \right] \mathbf{e}_j.
 \end{aligned} \quad (5.8)$$

A comparison of coefficient (and a renaming of the indices  $i \leftrightarrow j$ ) yields the transformation laws of vector components [see also Eq. (4.90)]

$$X^j = \sum_{i=1}^n a_i^j X'^i. \quad (5.9)$$

The matrix  $a = \{a_i^j\}$  is called the *transformation matrix*.

If the basis transformations involve nonlinear coordinate changes – such as from the Cartesian to the polar or spherical coordinates discussed later – we have to employ differentials

$$dX^j = \sum_{i=1}^n a_i^j dX'^i, \quad (5.10)$$

as well as

$$a_i^j = \frac{\partial X^j}{\partial X'^i}. \quad (5.11)$$

By assuming that the coordinate transformations are linear  $a_i^j$  can be expressed as in terms of the coordinates  $X^j$

$$a_i^j = \frac{X^j}{X'^i}. \quad (5.12)$$

A similar argument using

$$\mathbf{e}_i = \sum_{j=1}^n a'_i{}^j \mathbf{e}'_j, \quad i = 1, \dots, n \quad (5.13)$$

yields the inverse transformation laws

$$X'^j = \sum_{i=1}^n a'_i{}^j X^i. \quad (5.14)$$

Thereby,

$$\mathbf{e}_i = \sum_{j=1}^n a'_i{}^j \mathbf{e}'_j = \sum_{j=1}^n a'_i{}^j \sum_{k=1}^n a_j^k \mathbf{e}_k = \sum_{j=1}^n \sum_{k=1}^n [a'_i{}^j a_j^k] \mathbf{e}_k, \quad (5.15)$$

which, due to the linear independence of the basis vectors  $\mathbf{e}_i$  of  $\mathfrak{B}$ , is only satisfied if

$$a'_i{}^j a_j^k = \delta_i^k \quad \text{or} \quad \mathbf{A}' \mathbf{A} = \mathbb{I}. \quad (5.16)$$

That is,  $\mathbf{A}'$  is the *inverse matrix*  $\mathbf{A}^{-1}$  of  $\mathbf{A}$ . In index notation,

$$(a^{-1})_i{}^j = a'_i{}^j = \frac{X'^j}{X^i} \quad (5.17)$$

for linear coordinate transformations and

$$dX'^j = \sum_{i=1}^n a'_i{}^j dX^i = \sum_{i=1}^n (a^{-1})_i{}^j dX^i, \quad (5.18)$$

as well as

$$(a^{-1})_i{}^j = a'_i{}^j = \frac{\partial X'^j}{\partial X^i} = J_{ij}, \quad (5.19)$$

where  $J_{ij}$  stands for the *Jacobian matrix*

$$J \equiv J_{ij} = \frac{\partial X'^i}{\partial X^j} \equiv \begin{pmatrix} \frac{\partial X'^1}{\partial X^1} & \cdots & \frac{\partial X'^1}{\partial X^n} \\ \vdots & \ddots & \vdots \\ \frac{\partial X'^n}{\partial X^1} & \cdots & \frac{\partial X'^n}{\partial X^n} \end{pmatrix}. \quad (5.20)$$

### 5.3.2 Transformation of tensor components

Because of multilinearity and by insertion into (5.6),

$$\begin{aligned} \alpha(\mathbf{e}'_{j_1}, \mathbf{e}'_{j_2}, \dots, \mathbf{e}'_{j_k}) &= \alpha \left( \sum_{i_1=1}^n a_{j_1}^{i_1} \mathbf{e}_{i_1}, \sum_{i_2=1}^n a_{j_2}^{i_2} \mathbf{e}_{i_2}, \dots, \sum_{i_k=1}^n a_{j_k}^{i_k} \mathbf{e}_{i_k} \right) \\ &= \sum_{i_1=1}^n \sum_{i_2=1}^n \cdots \sum_{i_k=1}^n a_{j_1}^{i_1} a_{j_2}^{i_2} \cdots a_{j_k}^{i_k} \alpha(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \dots, \mathbf{e}_{i_k}) \end{aligned} \quad (5.21)$$

or

$$A'_{j_1 j_2 \dots j_k} = \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_k}. \quad (5.22)$$

## 5.4 Contravariant tensors

### 5.4.1 Definition of contravariant basis

Consider again a covariant basis  $\mathfrak{B} = \{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$  consisting of  $n$  basis vectors  $\mathbf{e}_i$ . Just as on page 30 earlier, we shall define a *contravariant* basis  $\mathfrak{B}^* = \{\mathbf{e}^1, \mathbf{e}^2, \dots, \mathbf{e}^n\}$  consisting of  $n$  basis vectors  $\mathbf{e}^i$  by the requirement that the scalar product obeys

$$\delta_i^j = \mathbf{e}^i \cdot \mathbf{e}_j \equiv (\mathbf{e}^i, \mathbf{e}_j) \equiv \langle \mathbf{e}^i | \mathbf{e}_j \rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}. \quad (5.23)$$

To distinguish elements of the two bases, the covariant vectors are denoted by *subscripts*, whereas the contravariant vectors are denoted by *superscripts*. The last terms  $\mathbf{e}^i \cdot \mathbf{e}_j \equiv (\mathbf{e}^i, \mathbf{e}_j) \equiv \langle \mathbf{e}^i | \mathbf{e}_j \rangle$  recall different notations of the scalar product.

Again, note that (the coordinates of) the dual basis vectors of an orthonormal basis can be coded identically as (the coordinates of) the original basis vectors; that is, in this case, (the coordinates of) the dual basis vectors are just rearranged as the transposed form of the original basis vectors.

The entire tensor formalism developed so far can be transferred and applied to define *contravariant* tensors as multilinear forms

$$\beta : \mathfrak{V}^{*k} \mapsto \mathbb{R} \quad (5.24)$$

by

$$\beta(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^k) = \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n \Xi_{i_1}^1 \Xi_{i_2}^2 \dots \Xi_{i_k}^k \beta(\mathbf{e}^{i_1}, \mathbf{e}^{i_2}, \dots, \mathbf{e}^{i_k}). \quad (5.25)$$

The

$$B^{i_1 i_2 \dots i_k} = \beta(\mathbf{e}^{i_1}, \mathbf{e}^{i_2}, \dots, \mathbf{e}^{i_k}) \quad (5.26)$$

are the *components* of the contravariant tensor  $\beta$  with respect to the basis  $\mathfrak{B}^*$ .

More generally, suppose  $\mathfrak{V}$  is an  $n$ -dimensional vector space, and  $\mathfrak{B} = \{\mathbf{f}_1, \dots, \mathbf{f}_n\}$  is a basis of  $\mathfrak{V}$ ; if  $g_{ij}$  is the *metric tensor*, the dual basis is defined by

$$g(f_i^*, f_j) = g(f^i, f_j) = \delta^i_j, \quad (5.27)$$

where again  $\delta^i_j$  is Kronecker delta function, which is defined

$$\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j, \\ 1 & \text{for } i = j. \end{cases} \quad (5.28)$$

regardless of the order of indices, and regardless of whether these indices represent covariance and contravariance.

#### 5.4.2 Connection between the transformation of covariant and contravariant entities

Because of linearity, we can make the formal *Ansatz*

$$\mathbf{e}'^j = \sum_i b_i^j \mathbf{e}^i, \quad (5.29)$$

where  $[b_i^j] = \mathbf{B}$  is the transformation matrix associated with the contravariant basis. How is  $b$  related to  $a$ , the transformation matrix associated with the covariant basis?

By exploiting (5.23) one can find the connection between the transformation of covariant and contravariant basis elements and thus tensor components; that is,

$$\delta_i^j = \mathbf{e}'_i \cdot \mathbf{e}'^j = (a_i^k \mathbf{e}_k) \cdot (b_l^j \mathbf{e}^l) = a_i^k b_l^j \mathbf{e}_k \cdot \mathbf{e}^l = a_i^k b_l^j \delta_k^l = a_i^k b_k^j, \quad (5.30)$$

and thus, if  $\mathbf{B}$  represents the transformation (matrix) whose components are  $b_i^j$ ,

$$\mathbf{B} = \mathbf{A}^{-1} = \mathbf{A}', \text{ and } \mathbf{e}'^j = \sum_i (a^{-1})_i^j \mathbf{e}^i = \sum_i a_i'^j \mathbf{e}^i. \quad (5.31)$$

The argument concerning transformations of covariant tensors and components can be carried through to the contravariant case. Hence, the contravariant components transform as

$$\begin{aligned} \beta(\mathbf{e}'^{j_1}, \mathbf{e}'^{j_2}, \dots, \mathbf{e}'^{j_k}) &= \beta\left(\sum_{i_1=1}^n a_{i_1}'^{j_1} \mathbf{e}^{i_1}, \sum_{i_2=1}^n a_{i_2}'^{j_2} \mathbf{e}^{i_2}, \dots, \sum_{i_k=1}^n a_{i_k}'^{j_k} \mathbf{e}^{i_k}\right) \\ &= \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n a_{i_1}'^{j_1} a_{i_2}'^{j_2} \dots a_{i_k}'^{j_k} \beta(\mathbf{e}^{i_1}, \mathbf{e}^{i_2}, \dots, \mathbf{e}^{i_k}) \end{aligned} \quad (5.32)$$

or

$$B'^{j_1 j_2 \dots j_k} = \sum_{i_1=1}^n \sum_{i_2=1}^n \dots \sum_{i_k=1}^n a_{i_1}'^{j_1} a_{i_2}'^{j_2} \dots a_{i_k}'^{j_k} B^{i_1 i_2 \dots i_k}. \quad (5.33)$$

### 5.5 Orthonormal bases

For orthonormal bases of  $n$ -dimensional Hilbert space,

$$\delta_i^j = \mathbf{e}_i \cdot \mathbf{e}^j \text{ if and only if } \mathbf{e}_i = \mathbf{e}^i \text{ for all } 1 \leq i, j \leq n. \quad (5.34)$$

Therefore, the vector space and its dual vector space are “identical” in the sense that the coordinate tuples representing their bases are identical (though relatively transposed). That is, besides transposition, the two bases are identical

$$\mathfrak{B} \equiv \mathfrak{B}^* \quad (5.35)$$

and formally any distinction between covariant and contravariant vectors becomes irrelevant. Conceptually, such a distinction persists, though. In this sense, we might “forget about the difference between covariant and contravariant orders.”

## 5.6 Invariant tensors and physical motivation

### 5.7 Metric tensor

Metric tensors are defined in metric vector spaces. A metric vector space (sometimes also referred to as “vector space with metric” or “geometry”) is a vector space with some inner or scalar product. This includes (pseudo-) Euclidean spaces with indefinite metric. (I.e., the distance needs not be positive or zero.)

#### 5.7.1 Definition metric

A *metric*  $g$  is a functional  $\mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$  with the following properties:

- $g$  is symmetric; that is,  $g(x, y) = g(y, x)$ ;
- $g$  is bilinear; that is,  $g(\alpha x + \beta y, z) = \alpha g(x, z) + \beta g(y, z)$  (due to symmetry  $g$  is also bilinear in the second argument);
- $g$  is nondegenerate; that is, for every  $x \in \mathfrak{V}$ ,  $x \neq 0$ , there exists a  $y \in \mathfrak{V}$  such that  $g(x, y) \neq 0$ .

#### 5.7.2 Construction of a metric from a scalar product by metric tensor

In particular cases, the *metric* tensor may be defined *via* the scalar product

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j \equiv (\mathbf{e}_i, \mathbf{e}_j) \equiv \langle \mathbf{e}_i | \mathbf{e}_j \rangle. \quad (5.36)$$

and

$$g^{ij} = \mathbf{e}^i \cdot \mathbf{e}^j \equiv (\mathbf{e}^i, \mathbf{e}^j) \equiv \langle \mathbf{e}^i | \mathbf{e}^j \rangle. \quad (5.37)$$

By definition of the (dual) basis in Eq. (4.34) on page 30,

$$g^i_j = \mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j, \quad (5.38)$$

which is a reflection of the covariant and contravariant metric tensors being inverse, since the basis and the associated dual basis is inverse (and *vice versa*). Note that it is possible to change a covariant tensor into a contravariant one and *vice versa* by the application of a metric tensor. This can be seen as follows. Because of linearity, any contravariant basis vector  $\mathbf{e}^i$  can be written as a linear sum of covariant (transposed, but we do not mark transposition here) basis vectors:

$$\mathbf{e}^i = A^{ij} \mathbf{e}_j. \quad (5.39)$$



Then,

$$g^{ik} = \mathbf{e}^i \cdot \mathbf{e}^k = (A^{ij} \mathbf{e}_j) \cdot \mathbf{e}^k = A^{ij} (\mathbf{e}_j \cdot \mathbf{e}^k) = A^{ij} \delta_j^k = A^{ik} \quad (5.40)$$

and thus

$$\mathbf{e}^i = g^{ij} \mathbf{e}_j \quad (5.41)$$

and

$$\mathbf{e}_i = g_{ij} \mathbf{e}^j. \quad (5.42)$$

For orthonormal bases, the metric tensor can be represented as a Kronecker delta function, and thus remains form invariant. Moreover, its covariant and contravariant components are identical; that is,  $\delta_{ij} = \delta_j^i = \delta_i^j = \delta^{ij}$ .

### 5.7.3 What can the metric tensor do for us?

Most often it is used to raise or lower the indices; that is, to change from contravariant to covariant and conversely from covariant to contravariant.

For example,

$$\mathbf{x} = X^i \mathbf{e}_i = X^i g_{ij} \mathbf{e}^j = X_j \mathbf{e}^j, \quad (5.43)$$

and hence  $X_j = X^i g_{ij}$ .

In the previous section, the metric tensor has been derived from the scalar product. The converse can be true as well. (Note, however, that the metric need not be positive.) In Euclidean space with the dot (scalar, inner) product the metric tensor represents the scalar product between vectors: let  $\mathbf{x} = X^i \mathbf{e}_i \in \mathbb{R}^n$  and  $\mathbf{y} = Y^j \mathbf{e}_j \in \mathbb{R}^n$  be two vectors. Then ("T" stands for the transpose),

$$\mathbf{x} \cdot \mathbf{y} \equiv (\mathbf{x}, \mathbf{y}) \equiv \langle \mathbf{x} | \mathbf{y} \rangle = X^i \mathbf{e}_i \cdot Y^j \mathbf{e}_j = X^i Y^j \mathbf{e}_i \cdot \mathbf{e}_j = X^i Y^j g_{ij} = X^T g Y. \quad (5.44)$$

It also characterizes the length of a vector: in the above equation, set  $\mathbf{y} = \mathbf{x}$ . Then,

$$\mathbf{x} \cdot \mathbf{x} \equiv (\mathbf{x}, \mathbf{x}) \equiv \langle \mathbf{x} | \mathbf{x} \rangle = X^i X^j g_{ij} \equiv X^T g X, \quad (5.45)$$

and thus

$$||x|| = \sqrt{X^i X^j g_{ij}} = \sqrt{X^T g X}. \quad (5.46)$$

The square of an infinitesimal vector  $ds = ||d\mathbf{x}||$  is

$$(ds)^2 = g_{ij} d\mathbf{x}^i d\mathbf{x}^j = d\mathbf{x}^T g d\mathbf{x}. \quad (5.47)$$

### 5.7.4 Transformation of the metric tensor

Insertion into the definitions and coordinate transformations (5.13) as well as (5.17) yields

$$\begin{aligned} g_{ij} &= \mathbf{e}_i \cdot \mathbf{e}_j = a_i'^l \mathbf{e}'_l \cdot a_j'^m \mathbf{e}'_m = a_i'^l a_j'^m \mathbf{e}'_l \cdot \mathbf{e}'_m \\ &= a_i'^l a_j'^m g'_{lm} = \frac{\partial X'^l}{\partial X^i} \frac{\partial X'^m}{\partial X^j} g'_{lm}. \end{aligned} \quad (5.48)$$

Conversely, (5.6) as well as (5.12) yields

$$\begin{aligned} g'_{ij} &= \mathbf{e}'_i \cdot \mathbf{e}'_j = a_i^l \mathbf{e}_l \cdot a_j^m \mathbf{e}_m = a_i^l a_j^m \mathbf{e}_l \cdot \mathbf{e}_m \\ &= a_i^l a_j^m g_{lm} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X^m}{\partial X'^j} g_{lm}. \end{aligned} \quad (5.49)$$

If the geometry (i.e., the basis) is locally orthonormal,  $g_{lm} = \delta_{lm}$ , then  $g'_{ij} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X^l}{\partial X'^j}$ .

Just to check consistency with Eq. (5.38) we can compute, for suitable differentiable coordinates  $X$  and  $X'$ ,

$$\begin{aligned} g_i'^j &= \mathbf{e}'_i \cdot \mathbf{e}'^j = a_i^l \mathbf{e}_l \cdot (a^{-1})^j_m \mathbf{e}^m = a_i^l (a^{-1})^j_m \mathbf{e}_l \cdot \mathbf{e}^m \\ &= a_i^l (a^{-1})^j_m \delta_l^m = a_i^l (a^{-1})^j_l \\ &= \frac{\partial X^l}{\partial X'^i} \frac{\partial X'^l}{\partial X^j} = \frac{\partial X^l}{\partial X^j} \frac{\partial X'^l}{\partial X'^i} = \delta^{lj} \delta_{li} = \delta_i^l. \end{aligned} \quad (5.50)$$

In terms of the *Jacobian matrix* defined in Eq. (5.20) the metric tensor in Eq. (5.48) can be rewritten as

$$g = J^T g' J \equiv g_{ij} = J_{li} J_{mj} g'_{lm}. \quad (5.51)$$

The metric tensor and the Jacobian (determinant) are thus related by

$$\det g = (\det J^T)(\det g')(\det J). \quad (5.52)$$

If the manifold is embedded into an Euclidean space, then  $g'_{lm} = \delta_{lm}$  and  $g = J^T J$ .

### 5.7.5 Examples

In what follows a few metrics are enumerated and briefly commented. For a more systematic treatment, see, for instance, Snapper and Troyer's *Metric Affine geometry*<sup>2</sup>.

Note also that due to the properties of the metric tensor, its coordinate representation has to be a *symmetric matrix* with *nonzero diagonals*. For the symmetry  $g(\mathbf{x}, \mathbf{y}) = g(\mathbf{y}, \mathbf{x})$  implies that  $g_{ij} x_i y^j = g_{ij} y^i x_j = g_{ij} x_j y^i = g_{ji} x_i y^j$  for all coordinate tuples  $x^i$  and  $y^j$ . And for any zero diagonal entry (say, in the  $k$ 'th position of the diagonal we can choose a nonzero vector  $\mathbf{z}$  whose coordinates are all zero except the  $k$ 'th coordinate. Then  $g(\mathbf{z}, \mathbf{x}) = 0$  for all  $\mathbf{x}$  in the vector space.

#### *n-dimensional Euclidean space*

$$g \equiv \{g_{ij}\} = \text{diag}(\underbrace{1, 1, \dots, 1}_{n \text{ times}}) \quad (5.53)$$

One application in physics is quantum mechanics, where  $n$  stands for the dimension of a complex Hilbert space. Some definitions can be

<sup>2</sup> Ernst Snapper and Robert J. Troyer. *Metric Affine Geometry*. Academic Press, New York, 1971

easily adopted to accommodate the complex numbers. E.g., axiom 5 of the scalar product becomes  $(x, y) = \overline{(x, y)}$ , where “ $\overline{(x, y)}$ ” stands for complex conjugation of  $(x, y)$ . Axiom 4 of the scalar product becomes  $(x, \alpha y) = \overline{\alpha}(x, y)$ .

### *Lorentz plane*

$$g \equiv \{g_{ij}\} = \text{diag}(1, -1) \quad (5.54)$$

### *Minkowski space of dimension $n$*

In this case the metric tensor is called the *Minkowski metric* and is often denoted by “ $\eta$ ”:

$$\eta \equiv \{\eta_{ij}\} = \text{diag}(\underbrace{1, 1, \dots, 1}_{n-1 \text{ times}}, -1) \quad (5.55)$$

One application in physics is the theory of special relativity, where  $D = 4$ . Alexandrov’s theorem states that the mere requirement of the preservation of zero distance (i.e., lightcones), combined with bijectivity (one-to-oneness) of the transformation law yields the Lorentz transformations<sup>3</sup>.

### *Negative Euclidean space of dimension $n$*

$$g \equiv \{g_{ij}\} = \text{diag}(\underbrace{-1, -1, \dots, -1}_n) \quad (5.56)$$

### *Artinian four-space*

$$g \equiv \{g_{ij}\} = \text{diag}(+1, +1, -1, -1) \quad (5.57)$$

### *General relativity*

In general relativity, the metric tensor  $g$  is linked to the energy-mass distribution. There, it appears as the primary concept when compared to the scalar product. In the case of zero gravity,  $g$  is just the Minkowski metric (often denoted by “ $\eta$ ”)  $\text{diag}(1, 1, 1, -1)$  corresponding to “flat” space-time.

The best known non-flat metric is the Schwarzschild metric

$$g \equiv \begin{pmatrix} (1 - 2m/r)^{-1} & 0 & 0 & 0 \\ 0 & r^2 & 0 & 0 \\ 0 & 0 & r^2 \sin^2 \theta & 0 \\ 0 & 0 & 0 & -(1 - 2m/r) \end{pmatrix} \quad (5.58)$$

with respect to the spherical space-time coordinates  $r, \theta, \phi, t$ .

<sup>3</sup> A. D. Alexandrov. On Lorentz transformations. *Uspehi Mat. Nauk.*, 5(3):187, 1950; A. D. Alexandrov. A contribution to chronogeometry. *Canadian Journal of Math.*, 19:1119–1128, 1967; A. D. Alexandrov. Mappings of spaces with families of cones and space-time transformations. *Annali di Matematica Pura ed Applicata*, 103:229–257, 1975. ISSN 0373-3114. DOI: 10.1007/BF02414157. URL <http://dx.doi.org/10.1007/BF02414157>; A. D. Alexandrov. On the principles of relativity theory. In *Classics of Soviet Mathematics. Volume 4. A. D. Alexandrov. Selected Works*, pages 289–318. 1996; H. J. Borchers and G. C. Hegerfeldt. The structure of space-time transformations. *Communications in Mathematical Physics*, 28(3):259–266, 1972. URL <http://projecteuclid.org/euclid.cmp/1103858408>; Walter Benz. *Geometrische Transformationen*. BI Wissenschaftsverlag, Mannheim, 1992; June A. Lester. Distance preserving transformations. In Francis Buekenhout, editor, *Handbook of Incidence Geometry*, pages 921–944. Elsevier, Amsterdam, 1995; and Karl Svozil. Conventions in relativity theory and quantum mechanics. *Foundations of Physics*, 32:479–502, 2002. DOI: 10.1023/A:1015017831247. URL <http://dx.doi.org/10.1023/A:1015017831247>

*Computation of the metric tensor of the circle of radius  $r$*

Consider the transformation from the standard orthonormal threedimensional “Cartesian” coordinates  $X_1 = x$ ,  $X_2 = y$ , into polar coordinates  $X'_1 = r$ ,  $X'_2 = \varphi$ . In terms of  $r$  and  $\varphi$ , the Cartesian coordinates can be written as

$$\begin{aligned} X_1 &= r \cos \varphi \equiv X'_1 \cos X'_2, \\ X_2 &= r \sin \varphi \equiv X'_1 \sin X'_2. \end{aligned} \quad (5.59)$$

Furthermore, since the basis we start with is the Cartesian orthonormal basis,  $g_{ij} = \delta_{ij}$ ; therefore,

$$g'_{ij} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X_k}{\partial X'^j} g_{lk} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X_k}{\partial X'^j} \delta_{lk} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X_l}{\partial X'^j}. \quad (5.60)$$

More explicitly, we obtain for the coordinates of the transformed metric tensor  $g'$

$$\begin{aligned} g'_{11} &= \frac{\partial X^l}{\partial X'^1} \frac{\partial X_l}{\partial X'^1} \\ &= \frac{\partial(r \cos \varphi)}{\partial r} \frac{\partial(r \cos \varphi)}{\partial r} + \frac{\partial(r \sin \varphi)}{\partial r} \frac{\partial(r \sin \varphi)}{\partial r} \\ &= (\cos \varphi)^2 + (\sin \varphi)^2 = 1, \\ g'_{12} &= \frac{\partial X^l}{\partial X'^1} \frac{\partial X_l}{\partial X'^2} \\ &= \frac{\partial(r \cos \varphi)}{\partial r} \frac{\partial(r \cos \varphi)}{\partial \varphi} + \frac{\partial(r \sin \varphi)}{\partial r} \frac{\partial(r \sin \varphi)}{\partial \varphi} \\ &= (\cos \varphi)(-r \sin \varphi) + (\sin \varphi)(r \cos \varphi) = 0, \\ g'_{21} &= \frac{\partial X^l}{\partial X'^2} \frac{\partial X_l}{\partial X'^1} \\ &= \frac{\partial(r \cos \varphi)}{\partial \varphi} \frac{\partial(r \cos \varphi)}{\partial r} + \frac{\partial(r \sin \varphi)}{\partial \varphi} \frac{\partial(r \sin \varphi)}{\partial r} \\ &= (-r \sin \varphi)(\cos \varphi) + (r \cos \varphi)(\sin \varphi) = 0, \\ g'_{22} &= \frac{\partial X^l}{\partial X'^2} \frac{\partial X_l}{\partial X'^2} \\ &= \frac{\partial(r \cos \varphi)}{\partial \varphi} \frac{\partial(r \cos \varphi)}{\partial \varphi} + \frac{\partial(r \sin \varphi)}{\partial \varphi} \frac{\partial(r \sin \varphi)}{\partial \varphi} \\ &= (-r \sin \varphi)^2 + (r \cos \varphi)^2 = r^2; \end{aligned} \quad (5.61)$$

that is, in matrix notation,

$$g' = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}, \quad (5.62)$$

and thus

$$(ds')^2 = g'_{ij} d\mathbf{x}'^i d\mathbf{x}'^j = (dr)^2 + r^2(d\varphi)^2. \quad (5.63)$$

### Computation of the metric tensor of the ball

Consider the transformation from the standard orthonormal three-dimensional “Cartesian” coordinates  $X_1 = x$ ,  $X_2 = y$ ,  $X_3 = z$ , into spherical coordinates (for a definition of spherical coordinates, see also page 267)  $X'_1 = r$ ,  $X'_2 = \theta$ ,  $X'_3 = \varphi$ . In terms of  $r, \theta, \varphi$ , the Cartesian coordinates can be written as

$$\begin{aligned} X_1 &= r \sin \theta \cos \varphi \equiv X'_1 \sin X'_2 \cos X'_3, \\ X_2 &= r \sin \theta \sin \varphi \equiv X'_1 \sin X'_2 \sin X'_3, \\ X_3 &= r \cos \theta \equiv X'_1 \cos X'_2. \end{aligned} \quad (5.64)$$

Furthermore, since the basis we start with is the Cartesian orthonormal basis,  $g_{ij} = \delta_{ij}$ ; hence finally

$$g'_{ij} = \frac{\partial X^l}{\partial X'^i} \frac{\partial X_l}{\partial X'^j} \equiv \text{diag}(1, r^2, r^2 \sin^2 \theta), \quad (5.65)$$

and

$$(ds')^2 = (dr)^2 + r^2(d\theta)^2 + r^2 \sin^2 \theta (d\varphi)^2. \quad (5.66)$$

The expression  $(ds')^2 = (dr)^2 + r^2(d\varphi)^2$  for polar coordinates in two dimensions (i.e.,  $n = 2$ ) of Eq. (5.63) is recovered by setting  $\theta = \pi/2$  and  $d\theta = 0$ .

### Computation of the metric tensor of the Moebius strip

The parameter representation of the Moebius strip is

$$\Phi(u, v) = \begin{pmatrix} (1 + v \cos \frac{u}{2}) \sin u \\ (1 + v \cos \frac{u}{2}) \cos u \\ v \sin \frac{u}{2} \end{pmatrix}, \quad (5.67)$$

where  $u \in [0, 2\pi]$  represents the position of the point on the circle, and where  $2a > 0$  is the “width” of the Moebius strip, and where  $v \in [-a, a]$ .

$$\begin{aligned} \Phi_v &= \frac{\partial \Phi}{\partial v} = \begin{pmatrix} \cos \frac{u}{2} \sin u \\ \cos \frac{u}{2} \cos u \\ \sin \frac{u}{2} \end{pmatrix} \\ \Phi_u &= \frac{\partial \Phi}{\partial u} = \begin{pmatrix} -\frac{1}{2} v \sin \frac{u}{2} \sin u + (1 + v \cos \frac{u}{2}) \cos u \\ -\frac{1}{2} v \sin \frac{u}{2} \cos u - (1 + v \cos \frac{u}{2}) \sin u \\ \frac{1}{2} v \cos \frac{u}{2} \end{pmatrix} \\ \left(\frac{\partial \Phi}{\partial v}\right)^T \frac{\partial \Phi}{\partial u} &= \begin{pmatrix} \cos \frac{u}{2} \sin u \\ \cos \frac{u}{2} \cos u \\ \sin \frac{u}{2} \end{pmatrix}^T \begin{pmatrix} -\frac{1}{2} v \sin \frac{u}{2} \sin u + (1 + v \cos \frac{u}{2}) \cos u \\ -\frac{1}{2} v \sin \frac{u}{2} \cos u - (1 + v \cos \frac{u}{2}) \sin u \\ \frac{1}{2} v \cos \frac{u}{2} \end{pmatrix} \\ &= -\frac{1}{2} \left( \cos \frac{u}{2} \sin^2 u \right) v \sin \frac{u}{2} - \frac{1}{2} \left( \cos \frac{u}{2} \cos^2 u \right) v \sin \frac{u}{2} \\ &\quad + \frac{1}{2} \sin \frac{u}{2} v \cos \frac{u}{2} = 0 \end{aligned} \quad (5.69)$$

$$\begin{aligned}
\left(\frac{\partial\Phi}{\partial\nu}\right)^T \frac{\partial\Phi}{\partial\nu} &= \begin{pmatrix} \cos \frac{u}{2} \sin u \\ \cos \frac{u}{2} \cos u \\ \sin \frac{u}{2} \end{pmatrix}^T \begin{pmatrix} \cos \frac{u}{2} \sin u \\ \cos \frac{u}{2} \cos u \\ \sin \frac{u}{2} \end{pmatrix} \\
&= \cos^2 \frac{u}{2} \sin^2 u + \cos^2 \frac{u}{2} \cos^2 u + \sin^2 \frac{u}{2} = 1
\end{aligned} \tag{5.70}$$

$$\begin{aligned}
&\left(\frac{\partial\Phi}{\partial u}\right)^T \frac{\partial\Phi}{\partial u} = \\
&\begin{pmatrix} -\frac{1}{2}\nu \sin \frac{u}{2} \sin u + (1 + \nu \cos \frac{u}{2}) \cos u \\ -\frac{1}{2}\nu \sin \frac{u}{2} \cos u - (1 + \nu \cos \frac{u}{2}) \sin u \\ \frac{1}{2}\nu \cos \frac{u}{2} \end{pmatrix}^T \cdot \\
&\cdot \begin{pmatrix} -\frac{1}{2}\nu \sin \frac{u}{2} \sin u + (1 + \nu \cos \frac{u}{2}) \cos u \\ -\frac{1}{2}\nu \sin \frac{u}{2} \cos u - (1 + \nu \cos \frac{u}{2}) \sin u \\ \frac{1}{2}\nu \cos \frac{u}{2} \end{pmatrix} \\
&= \frac{1}{4}\nu^2 \sin^2 \frac{u}{2} \sin^2 u + \cos^2 u + 2\nu \cos^2 u \cos \frac{u}{2} + \nu^2 \cos^2 u \cos^2 \frac{u}{2} \\
&+ \frac{1}{4}\nu^2 \sin^2 \frac{u}{2} \cos^2 u + \sin^2 u + 2\nu \sin^2 u \cos \frac{u}{2} + \nu^2 \sin^2 u \cos^2 \frac{u}{2} \\
&+ \frac{1}{4}\nu^2 \cos^2 \frac{1}{2} u = \frac{1}{4}\nu^2 + \nu^2 \cos^2 \frac{u}{2} + 1 + 2\nu \cos \frac{1}{2} u \\
&= \left(1 + \nu \cos \frac{u}{2}\right)^2 + \frac{1}{4}\nu^2
\end{aligned} \tag{5.71}$$

Thus the metric tensor is given by

$$\begin{aligned}
g'_{ij} &= \frac{\partial X^s}{\partial X'^i} \frac{\partial X^t}{\partial X'^j} g_{st} = \frac{\partial X^s}{\partial X'^i} \frac{\partial X^t}{\partial X'^j} \delta_{st} \\
&\equiv \begin{pmatrix} \Phi_u \cdot \Phi_u & \Phi_v \cdot \Phi_u \\ \Phi_v \cdot \Phi_u & \Phi_v \cdot \Phi_v \end{pmatrix} = \text{diag} \left( \left(1 + \nu \cos \frac{u}{2}\right)^2 + \frac{1}{4}\nu^2, 1 \right).
\end{aligned} \tag{5.72}$$

## 5.8 General tensor

A (general) Tensor  $T$  can be defined as a multilinear form on the  $r$ -fold product of a vector space  $\mathfrak{V}$ , times the  $s$ -fold product of the dual vector space  $\mathfrak{V}^*$ ; that is,

$$T : (\mathfrak{V})^r \times (\mathfrak{V}^*)^s = \underbrace{\mathfrak{V} \times \cdots \times \mathfrak{V}}_{r \text{ copies}} \times \underbrace{\mathfrak{V}^* \times \cdots \times \mathfrak{V}^*}_{s \text{ copies}} \mapsto \mathbb{F}, \tag{5.73}$$

where, most commonly, the scalar field  $\mathbb{F}$  will be identified with the set  $\mathbb{R}$  of reals, or with the set  $\mathbb{C}$  of complex numbers. Thereby,  $r$  is called the *covariant order*, and  $s$  is called the *contravariant order* of  $T$ . A tensor of covariant order  $r$  and contravariant order  $s$  is then pronounced a tensor of *type* (or *rank*)  $(r, s)$ . By convention, covariant indices are denoted by *subscripts*, whereas the contravariant indices are denoted by *superscripts*.

With the standard, “inherited” addition and scalar multiplication, the set  $\mathfrak{T}_r^s$  of all tensors of type  $(r, s)$  forms a linear vector space.

Note that a tensor of type  $(1, 0)$  is called a *covariant vector*, or just a *vector*. A tensor of type  $(0, 1)$  is called a *contravariant vector*.

Tensors can change their type by the invocation of the *metric tensor*. That is, a covariant tensor (index)  $i$  can be made into a contravariant tensor (index)  $j$  by summing over the index  $i$  in a product involving the tensor and  $g^{ij}$ . Likewise, a contravariant tensor (index)  $i$  can be made into a covariant tensor (index)  $j$  by summing over the index  $i$  in a product involving the tensor and  $g_{ij}$ .

Under basis or other linear transformations, covariant tensors with index  $i$  transform by summing over this index with (the transformation matrix)  $a_i^j$ . Contravariant tensors with index  $i$  transform by summing over this index with the inverse (transformation matrix)  $(a^{-1})_i^j$ .

### 5.9 Decomposition of tensors

Although a tensor of type (or rank)  $n$  transforms like the tensor product of  $n$  tensors of type 1, not all type- $n$  tensors can be decomposed into a single tensor product of  $n$  tensors of type (or rank) 1.

Nevertheless, by a generalized Schmidt decomposition (cf. page 73), any type-2 tensor can be decomposed into the sum of tensor products of two tensors of type 1.

### 5.10 Form invariance of tensors

A tensor (field) is form invariant with respect to some basis change if its representation in the new basis has the same form as in the old basis. For instance, if the “12122–component”  $T_{12122}(x)$  of the tensor  $T$  with respect to the old basis and old coordinates  $x$  equals some function  $f(x)$  (say,  $f(x) = x^2$ ), then, a necessary condition for  $T$  to be form invariant is that, in terms of the new basis, that component  $T'_{12122}(x')$  equals the same function  $f(x')$  as before, but in the new coordinates  $x'$ . A sufficient condition for form invariance of  $T$  is that *all* coordinates or components of  $T$  are form invariant in that way.

Although form invariance is a gratifying feature for the reasons explained shortly, a tensor (field) needs not necessarily be form invariant with respect to all or even any (symmetry) transformation(s).

A physical motivation for the use of form invariant tensors can be given as follows. What makes some tuples (or matrix, or tensor components in general) of numbers or scalar functions a tensor? It is the interpretation of the scalars as tensor components *with respect to a particular basis*. In another basis, if we were talking about the same tensor, the tensor components; that is, the numbers or scalar functions, would be different.

Pointedly stated, the tensor coordinates represent some encoding of a multilinear function with respect to a particular basis.

Formally, the tensor coordinates are numbers; that is, scalars, which are grouped together in vector tuples or matrices or whatever form we consider useful. As the tensor coordinates are scalars, they can be treated as scalars. For instance, due to commutativity and associativity, one can exchange their order. (Notice, though, that this is generally not the case for differential operators such as  $\partial_i = \partial/\partial x^i$ .)

A *form invariant* tensor with respect to certain transformations is a tensor which retains the same functional form if the transformations are performed; that is, if the basis changes accordingly. That is, in this case, the functional form of mapping numbers or coordinates or other entities remains unchanged, regardless of the coordinate change. Functions remain the same but with the new parameter components as argument. For instance;  $4 \mapsto 4$  and  $f(X_1, X_2, X_3) \mapsto f(X'_1, X'_2, X'_3)$ .

Furthermore, if a tensor is invariant with respect to one transformation, it need not be invariant with respect to another transformation, or with respect to changes of the scalar product; that is, the metric.

Nevertheless, totally symmetric (antisymmetric) tensors remain totally symmetric (antisymmetric) in all cases:

$$A_{i_1 i_2 \dots i_s i_t \dots i_k} = A_{i_1 i_2 \dots i_t i_s \dots i_k}$$

implies

$$\begin{aligned} A'_{j_1 i_2 \dots j_s j_t \dots j_k} &= a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_s}^{i_s} a_{j_t}^{i_t} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_s i_t \dots i_k} \\ &= a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_s}^{i_s} a_{j_t}^{i_t} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_t i_s \dots i_k} \\ &= a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_t}^{i_t} a_{j_s}^{i_s} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_t i_s \dots i_k} \\ &= A'_{j_1 i_2 \dots j_t j_s \dots j_k}. \end{aligned}$$

Likewise,

$$A_{i_1 i_2 \dots i_s i_t \dots i_k} = -A_{i_1 i_2 \dots i_t i_s \dots i_k}$$

implies

$$\begin{aligned} A'_{j_1 i_2 \dots j_s j_t \dots j_k} &= a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_s}^{i_s} a_{j_t}^{i_t} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_s i_t \dots i_k} \\ &= -a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_s}^{i_s} a_{j_t}^{i_t} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_t i_s \dots i_k} \\ &= -a_{j_1}^{i_1} a_{j_2}^{i_2} \dots a_{j_t}^{i_t} a_{j_s}^{i_s} \dots a_{j_k}^{i_k} A_{i_1 i_2 \dots i_t i_s \dots i_k} \\ &= -A'_{j_1 i_2 \dots j_t j_s \dots j_k}. \end{aligned}$$

In physics, it would be nice if the natural laws could be written into a form which does not depend on the particular reference frame or basis used. Form invariance thus is a gratifying physical feature, reflecting the *symmetry* against changes of coordinates and bases.

After all, physicists want the formalization of their fundamental laws not to artificially depend on, say, spacial directions, or on some particular basis, if there is no physical reason why this should be so. Therefore,



physicists tend to be crazy to write down everything in a form invariant manner.

One strategy to accomplish form invariance is to start out with form invariant tensors and compose – by tensor products and index reduction – everything from them. This method guarantees form invariance.

The “simplest” form invariant tensor under all transformations is the constant tensor of rank 0.

Another constant form invariant tensor under all transformations is represented by the Kronecker symbol  $\delta_j^i$ , because

$$(\delta')_j^i = (a^{-1})_{i'}^i a_j^{j'} \delta_{j'}^{i'} = (a^{-1})_{i'}^i a_j^{j'} = a_j^{i'} (a^{-1})_{i'}^i = \delta_j^i. \quad (5.74)$$

A simple form invariant tensor field is a vector  $\mathbf{x}$ , because if  $T(\mathbf{x}) = x^i t_i = x^i \mathbf{e}_i = \mathbf{x}$ , then the “inner transformation”  $\mathbf{x} \mapsto \mathbf{x}'$  and the “outer transformation”  $T \mapsto T' = \mathbf{A}T$  just compensate each other; that is, in coordinate representation, Eqs.(5.9) and (5.22) yield

$$T'(\mathbf{x}') = x'^i t'_i = (a^{-1})_l^i x^l a_i^j t_j = (a^{-1})_l^i a_i^j \mathbf{e}_j x^l = \delta_l^j \mathbf{e}_j x^l = \mathbf{x} = T(\mathbf{x}). \quad (5.75)$$

For the sake of another demonstration of form invariance, consider the following two factorizable tensor fields: while

$$S(x) = \begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} \otimes \begin{pmatrix} x_2 \\ -x_1 \end{pmatrix}^T = (x_2, -x_1)^T \otimes (x_2, -x_1) \equiv \begin{pmatrix} x_2^2 & -x_1 x_2 \\ -x_1 x_2 & x_1^2 \end{pmatrix} \quad (5.76)$$

is a form invariant tensor field with respect to the basis  $\{(0, 1), (1, 0)\}$  and orthogonal transformations (rotations around the origin)

$$\begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix}, \quad (5.77)$$

$$T(x) = \begin{pmatrix} x_2 \\ x_1 \end{pmatrix} \otimes \begin{pmatrix} x_2 \\ x_1 \end{pmatrix}^T = (x_2, x_1)^T \otimes (x_2, x_1) \equiv \begin{pmatrix} x_2^2 & x_1 x_2 \\ x_1 x_2 & x_1^2 \end{pmatrix} \quad (5.78)$$

is not.

This can be proven by considering the single factors from which  $S$  and  $T$  are composed. Eqs. (5.21)-(5.22) and (5.32)-(5.33) show that the form invariance of the factors implies the form invariance of the tensor products.

For instance, in our example, the factors  $(x_2, -x_1)^T$  of  $S$  are invariant, as they transform as

$$\begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} = \begin{pmatrix} x_2 \cos \varphi - x_1 \sin \varphi \\ -x_2 \sin \varphi - x_1 \cos \varphi \end{pmatrix} = \begin{pmatrix} x'_2 \\ -x'_1 \end{pmatrix},$$

where the transformation of the coordinates

$$\begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix} = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \cos \varphi + x_2 \sin \varphi \\ -x_1 \sin \varphi + x_2 \cos \varphi \end{pmatrix}$$

has been used.

Note that the notation identifying tensors of type (or rank) two with matrices, creates an “artifact” insofar as the transformation of the “second index” must then be represented by the exchanged multiplication order, together with the transposed transformation matrix; that is,

$$a_{ik}a_{jl}A_{kl} = a_{ik}A_{kl}a_{jl} = a_{ik}A_{kl}(a^T)_{lj} \equiv a \cdot A \cdot a^T.$$

Thus for a transformation of the transposed tuple  $(x_2, -x_1)$  we must consider the *transposed* transformation matrix arranged *after* the factor; that is,

$$(x_2, -x_1) \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} = (x_2 \cos \varphi - x_1 \sin \varphi, -x_2 \sin \varphi - x_1 \cos \varphi) = (x'_2, -x'_1).$$

In contrast, a similar calculation shows that the factors  $(x_2, x_1)^T$  of  $T$  do not transform invariantly. However, noninvariance with respect to certain transformations does not imply that  $T$  is not a valid, “respectable” tensor field; it is just not form invariant under rotations.

Nevertheless, note again that, while the tensor product of form invariant tensors is again a form invariant tensor, not every form invariant tensor might be decomposed into products of form invariant tensors.

Let  $|+\rangle \equiv (0, 1)$  and  $|-\rangle \equiv (1, 0)$ . For a nondecomposable tensor, consider the sum of two-partite tensor products (associated with two “entangled” particles) Bell state (cf. Eq. (A.28) on page 271) in the standard basis

$$\begin{aligned} |\Psi^-\rangle &= \frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle) \\ &\equiv \left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right) \\ &\equiv \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{5.79}$$

Why is  $|\Psi^-\rangle$  not decomposable? In order to be able to answer this question (see also Section 4.10.3 on page 37), consider the most general two-partite state

$$|\psi\rangle = \psi_{--} |--\rangle + \psi_{-+} | -+\rangle + \psi_{+-} | +-\rangle + \psi_{++} | ++\rangle, \tag{5.80}$$

with  $\psi_{ij} \in \mathbb{C}$ , and compare it to the most general state obtainable through products of single-partite states  $|\phi_1\rangle = \alpha_- |-\rangle + \alpha_+ |+\rangle$ , and  $|\phi_2\rangle = \beta_- |-\rangle + \beta_+ |+\rangle$  with  $\alpha_i, \beta_i \in \mathbb{C}$ ; that is,

$$\begin{aligned} |\phi\rangle &= |\phi_1\rangle |\phi_2\rangle \\ &= (\alpha_- |-\rangle + \alpha_+ |+\rangle)(\beta_- |-\rangle + \beta_+ |+\rangle) \\ &= \alpha_- \beta_- |--\rangle + \alpha_- \beta_+ | -+\rangle + \alpha_+ \beta_- | +-\rangle + \alpha_+ \beta_+ | ++\rangle. \end{aligned} \tag{5.81}$$

$|\Psi^-\rangle$ , together with the other three Bell states  $|\Psi^+\rangle = \frac{1}{\sqrt{2}} (|+-\rangle + |-+\rangle)$ ,  $|\Phi^+\rangle = \frac{1}{\sqrt{2}} (|--\rangle + |++\rangle)$ , and  $|\Phi^-\rangle = \frac{1}{\sqrt{2}} (|--\rangle - |++\rangle)$ , forms an orthonormal basis of  $\mathbb{C}^4$ .

Since the two-partite basis states

$$\begin{aligned} |--\rangle &\equiv (1, 0, 0, 0), \\ |-\rangle &\equiv (0, 1, 0, 0), \\ |+-\rangle &\equiv (0, 0, 1, 0), \\ |++\rangle &\equiv (0, 0, 0, 1) \end{aligned} \quad (5.82)$$

are linear independent (indeed, orthonormal), a comparison of  $|\psi\rangle$  with  $|\phi\rangle$  yields

$$\begin{aligned} \psi_{--} &= \alpha_- \beta_-, \\ \psi_{-+} &= \alpha_- \beta_+, \\ \psi_{+-} &= \alpha_+ \beta_-, \\ \psi_{++} &= \alpha_+ \beta_+. \end{aligned} \quad (5.83)$$

Hence,  $\psi_{--}/\psi_{-+} = \beta_-/\beta_+ = \psi_{+-}/\psi_{++}$ , and thus a necessary and sufficient condition for a two-partite quantum state to be decomposable into a product of single-particle quantum states is that its amplitudes obey

$$\psi_{--}\psi_{++} = \psi_{-+}\psi_{+-}. \quad (5.84)$$

This is not satisfied for the Bell state  $|\Psi^-\rangle$  in Eq. (5.79), because in this case  $\psi_{--} = \psi_{++} = 0$  and  $\psi_{-+} = -\psi_{+-} = 1/\sqrt{2}$ . Such nondecomposability is in physics referred to as *entanglement*<sup>4</sup>.

Note also that  $|\Psi^-\rangle$  is a *singlet state*, as it is form invariant under the following generalized rotations in two-dimensional complex Hilbert sub-space; that is, (if you do not believe this please check yourself)

$$\begin{aligned} |+\rangle &= e^{i\frac{\varphi}{2}} \left( \cos \frac{\theta}{2} |+\rangle - \sin \frac{\theta}{2} |-\rangle \right), \\ |-\rangle &= e^{-i\frac{\varphi}{2}} \left( \sin \frac{\theta}{2} |+\rangle + \cos \frac{\theta}{2} |-\rangle \right) \end{aligned} \quad (5.85)$$

in the spherical coordinates  $\theta, \varphi$  defined on page 267, but it cannot be composed or written as a product of a *single* (let alone form invariant) two-partite tensor product.

In order to prove form invariance of a constant tensor, one has to transform the tensor according to the standard transformation laws (5.22) and (5.26), and compare the result with the input; that is, with the untransformed, original, tensor. This is sometimes referred to as the “outer transformation.”

In order to prove form invariance of a tensor field, one has to additionally transform the spatial coordinates on which the field depends; that is, the arguments of that field; and then compare. This is sometimes referred to as the “inner transformation.” This will become clearer with the following example.

<sup>4</sup> Erwin Schrödinger. Discussion of probability relations between separated systems. *Mathematical Proceedings of the Cambridge Philosophical Society*, 31(04):555–563, 1935a. DOI: 10.1017/S0305004100013554. URL <http://dx.doi.org/10.1017/S0305004100013554>; Erwin Schrödinger. Probability relations between separated systems. *Mathematical Proceedings of the Cambridge Philosophical Society*, 32(03):446–452, 1936. DOI: 10.1017/S0305004100019137. URL <http://dx.doi.org/10.1017/S0305004100019137>; and Erwin Schrödinger. Die gegenwärtige Situation in der Quantenmechanik. *Naturwissenschaften*, 23:807–812, 823–828, 844–849, 1935b. DOI: 10.1007/BF01491891, 10.1007/BF01491914, 10.1007/BF01491987. URL <http://dx.doi.org/10.1007/BF01491891>, <http://dx.doi.org/10.1007/BF01491914>, <http://dx.doi.org/10.1007/BF01491987>

Consider again the tensor field defined earlier in Eq. (5.76), but let us not choose the “elegant” ways of proving form invariance by factoring; rather we explicitly consider the transformation of all the components

$$S_{ij}(x_1, x_2) = \begin{pmatrix} -x_1 x_2 & -x_2^2 \\ x_1^2 & x_1 x_2 \end{pmatrix}$$

with respect to the standard basis  $\{(1, 0), (0, 1)\}$ .

Is  $S$  form invariant with respect to rotations around the origin? That is,  $S$  should be form invariant with respect to transformations  $x'_i = a_{ij}x_j$  with

$$a_{ij} = \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix}.$$

Consider the “outer” transformation first. As has been pointed out earlier, the term on the right hand side in  $S'_{ij} = a_{ik}a_{jl}S_{kl}$  can be rewritten as a product of three matrices; that is,

$$a_{ik}a_{jl}S_{kl}(x_n) = a_{ik}S_{kl}a_{jl} = a_{ik}S_{kl}(a^T)_{lj} \equiv a \cdot S \cdot a^T.$$

$a^T$  stands for the transposed matrix; that is,  $(a^T)_{ij} = a_{ji}$ .

$$\begin{aligned} & \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} -x_1 x_2 & -x_2^2 \\ x_1^2 & x_1 x_2 \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} = \\ & = \begin{pmatrix} -x_1 x_2 \cos \varphi + x_1^2 \sin \varphi & -x_2^2 \cos \varphi + x_1 x_2 \sin \varphi \\ x_1 x_2 \sin \varphi + x_1^2 \cos \varphi & x_2^2 \sin \varphi + x_1 x_2 \cos \varphi \end{pmatrix} \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} = \\ & = \begin{pmatrix} \cos \varphi (-x_1 x_2 \cos \varphi + x_1^2 \sin \varphi) + & -\sin \varphi (-x_1 x_2 \cos \varphi + x_1^2 \sin \varphi) + \\ + \sin \varphi (-x_2^2 \cos \varphi + x_1 x_2 \sin \varphi) & + \cos \varphi (-x_2^2 \cos \varphi + x_1 x_2 \sin \varphi) \end{pmatrix} = \\ & = \begin{pmatrix} \cos \varphi (x_1 x_2 \sin \varphi + x_1^2 \cos \varphi) + & -\sin \varphi (x_1 x_2 \sin \varphi + x_1^2 \cos \varphi) + \\ + \sin \varphi (x_2^2 \sin \varphi + x_1 x_2 \cos \varphi) & + \cos \varphi (x_2^2 \sin \varphi + x_1 x_2 \cos \varphi) \end{pmatrix} = \\ & = \begin{pmatrix} x_1 x_2 (\sin^2 \varphi - \cos^2 \varphi) + & 2x_1 x_2 \sin \varphi \cos \varphi \\ + (x_1^2 - x_2^2) \sin \varphi \cos \varphi & -x_1^2 \sin^2 \varphi - x_2^2 \cos^2 \varphi \end{pmatrix} \\ & = \begin{pmatrix} 2x_1 x_2 \sin \varphi \cos \varphi + & -x_1 x_2 (\sin^2 \varphi - \cos^2 \varphi) - \\ + x_1^2 \cos^2 \varphi + x_2^2 \sin^2 \varphi & - (x_1^2 - x_2^2) \sin \varphi \cos \varphi \end{pmatrix} \end{aligned}$$

Let us now perform the “inner” transform

$$x'_i = a_{ij}x_j \implies \begin{aligned} x'_1 &= x_1 \cos \varphi + x_2 \sin \varphi \\ x'_2 &= -x_1 \sin \varphi + x_2 \cos \varphi. \end{aligned}$$

Thereby we assume (to be corroborated) that the functional form in the new coordinates are identical to the functional form of the old coordinates. A comparison yields

$$\begin{aligned}
 -x'_1 x'_2 &= -(x_1 \cos \varphi + x_2 \sin \varphi)(-x_1 \sin \varphi + x_2 \cos \varphi) = \\
 &= -(-x_1^2 \sin \varphi \cos \varphi + x_2^2 \sin \varphi \cos \varphi - x_1 x_2 \sin^2 \varphi + x_1 x_2 \cos^2 \varphi) = \\
 &= x_1 x_2 (\sin^2 \varphi - \cos^2 \varphi) + (x_1^2 - x_2^2) \sin \varphi \cos \varphi \\
 (x'_1)^2 &= (x_1 \cos \varphi + x_2 \sin \varphi)(x_1 \cos \varphi + x_2 \sin \varphi) = \\
 &= x_1^2 \cos^2 \varphi + x_2^2 \sin^2 \varphi + 2x_1 x_2 \sin \varphi \cos \varphi \\
 (x'_2)^2 &= (-x_1 \sin \varphi + x_2 \cos \varphi)(-x_1 \sin \varphi + x_2 \cos \varphi) = \\
 &= x_1^2 \sin^2 \varphi + x_2^2 \cos^2 \varphi - 2x_1 x_2 \sin \varphi \cos \varphi
 \end{aligned}$$

and hence

$$S'(x'_1, x'_2) = \begin{pmatrix} -x'_1 x'_2 & -(x'_2)^2 \\ (x'_1)^2 & x'_1 x'_2 \end{pmatrix}$$

is invariant with respect to rotations by angles  $\varphi$ , yielding the new basis  $\{(\cos \varphi, -\sin \varphi), (\sin \varphi, \cos \varphi)\}$ .

Incidentally, as has been stated earlier,  $S(x)$  can be written as the product of two invariant tensors  $b_i(x)$  and  $c_j(x)$ :

$$S_{ij}(x) = b_i(x)c_j(x),$$

with  $b(x_1, x_2) = (-x_2, x_1)$ , and  $c(x_1, x_2) = (x_1, x_2)$ . This can be easily checked by comparing the components:

$$\begin{aligned}
 b_1 c_1 &= -x_1 x_2 = S_{11}, \\
 b_1 c_2 &= -x_2^2 = S_{12}, \\
 b_2 c_1 &= x_1^2 = S_{21}, \\
 b_2 c_2 &= x_1 x_2 = S_{22}.
 \end{aligned}$$

Under rotations,  $b$  and  $c$  transform into

$$\begin{aligned}
 a_{ij} b_j &= \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} -x_2 \\ x_1 \end{pmatrix} = \begin{pmatrix} -x_2 \cos \varphi + x_1 \sin \varphi \\ x_2 \sin \varphi + x_1 \cos \varphi \end{pmatrix} = \begin{pmatrix} -x'_2 \\ x'_1 \end{pmatrix} \\
 a_{ij} c_j &= \begin{pmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \cos \varphi + x_2 \sin \varphi \\ -x_1 \sin \varphi + x_2 \cos \varphi \end{pmatrix} = \begin{pmatrix} x'_1 \\ x'_2 \end{pmatrix}.
 \end{aligned}$$

This factorization of  $S$  is nonunique, since Eq. (5.76) uses a different factorization; also,  $S$  is decomposable into, for example,

$$S(x_1, x_2) = \begin{pmatrix} -x_1 x_2 & -x_2^2 \\ x_1^2 & x_1 x_2 \end{pmatrix} = \begin{pmatrix} -x_2^2 \\ x_1 x_2 \end{pmatrix} \otimes \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}.$$

### 5.11 The Kronecker symbol $\delta$

For vector spaces of dimension  $n$  the totally symmetric Kronecker symbol  $\delta$ , sometimes referred to as the delta symbol  $\delta$ -tensor, can be defined by

$$\delta_{i_1 i_2 \dots i_k} = \begin{cases} +1 & \text{if } i_1 = i_2 = \dots = i_k \\ 0 & \text{otherwise (that is, some indices are not identical).} \end{cases} \quad (5.86)$$

Note that, with the Einstein summation convention,

$$\begin{aligned} \delta_{ij} a_j &= a_j \delta_{ij} = \delta_{i1} a_1 + \delta_{i2} a_2 + \dots + \delta_{in} a_n = a_i, \\ \delta_{ji} a_j &= a_j \delta_{ji} = \delta_{1i} a_1 + \delta_{2i} a_2 + \dots + \delta_{ni} a_n = a_i. \end{aligned} \quad (5.87)$$

### 5.12 The Levi-Civita symbol $\varepsilon$

For vector spaces of dimension  $n$  the totally antisymmetric Levi-Civita symbol  $\varepsilon$ , sometimes referred to as the Levi-Civita symbol  $\varepsilon$ -tensor, can be defined by the number of permutations of its indices; that is,

$$\varepsilon_{i_1 i_2 \dots i_k} = \begin{cases} +1 & \text{if } (i_1 i_2 \dots i_k) \text{ is an even permutation of } (1, 2, \dots, k) \\ -1 & \text{if } (i_1 i_2 \dots i_k) \text{ is an odd permutation of } (1, 2, \dots, k) \\ 0 & \text{otherwise (that is, some indices are identical).} \end{cases} \quad (5.88)$$

Hence,  $\varepsilon_{i_1 i_2 \dots i_k}$  stands for the the sign of the permutation in the case of a permutation, and zero otherwise.

In two dimensions,

$$\varepsilon_{ij} \equiv \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

In three-dimensional Euclidean space, the cross product, or vector product of two vectors  $\mathbf{x} \equiv x_i$  and  $\mathbf{y} \equiv y_i$  can be written as  $\mathbf{x} \times \mathbf{y} \equiv \varepsilon_{ijk} x_j y_k$ .

For a direct proof, consider, for arbitrary three-dimensional vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and by enumerating all nonvanishing terms; that is, all permutations,

$$\begin{aligned} \mathbf{x} \times \mathbf{y} &\equiv \varepsilon_{ijk} x_j y_k \equiv \begin{pmatrix} \varepsilon_{123} x_2 y_3 + \varepsilon_{132} x_3 y_2 \\ \varepsilon_{213} x_1 y_3 + \varepsilon_{231} x_3 y_1 \\ \varepsilon_{312} x_2 y_3 + \varepsilon_{321} x_3 y_2 \end{pmatrix} \\ &= \begin{pmatrix} \varepsilon_{123} x_2 y_3 - \varepsilon_{123} x_3 y_2 \\ -\varepsilon_{123} x_1 y_3 + \varepsilon_{123} x_3 y_1 \\ \varepsilon_{123} x_2 y_3 - \varepsilon_{123} x_3 y_2 \end{pmatrix} = \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ -x_1 y_3 + x_3 y_1 \\ x_2 y_3 - x_3 y_2 \end{pmatrix}. \end{aligned} \quad (5.89)$$

### 5.13 The nabla, Laplace, and D'Alembert operators

The nabla operator

$$\nabla = \left( \frac{\partial}{\partial X_1}, \frac{\partial}{\partial X_2}, \dots, \frac{\partial}{\partial X_n} \right). \quad (5.90)$$

is a vector differential operator in an  $n$ -dimensional vector space  $\mathfrak{V}$ . In index notation,  $\nabla_i = \partial_i = \partial_{X^i}$ .

The nabla operator transforms in the following manners:  $\nabla_i = \partial_i = \partial_{X^i}$  transforms like a *covariant* vector, since

$$\partial_i = \frac{\partial}{\partial X^i} = \frac{\partial X'^j}{\partial X^i} \frac{\partial}{\partial X'^j} = (a^{-1})_i^j \frac{\partial}{\partial X'^j} = J_{ij} \frac{\partial}{\partial X'^j}, \quad (5.91)$$

where  $J_{ij}$  stands for the *Jacobian matrix* defined in Eq. (5.20).

As very similar calculation demonstrates that  $\partial^i = \frac{\partial}{\partial X_i}$  transforms like a *contravariant* vector.

In three dimensions and in the standard Cartesian basis,

$$\nabla = \left( \frac{\partial}{\partial X_1}, \frac{\partial}{\partial X_2}, \frac{\partial}{\partial X_3} \right) = \mathbf{e}_1 \frac{\partial}{\partial X_1} + \mathbf{e}_2 \frac{\partial}{\partial X_2} + \mathbf{e}_3 \frac{\partial}{\partial X_3}. \quad (5.92)$$

It is often used to define basic differential operations; in particular, (i) to denote the *gradient* of a scalar field  $f(X_1, X_2, X_3)$  (rendering a vector field with respect to a particular basis), (ii) the *divergence* of a vector field  $\mathbf{v}(X_1, X_2, X_3)$  (rendering a scalar field with respect to a particular basis), and (iii) the *curl* (rotation) of a vector field  $\mathbf{v}(X_1, X_2, X_3)$  (rendering a vector field with respect to a particular basis) as follows:

$$\text{grad } f = \nabla f = \left( \frac{\partial f}{\partial X_1}, \frac{\partial f}{\partial X_2}, \frac{\partial f}{\partial X_3} \right), \quad (5.93)$$

$$\text{div } \mathbf{v} = \nabla \cdot \mathbf{v} = \frac{\partial v_1}{\partial X_1} + \frac{\partial v_2}{\partial X_2} + \frac{\partial v_3}{\partial X_3}, \quad (5.94)$$

$$\text{rot } \mathbf{v} = \nabla \times \mathbf{v} = \left( \frac{\partial v_3}{\partial X_2} - \frac{\partial v_2}{\partial X_3}, \frac{\partial v_1}{\partial X_3} - \frac{\partial v_3}{\partial X_1}, \frac{\partial v_2}{\partial X_1} - \frac{\partial v_1}{\partial X_2} \right) \quad (5.95)$$

$$\equiv \varepsilon_{ijk} \partial_j v_k. \quad (5.96)$$

The *Laplace operator* is defined by

$$\Delta = \nabla^2 = \nabla \cdot \nabla = \frac{\partial^2}{\partial^2 X_1} + \frac{\partial^2}{\partial^2 X_2} + \frac{\partial^2}{\partial^2 X_3}. \quad (5.97)$$

In special relativity and electrodynamics, as well as in wave theory and quantized field theory, with the Minkowski space-time of dimension four (referring to the metric tensor with the signature “ $\pm, \pm, \pm, \mp$ ”), the *D'Alembert operator* is defined by the Minkowski metric  $\eta = \text{diag}(1, 1, 1, -1)$

$$\square = \partial_i \partial^i = \eta_{ij} \partial^i \partial^j = \nabla^2 - \frac{\partial^2}{\partial^2 t} = \nabla \cdot \nabla - \frac{\partial^2}{\partial^2 t} = \frac{\partial^2}{\partial^2 X_1} + \frac{\partial^2}{\partial^2 X_2} + \frac{\partial^2}{\partial^2 X_3} - \frac{\partial^2}{\partial^2 t}. \quad (5.98)$$

### 5.14 Some tricks and examples

There are some tricks which are commonly used. Here, some of them are enumerated:

- (i) Indices which appear as internal sums can be renamed arbitrarily (provided their name is not already taken by some other index). That is,  $a_i b^i = a_j b^j$  for arbitrary  $a, b, i, j$ .
- (ii) With the Euclidean metric,  $\delta_{ii} = n$ .
- (iii)  $\frac{\partial X^i}{\partial X^j} = \delta_j^i$ .
- (iv) With the Euclidean metric,  $\frac{\partial X^i}{\partial X^i} = n$ .
- (v)  $\varepsilon_{ij} \delta_{ij} = -\varepsilon_{ji} \delta_{ij} = -\varepsilon_{ji} \delta_{ji} = (i \leftrightarrow j) = -\varepsilon_{ij} \delta_{ij} = 0$ , since  $a = -a$  implies  $a = 0$ ; likewise,  $\varepsilon_{ij} x_i x_j = 0$ . In general, the Einstein summations  $s_{ij} \dots a_{ij} \dots$  over objects  $s_{ij} \dots$  which are *symmetric* with respect to index exchanges over objects  $a_{ij} \dots$  which are *antisymmetric* with respect to index exchanges yields zero.
- (vi) For threedimensional vector spaces ( $n = 3$ ) and the Euclidean metric, the *Grassmann identity* holds:

$$\varepsilon_{ijk} \varepsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}. \quad (5.99)$$

For the sake of a proof, consider

$$\begin{aligned}
 & \mathbf{x} \times (\mathbf{y} \times \mathbf{z}) \equiv \\
 & \text{in index notation} \\
 & x_j \varepsilon_{ijk} y_l z_m \varepsilon_{klm} = x_j y_l z_m \varepsilon_{ijk} \varepsilon_{klm} \equiv \\
 & \text{in coordinate notation} \\
 & \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \times \left[ \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \times \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} \right] = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \times \begin{pmatrix} y_2 z_3 - y_3 z_2 \\ y_3 z_1 - y_1 z_3 \\ y_1 z_2 - y_2 z_1 \end{pmatrix} = \\
 & \begin{pmatrix} x_2(y_1 z_2 - y_2 z_1) - x_3(y_3 z_1 - y_1 z_3) \\ x_3(y_2 z_3 - y_3 z_2) - x_1(y_1 z_2 - y_2 z_1) \\ x_1(y_3 z_1 - y_1 z_3) - x_2(y_2 z_3 - y_3 z_2) \end{pmatrix} = \\
 & \begin{pmatrix} x_2 y_1 z_2 - x_2 y_2 z_1 - x_3 y_3 z_1 + x_3 y_1 z_3 \\ x_3 y_2 z_3 - x_3 y_3 z_2 - x_1 y_1 z_2 + x_1 y_2 z_1 \\ x_1 y_3 z_1 - x_1 y_1 z_3 - x_2 y_2 z_3 + x_2 y_3 z_2 \end{pmatrix} = \\
 & \begin{pmatrix} y_1(x_2 z_2 + x_3 z_3) - z_1(x_2 y_2 + x_3 y_3) \\ y_2(x_3 z_3 + x_1 z_1) - z_2(x_1 y_1 + x_3 y_3) \\ y_3(x_1 z_1 + x_2 z_2) - z_3(x_1 y_1 + x_2 y_2) \end{pmatrix}
 \end{aligned} \quad (5.100)$$

The “incomplete” dot products can be completed through addition and



subtraction of the same term, respectively; that is,

$$\begin{pmatrix} y_1(x_1 z_1 + x_2 z_2 + x_3 z_3) - z_1(x_1 y_1 + x_2 y_2 + x_3 y_3) \\ y_2(x_1 z_1 + x_2 z_2 + x_3 z_3) - z_2(x_1 y_1 + x_2 y_2 + x_3 y_3) \\ y_3(x_1 z_1 + x_2 z_2 + x_3 z_3) - z_3(x_1 y_1 + x_2 y_2 + x_3 y_3) \end{pmatrix} \equiv$$

in vector notation (5.101)

$$\mathbf{y}(\mathbf{x} \cdot \mathbf{z}) - \mathbf{z}(\mathbf{x} \cdot \mathbf{y}) \equiv$$

in index notation

$$x_j y_l z_m (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}).$$

(vii) For threedimensional vector spaces ( $n = 3$ ) and the Euclidean metric,

$$|a \times b| = \sqrt{\varepsilon_{ijk} \varepsilon_{ist} a_j a_s b_k b_t} = \sqrt{|a|^2 |b|^2 - (a \cdot b)^2} = \sqrt{\det \begin{pmatrix} a \cdot a & a \cdot b \\ a \cdot b & b \cdot b \end{pmatrix}} = |a||b| \sin \theta_{ab}.$$

(viii) Let  $u, v \equiv X'_1, X'_2$  be two parameters associated with an orthonormal Cartesian basis  $\{(0, 1), (1, 0)\}$ , and let  $\Phi : (u, v) \mapsto \mathbb{R}^3$  be a mapping from some area of  $\mathbb{R}^2$  into a twodimensional surface of  $\mathbb{R}^3$ . Then the metric tensor is given by  $g_{ij} = \frac{\partial \Phi^k}{\partial X'^i} \frac{\partial \Phi^m}{\partial X'^j} \delta_{km}$ .

Consider the following examples in threedimensional vector space. Let  $r^2 = \sum_{i=1}^3 x_i^2$ .

1.

$$\partial_j r = \partial_j \sqrt{\sum_i x_i^2} = \frac{1}{2} \frac{1}{\sqrt{\sum_i x_i^2}} 2x_j = \frac{x_j}{r} \quad (5.102)$$

By using the chain rule one obtains

$$\partial_j r^\alpha = \alpha r^{\alpha-1} (\partial_j r) = \alpha r^{\alpha-1} \left( \frac{x_j}{r} \right) = \alpha r^{\alpha-2} x_j \quad (5.103)$$

and thus  $\nabla r^\alpha = \alpha r^{\alpha-2} \mathbf{x}$ .

2.

$$\partial_j \log r = \frac{1}{r} (\partial_j r) \quad (5.104)$$

With  $\partial_j r = \frac{x_j}{r}$  derived earlier in Eq. (5.103) one obtains  $\partial_j \log r = \frac{1}{r} \frac{x_j}{r} = \frac{x_j}{r^2}$ , and thus  $\nabla \log r = \frac{\mathbf{x}}{r^2}$ .

3.

$$\begin{aligned}
& \partial_j \left[ \left( \sum_i (x_i - a_i)^2 \right)^{-\frac{1}{2}} + \left( \sum_i (x_i + a_i)^2 \right)^{-\frac{1}{2}} \right] = \\
& = -\frac{1}{2} \left[ \frac{1}{\left( \sum_i (x_i - a_i)^2 \right)^{\frac{3}{2}}} 2(x_j - a_j) + \frac{1}{\left( \sum_i (x_i + a_i)^2 \right)^{\frac{3}{2}}} 2(x_j + a_j) \right] = \\
& \quad - \left( \sum_i (x_i - a_i)^2 \right)^{-\frac{3}{2}} (x_j - a_j) - \left( \sum_i (x_i + a_i)^2 \right)^{-\frac{3}{2}} (x_j + a_j).
\end{aligned} \tag{5.105}$$

4. For three dimensions and for  $r \neq 0$ ,

$$\nabla \left( \frac{\mathbf{r}}{r^3} \right) \equiv \partial_i \left( \frac{r_i}{r^3} \right) = \frac{1}{r^3} \underbrace{\partial_i r_i}_{=3} + r_i \left( -3 \frac{1}{r^4} \right) \left( \frac{1}{2r} \right) 2r_i = 3 \frac{1}{r^3} - 3 \frac{1}{r^3} = 0. \tag{5.106}$$

5. With this solution (5.106) one obtains, for three dimensions and  $r \neq 0$ ,

$$\Delta \left( \frac{1}{r} \right) \equiv \partial_i \partial_i \frac{1}{r} = \partial_i \left( -\frac{1}{r^2} \right) \left( \frac{1}{2r} \right) 2r_i = -\partial_i \frac{r_i}{r^3} = 0. \tag{5.107}$$

6. With the earlier solution (5.106) one obtains

$$\begin{aligned}
& \Delta \left( \frac{\mathbf{r}\mathbf{p}}{r^3} \right) \equiv \\
& \partial_i \partial_i \frac{r_j p_j}{r^3} = \partial_i \left[ \frac{p_i}{r^3} + r_j p_j \left( -3 \frac{1}{r^5} \right) r_i \right] = \\
& = p_i \left( -3 \frac{1}{r^5} \right) r_i + p_i \left( -3 \frac{1}{r^5} \right) r_i + \\
& + r_j p_j \left[ \left( 15 \frac{1}{r^6} \right) \left( \frac{1}{2r} \right) 2r_i \right] r_i + r_j p_j \left( -3 \frac{1}{r^5} \right) \underbrace{\partial_i r_i}_{=3} = \\
& = r_i p_i \frac{1}{r^5} (-3 - 3 + 15 - 9) = 0
\end{aligned} \tag{5.108}$$

7. With  $r \neq 0$  and constant  $\mathbf{p}$  one obtains

$$\begin{aligned}
& \nabla \times (\mathbf{p} \times \frac{\mathbf{r}}{r^3}) \equiv \varepsilon_{ijk} \partial_j \varepsilon_{klm} p_l \frac{r_m}{r^3} = p_l \varepsilon_{ijk} \varepsilon_{klm} \left[ \partial_j \frac{r_m}{r^3} \right] \\
& = p_l \varepsilon_{ijk} \varepsilon_{klm} \left[ \frac{1}{r^3} \partial_j r_m + r_m \left( -3 \frac{1}{r^4} \right) \left( \frac{1}{2r} \right) 2r_j \right] \\
& = p_l \varepsilon_{ijk} \varepsilon_{klm} \left[ \frac{1}{r^3} \delta_{jm} - 3 \frac{r_j r_m}{r^5} \right] \\
& = p_l (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \left[ \frac{1}{r^3} \delta_{jm} - 3 \frac{r_j r_m}{r^5} \right] \\
& = p_i \underbrace{\left( 3 \frac{1}{r^3} - 3 \frac{1}{r^3} \right)}_{=0} - p_j \underbrace{\left( \frac{1}{r^3} \partial_j r_i - 3 \frac{r_j r_i}{r^5} \right)}_{=\delta_{ij}} \\
& = -\frac{\mathbf{p}}{r^3} + 3 \frac{(\mathbf{r}\mathbf{p})\mathbf{r}}{r^5}.
\end{aligned} \tag{5.109}$$

Note that, in three dimensions, the Grassmann identity (5.99)  $\varepsilon_{ijk} \varepsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}$  holds.

8.

$$\begin{aligned}
& \nabla \times (\nabla \Phi) \\
& \equiv \varepsilon_{ijk} \partial_j \partial_k \Phi \\
& = \varepsilon_{ikj} \partial_k \partial_j \Phi \\
& = \varepsilon_{ikj} \partial_j \partial_k \Phi \\
& = -\varepsilon_{ijk} \partial_j \partial_k \Phi = 0.
\end{aligned} \tag{5.110}$$

This is due to the fact that  $\partial_j \partial_k$  is symmetric, whereas  $\varepsilon_{ijk}$  is totally antisymmetric.

9. For a proof that  $(\mathbf{x} \times \mathbf{y}) \times \mathbf{z} \neq \mathbf{x} \times (\mathbf{y} \times \mathbf{z})$  consider

$$\begin{aligned}
& (\mathbf{x} \times \mathbf{y}) \times \mathbf{z} \\
& \equiv \varepsilon_{ijl} \varepsilon_{jkm} x_k y_m z_l \\
& = -\varepsilon_{ilj} \varepsilon_{jkm} x_k y_m z_l \\
& = -(\delta_{ik} \delta_{lm} - \delta_{im} \delta_{lk}) x_k y_m z_l \\
& = -x_i \mathbf{y} \cdot \mathbf{z} + y_i \mathbf{x} \cdot \mathbf{z}.
\end{aligned} \tag{5.111}$$

versus

$$\begin{aligned}
& \mathbf{x} \times (\mathbf{y} \times \mathbf{z}) \\
& \equiv \varepsilon_{ilj} \varepsilon_{jkm} x_l y_k z_m \\
& = (\delta_{ik} \delta_{lm} - \delta_{im} \delta_{lk}) x_l y_k z_m \\
& = y_i \mathbf{x} \cdot \mathbf{z} - z_i \mathbf{x} \cdot \mathbf{y}.
\end{aligned} \tag{5.112}$$

10. Let  $\mathbf{w} = \frac{\mathbf{p}}{r}$  with  $p_i = p_i(t - \frac{r}{c})$ , whereby  $t$  and  $c$  are constants. Then,

$$\begin{aligned}
\text{div } \mathbf{w} &= \nabla \cdot \mathbf{w} \\
\equiv \partial_i w_i &= \partial_i \left[ \frac{1}{r} p_i \left( t - \frac{r}{c} \right) \right] = \\
&= \left( -\frac{1}{r^2} \right) \left( \frac{1}{2r} \right) 2r_i p_i + \frac{1}{r} p'_i \left( -\frac{1}{c} \right) \left( \frac{1}{2r} \right) 2r_i = \\
&= -\frac{r_i p_i}{r^3} - \frac{1}{cr^2} p'_i r_i.
\end{aligned}$$

Hence,  $\text{div } \mathbf{w} = \nabla \cdot \mathbf{w} = -\left( \frac{\mathbf{r} \cdot \mathbf{p}}{r^3} + \frac{\mathbf{r} \cdot \mathbf{p}'}{cr^2} \right)$ .

$$\begin{aligned}
\text{rot } \mathbf{w} &= \nabla \times \mathbf{w} \\
\varepsilon_{ijk} \partial_j w_k &= \varepsilon_{ijk} \left[ \left( -\frac{1}{r^2} \right) \left( \frac{1}{2r} \right) 2r_j p_k + \frac{1}{r} p'_k \left( -\frac{1}{c} \right) \left( \frac{1}{2r} \right) 2r_j \right] = \\
&= -\frac{1}{r^3} \varepsilon_{ijk} r_j p_k - \frac{1}{cr^2} \varepsilon_{ijk} r_j p'_k = \\
&\equiv -\frac{1}{r^3} (\mathbf{r} \times \mathbf{p}) - \frac{1}{cr^2} (\mathbf{r} \times \mathbf{p}').
\end{aligned}$$

11. Let us verify some specific examples of Gauss' (divergence) theorem, stating that the outward flux of a vector field through a closed surface is

equal to the volume integral of the divergence of the region inside the surface. That is, the sum of all sources subtracted by the sum of all sinks represents the net flow out of a region or volume of threedimensional space:

$$\int_V \nabla \cdot \mathbf{w} dv = \int_F \mathbf{w} \cdot d\mathbf{f}. \quad (5.113)$$

Consider the vector field  $\mathbf{w} = (4x, -2y^2, z^2)$  and the (cylindric) volume bounded by the planes  $z = 0$  und  $z = 3$ , as well as by the surface  $x^2 + y^2 = 4$ .

Let us first look at the left hand side  $\int_V \nabla \cdot \mathbf{w} dv$  of Eq. (5.113):

$$\begin{aligned} \nabla \mathbf{w} &= \text{div } \mathbf{w} = 4 - 4y + 2z \\ \Rightarrow \int_V \text{div } \mathbf{w} dv &= \int_{z=0}^3 dz \int_{x=-2}^2 dx \int_{y=-\sqrt{4-x^2}}^{\sqrt{4-x^2}} dy (4 - 4y + 2z) = \\ &\quad \text{cylindric coordinates: } \begin{bmatrix} x &= & r \cos \varphi \\ y &= & r \sin \varphi \\ z &= & z \end{bmatrix} \\ &= \int_{z=0}^3 dz \int_0^2 r dr \int_0^{2\pi} d\varphi (4 - 4r \sin \varphi + 2z) = \\ &= \int_{z=0}^3 dz \int_0^2 r dr (4\varphi + 4r \cos \varphi + 2\varphi z) \Big|_{\varphi=0}^{2\pi} = \\ &= \int_{z=0}^3 dz \int_0^2 r dr (8\pi + 4r + 4\pi z - 4r) = \\ &= \int_{z=0}^3 dz \int_0^2 r dr (8\pi + 4\pi z) \\ &= 2 \left( 8\pi z + 4\pi \frac{z^2}{2} \right) \Big|_{z=0}^{z=3} = 2(24 + 18)\pi = 84\pi \end{aligned}$$

Now consider the right hand side  $\int_F \mathbf{w} \cdot d\mathbf{f}$  of Eq. (5.113). The surface consists of three parts: the lower plane  $F_1$  of the cylinder is characterized by  $z = 0$ ; the upper plane  $F_2$  of the cylinder is characterized by  $z = 3$ ; the surface on the side of the cylinder  $F_3$  is characterized by  $x^2 + y^2 = 4$ .

$d\mathbf{f}$  must be normal to these surfaces, pointing outwards; hence

$$\begin{aligned}
 F_1 : \int_{\mathcal{F}_1} \mathbf{w} \cdot d\mathbf{f}_1 &= \int_{\mathcal{F}_1} \begin{pmatrix} 4x \\ -2y^2 \\ z^2=0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} dx dy = 0 \\
 F_2 : \int_{\mathcal{F}_2} \mathbf{w} \cdot d\mathbf{f}_2 &= \int_{\mathcal{F}_2} \begin{pmatrix} 4x \\ -2y^2 \\ z^2=9 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} dx dy = \\
 &= 9 \int_{K_{r=2}} df = 9 \cdot 4\pi = 36\pi \\
 F_3 : \int_{\mathcal{F}_3} \mathbf{w} \cdot d\mathbf{f}_3 &= \int_{\mathcal{F}_3} \begin{pmatrix} 4x \\ -2y^2 \\ z^2 \end{pmatrix} \left( \frac{\partial \mathbf{x}}{\partial \varphi} \times \frac{\partial \mathbf{x}}{\partial z} \right) d\varphi dz \quad (r=2=\text{const.}) \\
 \frac{\partial \mathbf{x}}{\partial \varphi} &= \begin{pmatrix} -r \sin \varphi \\ r \cos \varphi \\ 0 \end{pmatrix} = \begin{pmatrix} -2 \sin \varphi \\ 2 \cos \varphi \\ 0 \end{pmatrix}; \quad \frac{\partial \mathbf{x}}{\partial z} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\
 &\Rightarrow \left( \frac{\partial \mathbf{x}}{\partial \varphi} \times \frac{\partial \mathbf{x}}{\partial z} \right) = \begin{pmatrix} 2 \cos \varphi \\ 2 \sin \varphi \\ 0 \end{pmatrix} \\
 \Rightarrow F_3 &= \int_{\varphi=0}^{2\pi} d\varphi \int_{z=0}^3 dz \begin{pmatrix} 4 \cdot 2 \cos \varphi \\ -2(2 \sin \varphi)^2 \\ z^2 \end{pmatrix} \begin{pmatrix} 2 \cos \varphi \\ 2 \sin \varphi \\ 0 \end{pmatrix} = \\
 &= \int_{\varphi=0}^{2\pi} d\varphi \int_{z=0}^3 dz (16 \cos^2 \varphi - 16 \sin^3 \varphi) = \\
 &= 3 \cdot 16 \int_{\varphi=0}^{2\pi} d\varphi (\cos^2 \varphi - \sin^3 \varphi) = \\
 &= \begin{bmatrix} \int \cos^2 \varphi d\varphi &= \frac{\varphi}{2} + \frac{1}{4} \sin 2\varphi \\ \int \sin^3 \varphi d\varphi &= -\cos \varphi + \frac{1}{3} \cos^3 \varphi \end{bmatrix} = \\
 &= 3 \cdot 16 \left\{ \frac{2\pi}{2} - \underbrace{\left[ \left(1 + \frac{1}{3}\right) - \left(1 + \frac{1}{3}\right) \right]}_{=0} \right\} = 48\pi
 \end{aligned}$$

For the flux through the surfaces one thus obtains

$$\oint_F \mathbf{w} \cdot d\mathbf{f} = F_1 + F_2 + F_3 = 84\pi.$$

12. Let us verify some specific examples of Stokes' theorem in three dimensions, stating that

$$\int_{\mathcal{F}} \text{rot } \mathbf{b} \cdot d\mathbf{f} = \oint_{\mathcal{C}_{\mathcal{F}}} \mathbf{b} \cdot d\mathbf{s}. \quad (5.114)$$

Consider the vector field  $\mathbf{b} = (yz, -xz, 0)$  and the (cylindric) volume bounded by spherical cap formed by the plane at  $z = a/\sqrt{2}$  of a sphere of radius  $a$  centered around the origin.

Let us first look at the left hand side  $\int_{\mathcal{F}} \text{rot } \mathbf{b} \cdot d\mathbf{f}$  of Eq. (5.114):

$$\mathbf{b} = \begin{pmatrix} yz \\ -xz \\ 0 \end{pmatrix} \Rightarrow \text{rot } \mathbf{b} = \nabla \times \mathbf{b} = \begin{pmatrix} x \\ y \\ -2z \end{pmatrix}$$

Let us transform this into spherical coordinates:

$$\mathbf{x} = \begin{pmatrix} r \sin \theta \cos \varphi \\ r \sin \theta \sin \varphi \\ r \cos \theta \end{pmatrix}$$

$$\Rightarrow \frac{\partial \mathbf{x}}{\partial \theta} = r \begin{pmatrix} \cos \theta \cos \varphi \\ \cos \theta \sin \varphi \\ -\sin \theta \end{pmatrix}; \quad \frac{\partial \mathbf{x}}{\partial \varphi} = r \begin{pmatrix} -\sin \theta \sin \varphi \\ \sin \theta \cos \varphi \\ 0 \end{pmatrix}$$

$$d\mathbf{f} = \left( \frac{\partial \mathbf{x}}{\partial \theta} \times \frac{\partial \mathbf{x}}{\partial \varphi} \right) d\theta d\varphi = r^2 \begin{pmatrix} \sin^2 \theta \cos \varphi \\ \sin^2 \theta \sin \varphi \\ \sin \theta \cos \theta \end{pmatrix} d\theta d\varphi$$

$$\nabla \times \mathbf{b} = r \begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ -2 \cos \theta \end{pmatrix}$$

$$\begin{aligned} \int_{\mathcal{F}} \text{rot } \mathbf{b} \cdot d\mathbf{f} &= \int_{\theta=0}^{\pi/4} d\theta \int_{\varphi=0}^{2\pi} d\varphi a^3 \begin{pmatrix} \sin \theta \cos \varphi \\ \sin \theta \sin \varphi \\ -2 \cos \theta \end{pmatrix} \begin{pmatrix} \sin^2 \theta \cos \varphi \\ \sin^2 \theta \sin \varphi \\ \sin \theta \cos \theta \end{pmatrix} = \\ &= a^3 \int_{\theta=0}^{\pi/4} d\theta \int_{\varphi=0}^{2\pi} d\varphi \left[ \sin^3 \theta \underbrace{(\cos^2 \varphi + \sin^2 \varphi)}_{=1} - 2 \sin \theta \cos^2 \theta \right] = \\ &= 2\pi a^3 \left[ \int_{\theta=0}^{\pi/4} d\theta (1 - \cos^2 \theta) \sin \theta - 2 \int_{\theta=0}^{\pi/4} d\theta \sin \theta \cos^2 \theta \right] = \\ &= 2\pi a^3 \int_{\theta=0}^{\pi/4} d\theta \sin \theta (1 - 3 \cos^2 \theta) = \\ &\quad \left[ \begin{array}{l} \text{transformation of variables:} \\ \cos \theta = u \Rightarrow du = -\sin \theta d\theta \Rightarrow d\theta = -\frac{du}{\sin \theta} \end{array} \right] \\ &= 2\pi a^3 \int_{\theta=0}^{\pi/4} (-du) (1 - 3u^2) = 2\pi a^3 \left( \frac{3u^3}{3} - u \right) \Big|_{\theta=0}^{\pi/4} = \\ &= 2\pi a^3 (\cos^3 \theta - \cos \theta) \Big|_{\theta=0}^{\pi/4} = 2\pi a^3 \left( \frac{2\sqrt{2}}{8} - \frac{\sqrt{2}}{2} \right) = \\ &= \frac{2\pi a^3}{8} (-2\sqrt{2}) = -\frac{\pi a^3 \sqrt{2}}{2} \end{aligned}$$

Now consider the right hand side  $\oint_{\mathcal{C}_{\mathcal{F}}} \mathbf{b} \cdot d\mathbf{s}$  of Eq. (5.114). The radius  $r'$  of the circle surface  $\{(x, y, z) \mid x, y \in \mathbb{R}, z = a/\sqrt{2}\}$  bounded by the sphere with radius  $a$  is determined by  $a^2 = (r')^2 + \frac{a^2}{2}$ ; hence,  $r' = a/\sqrt{2}$ . The curve of integration  $\mathcal{C}_{\mathcal{F}}$  can be parameterized by

$$\{(x, y, z) \mid x = \frac{a}{\sqrt{2}} \cos \varphi, y = \frac{a}{\sqrt{2}} \sin \varphi, z = \frac{a}{\sqrt{2}}\}.$$

Therefore,

$$\mathbf{x} = a \begin{pmatrix} \frac{1}{\sqrt{2}} \cos \varphi \\ \frac{1}{\sqrt{2}} \sin \varphi \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{a}{\sqrt{2}} \begin{pmatrix} \cos \varphi \\ \sin \varphi \\ 1 \end{pmatrix} \in \mathcal{C}_{\mathcal{F}}$$

Let us transform this into polar coordinates:

$$d\mathbf{s} = \frac{d\mathbf{x}}{d\varphi} d\varphi = \frac{a}{\sqrt{2}} \begin{pmatrix} -\sin \varphi \\ \cos \varphi \\ 0 \end{pmatrix} d\varphi$$

$$\mathbf{b} = \begin{pmatrix} \frac{a}{\sqrt{2}} \sin \varphi \cdot \frac{a}{\sqrt{2}} \\ -\frac{a}{\sqrt{2}} \cos \varphi \cdot \frac{a}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{a^2}{2} \begin{pmatrix} \sin \varphi \\ -\cos \varphi \\ 0 \end{pmatrix}$$

Hence the circular integral is given by

$$\oint_{\mathcal{C}_{\mathcal{F}}} \mathbf{b} \cdot d\mathbf{s} = \frac{a^2}{2} \frac{a}{\sqrt{2}} \int_{\varphi=0}^{2\pi} \underbrace{(-\sin^2 \varphi - \cos^2 \varphi)}_{=-1} d\varphi = -\frac{a^3}{2\sqrt{2}} 2\pi = -\frac{a^3 \pi}{\sqrt{2}}.$$

## 5.15 Some common misconceptions

### 5.15.1 Confusion between component representation and “the real thing”

Given a particular basis, a tensor is uniquely characterized by its components. However, without reference to a particular basis, any components are just blurbs.

Example (wrong!): a type-1 tensor (i.e., a vector) is given by (1, 2).

Correct: with respect to the basis  $\{(0, 1), (1, 0)\}$ , a rank-1 tensor (i.e., a vector) is given by (1, 2).

### 5.15.2 A matrix is a tensor

See the above section. **Example (wrong!): A matrix is a tensor of type (or rank) 2.** Correct: with respect to the basis  $\{(0, 1), (1, 0)\}$ , a matrix represents a type-2 tensor. The matrix components are the tensor components.

Also, for non-orthogonal bases, covariant, contravariant, and mixed tensors correspond to different matrices.



# 6

## Projective and incidence geometry

PROJECTIVE GEOMETRY is about the *geometric properties* that are invariant under *projective transformations*. *Incidence geometry* is about which points lie on which line.

### 6.1 Notation

In what follows, for the sake of being able to formally represent *geometric transformations* as “*quasi-linear*” transformations and matrices, the coordinates of  $n$ -dimensional Euclidean space will be augmented with one additional coordinate which is set to one. For instance, in the plane  $\mathbb{R}^2$ , we define new “three-component” coordinates by

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \equiv \begin{pmatrix} x_1 \\ x_2 \\ 1 \end{pmatrix} = \mathbf{X}. \quad (6.1)$$

In order to differentiate these new coordinates  $\mathbf{X}$  from the usual ones  $\mathbf{x}$ , they will be written in capital letters.

### 6.2 Affine transformations

*Affine transformations*

$$f(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{t} \quad (6.2)$$

with the *translation*  $\mathbf{t}$ , and encoded by a tuple  $(t_1, t_2)^T$ , and an arbitrary linear transformation  $\mathbf{A}$  encoding *rotations*, as well as *dilatation and skewing transformations* and represented by an arbitrary matrix  $A$ , can be “wrapped together” to form the new transformation matrix (“ $\mathbf{0}^T$ ” indicates a row matrix with entries zero)

$$\mathbf{f} = \left( \begin{array}{c|c} \mathbf{A} & \mathbf{t} \\ \hline \mathbf{0}^T & 1 \end{array} \right) \equiv \left( \begin{array}{cc|c} a_{11} & a_{12} & t_1 \\ a_{21} & a_{22} & t_2 \\ \hline 0 & 0 & 1 \end{array} \right). \quad (6.3)$$



As a result, the affine transformation  $f$  can be represented in the “quasi-linear” form

$$\mathbf{f}(\mathbf{X}) = \mathbf{f}\mathbf{X} = \left( \begin{array}{c|c} \mathbf{A} & \mathbf{t} \\ \hline \mathbf{0}^T & 1 \end{array} \right) \mathbf{X}. \quad (6.4)$$

### 6.2.1 One-dimensional case

In one dimension, that is, for  $\mathbf{z} \in \mathbb{C}$ , among the five basic operations

- (i) scaling:  $\mathbf{f}(\mathbf{z}) = r\mathbf{z}$  for  $r \in \mathbb{R}$ ,
- (ii) translation:  $\mathbf{f}(\mathbf{z}) = \mathbf{z} + \mathbf{w}$  for  $w \in \mathbb{C}$ ,
- (iii) rotation:  $\mathbf{f}(\mathbf{z}) = e^{i\varphi}\mathbf{z}$  for  $\varphi \in \mathbb{R}$ ,
- (iv) complex conjugation:  $\mathbf{f}(\mathbf{z}) = \bar{\mathbf{z}}$ ,
- (v) inversion:  $\mathbf{f}(\mathbf{z}) = \mathbf{z}^{-1}$ ,

there are three types of affine transformations (i)–(iii) which can be combined.

### 6.3 Similarity transformations

Similarity transformations involve translations  $\mathbf{t}$ , rotations  $\mathbf{R}$  and a dilatation  $r$  and can be represented by the matrix

$$\left( \begin{array}{c|c} r\mathbf{R} & \mathbf{t} \\ \hline \mathbf{0}^T & 1 \end{array} \right) \equiv \left( \begin{array}{cc|c} m \cos \varphi & -m \sin \varphi & t_1 \\ m \sin \varphi & m \cos \varphi & t_2 \\ \hline 0 & 0 & 1 \end{array} \right). \quad (6.5)$$

### 6.4 Fundamental theorem of affine geometry

Any bijection from  $\mathbb{R}^n$ ,  $n \geq 2$ , onto itself which maps all lines onto lines is an affine transformation.

### 6.5 Alexandrov's theorem

Consider the Minkowski space-time  $\mathbb{M}^n$ ; that is,  $\mathbb{R}^n$ ,  $n \geq 3$ , and the Minkowski metric [cf. (5.55) on page 92]  $\eta \equiv \{\eta_{ij}\} = \text{diag}(\underbrace{1, 1, \dots, 1}_{n-1 \text{ times}}, -1)$ . Consider further bijections  $\mathbf{f}$  from  $\mathbb{M}^n$  onto itself preserving light cones; that is for all  $\mathbf{x}, \mathbf{y} \in \mathbb{M}^n$ ,

$$\eta_{ij}(x^i - y^i)(x^j - y^j) = 0 \text{ if and only if } \eta_{ij}(\mathbf{f}^i(x) - \mathbf{f}^i(y))(\mathbf{f}^j(x) - \mathbf{f}^j(y)) = 0.$$

Then  $\mathbf{f}(x)$  is the product of a Lorentz transformation and a positive scale factor.

For a proof and further references, see

June A. Lester. Distance preserving transformations. In Francis Buekenhout, editor, *Handbook of Incidence Geometry*, pages 921–944. Elsevier, Amsterdam, 1995

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# 7

## Group theory

GROUP THEORY is about *transformations* and *symmetries*.

### 7.1 Definition

A *group* is a set of objects  $\mathfrak{G}$  which satisfy the following conditions (or, stated differently, axioms):

- (i) closedness: There exists a *composition rule* “ $\circ$ ” such that  $\mathfrak{G}$  is *closed* under any composition of elements; that is, the combination of any two elements  $a, b \in \mathfrak{G}$  results in an element of the group  $\mathfrak{G}$ .
- (ii) associativity: for all  $a, b$ , and  $c$  in  $\mathfrak{G}$ , the following equality holds:  
$$a \circ (b \circ c) = (a \circ b) \circ c;$$
- (iii) identity (element): there exists an element of  $\mathfrak{G}$ , called the *identity* (element) and denoted by  $I$ , such that for all  $a$  in  $\mathfrak{G}$ ,  $a \circ I = a$ .
- (iv) inverse (element): for every  $a$  in  $\mathfrak{G}$ , there exists an element  $a^{-1}$  in  $\mathfrak{G}$ , such that  $a^{-1} \circ a = I$ .
- (v) (optional) commutativity: if, for all  $a$  and  $b$  in  $\mathfrak{G}$ , the following equalities hold:  $a \circ b = b \circ a$ , then the group  $\mathfrak{G}$  is called *Abelian (group)*; otherwise it is called *non-Abelian (group)*.

A *subgroup* of a group is a subset which also satisfies the above axioms.

The *order* of a group is the number of distinct elements of that group.

In discussing groups one should keep in mind that there are two abstract spaces involved:

- (i) *Representation space* is the space of elements on which the group elements – that is, the group transformations – act.
- (ii) *Group space* is the space of elements of the group transformations. Its *dimension* is the number of independent transformations which

the group is composed of. These independent elements – also called the *generators* of the group – form a basis for all group elements. The coordinates in this space are defined relative (in terms of) the (basis elements, also called) generators. A *continuous group* can geometrically be imagined as a linear space (e.g., a linear vector or matrix space) *continuous group linear space* in which every point in this linear space is an element of the group.

Suppose we can find a structure- and distinction-preserving mapping  $U$  – that is, an injective mapping preserving the group operation  $\circ$  – between elements of a group  $\mathfrak{G}$  and the groups of general either real or complex non-singular matrices  $GL(n, \mathbb{R})$  or  $GL(n, \mathbb{C})$ , respectively. Then this mapping is called a *representation* of the group  $\mathfrak{G}$ . In particular, for this  $U : \mathfrak{G} \mapsto GL(n, \mathbb{R})$  or  $U : \mathfrak{G} \mapsto GL(n, \mathbb{C})$ ,

$$U(a \circ b) = U(a) \cdot U(b), \quad (7.1)$$

for all  $a, b, a \circ b \in \mathfrak{G}$ .

Consider, for the sake of an example, the *Pauli spin matrices* which are proportional to the angular momentum operators along the  $x, y, z$ -axis <sup>1</sup>:

<sup>1</sup> Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

$$\begin{aligned} \sigma_1 = \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma_2 = \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \sigma_3 = \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (7.2)$$

Suppose these matrices  $\sigma_1, \sigma_2, \sigma_3$  serve as generators of a group. With respect to this basis system of matrices  $\{\sigma_1, \sigma_2, \sigma_3\}$  a general point in group in group space might be labelled by a three-dimensional vector with the coordinates  $(x_1, x_2, x_3)$  (relative to the basis  $\{\sigma_1, \sigma_2, \sigma_3\}$ ); that is,

$$\mathbf{x} = x_1 \sigma_1 + x_2 \sigma_2 + x_3 \sigma_3. \quad (7.3)$$

If we form the exponential  $A(\mathbf{x}) = e^{\frac{i}{2}\mathbf{x}}$ , we can show (no proof is given here) that  $A(\mathbf{x})$  is a two-dimensional matrix representation of the group  $SU(2)$ , the special unitary group of degree 2 of  $2 \times 2$  unitary matrices with determinant 1.

## 7.2 Lie theory

### 7.2.1 Generators

We can generalize this example by defining the *generators* of a continuous group as the first coefficient of a Taylor expansion around unity; that is, if

the dimension of the group is  $n$ , and the Taylor expansion is

$$G(\mathbf{X}) = \sum_{i=1}^n X_i T_i + \dots, \quad (7.4)$$

then the matrix generator  $T_i$  is defined by

$$T_i = \left. \frac{\partial G(\mathbf{X})}{\partial X_i} \right|_{\mathbf{X}=0}. \quad (7.5)$$

### 7.2.2 Exponential map

There is an exponential connection  $\exp : \mathfrak{X} \mapsto \mathfrak{G}$  between a matrix Lie group and the Lie algebra  $\mathfrak{X}$  generated by the generators  $T_i$ .

### 7.2.3 Lie algebra

A Lie algebra is a vector space  $\mathfrak{X}$ , together with a binary *Lie bracket* operation  $[\cdot, \cdot] : \mathfrak{X} \times \mathfrak{X} \mapsto \mathfrak{X}$  satisfying

- (i) bilinearity;
- (ii) antisymmetry:  $[X, Y] = -[Y, X]$ , in particular  $[X, X] = 0$ ;
- (iii) the Jacobi identity:  $[X, [Y, Z]] + [Z, [X, Y]] + [Y, [Z, X]] = 0$

for all  $X, Y, Z \in \mathfrak{X}$ .

## 7.3 Some important groups

### 7.3.1 General linear group $GL(n, \mathbb{C})$

The *general linear group*  $GL(n, \mathbb{C})$  contains all non-singular (i.e., invertible; there exist an inverse)  $n \times n$  matrices with complex entries. The composition rule “ $\circ$ ” is identified with matrix multiplication (which is associative); the neutral element is the unit matrix  $\mathbb{I}_n = \text{diag}(\underbrace{1, \dots, 1}_{n \text{ times}})$ .

### 7.3.2 Orthogonal group $O(n)$

The *orthogonal group*  $O(n)$ <sup>2</sup> contains all orthogonal [i.e.,  $A^{-1} = A^T$ ]  $n \times n$  matrices. The composition rule “ $\circ$ ” is identified with matrix multiplication (which is associative); the neutral element is the unit matrix  $\mathbb{I}_n = \text{diag}(\underbrace{1, \dots, 1}_{n \text{ times}})$ .

Because of orthogonality, only half of the off-diagonal entries are independent of one another; also the diagonal elements must be real; that leaves us with the liberty of dimension  $n(n+1)/2$ :  $(n^2 - n)/2$  complex numbers from the off-diagonal elements, plus  $n$  reals from the diagonal.

<sup>2</sup> F. D. Murnaghan. *The Unitary and Rotation Groups*. Spartan Books, Washington, D.C., 1962

### 7.3.3 Rotation group $SO(n)$

The *special orthogonal group* or, by another name, the *rotation group*  $SO(n)$  contains all orthogonal  $n \times n$  matrices with unit determinant.  $SO(n)$  is a subgroup of  $O(n)$ .

The rotation group in two-dimensional configuration space  $SO(2)$  corresponds to planar rotations around the origin. It has dimension 1 corresponding to one parameter  $\theta$ . Its elements can be written as

$$R(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}. \quad (7.6)$$

### 7.3.4 Unitary group $U(n)$

The *unitary group*  $U(n)$ <sup>3</sup> contains all unitary [i.e.,  $A^{-1} = A^\dagger = (\bar{A})^T$ ]  $n \times n$  matrices. The composition rule “ $\circ$ ” is identified with matrix multiplication (which is associative); the neutral element is the unit matrix  $\mathbb{I}_n = \text{diag}(\underbrace{1, \dots, 1}_{n \text{ times}})$ .

Because of unitarity, only half of the off-diagonal entries are independent of one another; also the diagonal elements must be real; that leaves us with the liberty of dimension  $n^2$ :  $(n^2 - n)/2$  complex numbers from the off-diagonal elements, plus  $n$  reals from the diagonal yield  $n^2$  real parameters.

Not that, for instance,  $U(1)$  is the set of complex numbers  $z = e^{i\theta}$  of unit modulus  $|z|^2 = 1$ . It forms an Abelian group.

<sup>3</sup> F. D. Murnaghan. *The Unitary and Rotation Groups*. Spartan Books, Washington, D.C., 1962

### 7.3.5 Special unitary group $SU(n)$

The *special unitary group*  $SU(n)$  contains all unitary  $n \times n$  matrices with unit determinant.  $SU(n)$  is a subgroup of  $U(n)$ .

### 7.3.6 Symmetric group $S(n)$

The *symmetric group*  $S(n)$  on a finite set of  $n$  elements (or symbols) is the group whose elements are all the permutations of the  $n$  elements, and whose group operation is the composition of such permutations. The identity is the identity permutation. The *permutations* are bijective functions from the set of elements onto itself. The order (number of elements) of  $S(n)$  is  $n!$ . Generalizing these groups to an infinite number of elements  $S_\infty$  is straightforward.

The symmetric group should not be confused with a symmetry group.

### 7.3.7 Poincaré group

The Poincaré group is the group of *isometries* – that is, bijective maps preserving distances – in space-time modelled by  $\mathbb{R}^4$  endowed with a scalar product and thus of a norm induced by the *Minkowski metric*  $\eta \equiv \{\eta_{ij}\} = \text{diag}(1, 1, 1, -1)$  introduced in (5.55).

It has dimension ten ( $4 + 3 + 3 = 10$ ), associated with the ten fundamental (distance preserving) operations from which general isometries can be composed: (i) translation through time and any of the three dimensions of space ( $1 + 3 = 4$ ), (ii) rotation (by a fixed angle) around any of the three spatial axes (3), and a (Lorentz) boost, increasing the velocity in any of the three spatial directions of two uniformly moving bodies (3).

The rotations and Lorentz boosts form the *Lorentz group*.

#### 7.4 Cayley's representation theorem

*Cayley's theorem* states that every group  $\mathfrak{G}$  can be imbedded as – equivalently, is isomorphic to – a subgroup of the symmetric group; that is, it is isomorphic with some permutation group. In particular, every finite group  $\mathfrak{G}$  of order  $n$  can be imbedded as – equivalently, is isomorphic to – a subgroup of the symmetric group  $S(n)$ .

Stated pointedly: permutations exhaust the possible structures of (finite) groups. The study of subgroups of the symmetric groups is no less general than the study of all groups. No proof is given here.



For a proof, see

Joseph J. Rotman. *An Introduction to the Theory of Groups*, volume 148 of *Graduate texts in mathematics*. Springer, New York, fourth edition, 1995. ISBN 0387942858



*Part III:*

*Functional analysis*





## Brief review of complex analysis

Is it not amazing that complex numbers<sup>1</sup> can be used for physics? Robert Musil (a mathematician educated in Vienna), in “*Verwirrungen des Zöglings Törleß*”, expressed the amazement of a youngster confronted with the applicability of imaginaries, states that, at the beginning of any computation involving imaginary numbers are “solid” numbers which could represent something measurable, like lengths or weights, or something else tangible; or are at least real numbers. At the end of the computation there are also such “solid” numbers. But the beginning and the end of the computation are connected by something seemingly nonexistent. Does this not appear, Musil’s *Zöglings Törleß* wonders, like a bridge crossing an abyss with only a bridge pier at the very beginning and one at the very end, which could nevertheless be crossed with certainty and securely, as if this bridge would exist entirely?

In what follows, a very brief review of *complex analysis*, or, by another term, *function theory*, will be presented. For much more detailed introductions to complex analysis, including proofs, take, for instance, the “classical” books<sup>2</sup>, among a zillion of other very good ones<sup>3</sup>. We shall study complex analysis not only for its beauty, but also because it yields very important analytical methods and tools; for instance for the solution of (differential) equations and the computation of definite integrals. These methods will then be required for the computation of distributions and Green’s functions, as well for the solution of differential equations of mathematical physics – such as the Schrödinger equation.

One motivation for introducing *imaginary numbers* is the (if you perceive it that way) “malady” that not every polynomial such as  $P(x) = x^2 + 1$  has a root  $x$  – and thus not every (polynomial) equation  $P(x) = x^2 + 1 = 0$  has a solution  $x$  – which is a real number. Indeed, you need the imaginary unit  $i^2 = -1$  for a factorization  $P(x) = (x + i)(x - i)$  yielding the two roots  $\pm i$  to achieve this. In that way, the introduction of imaginary numbers is a further step towards omni-solvability. No wonder that the fundamental theorem of algebra, stating that every non-constant polynomial with complex coefficients has at least one complex root – and thus total factoriz-

<sup>1</sup> Edmund Hlawka. Zum Zahlbegriff. *Philosophia Naturalis*, 19:413–470, 1982

German original  
(<http://www.gutenberg.org/ebooks/34717>):  
“In solch einer Rechnung sind am Anfang ganz solide Zahlen, die Meter oder Gewichte, oder irgend etwas anderes Greifbares darstellen können und wenigstens wirkliche Zahlen sind. Am Ende der Rechnung stehen ebensolche. Aber diese beiden hängen miteinander durch etwas zusammen, das es gar nicht gibt. Ist das nicht wie eine Brücke, von der nur Anfangs- und Endpfeiler vorhanden sind und die man dennoch so sicher überschreitet, als ob sie ganz dastünde? Für mich hat so eine Rechnung etwas Schwindliges; als ob es ein Stück des Weges weiß Gott wohin ginge. Das eigentlich Unheimliche ist mir aber die Kraft, die in solch einer Rechnung steckt und einen so festhält, daß man doch wieder richtig landet.”

<sup>2</sup> Eberhard Freitag and Rolf Busam. *Funktionentheorie I*. Springer, Berlin, Heidelberg, fourth edition, 1993,1995,2000,2006. English translation in ; E. T. Whittaker and G. N. Watson. *A Course of Modern Analysis*. Cambridge University Press, Cambridge, 4th edition, 1927. URL <http://archive.org/details/ACourseOfModernAnalysis>. Reprinted in 1996. Table errata: Math. Comp. v. 36 (1981), no. 153, p. 319; Robert E. Greene and Stephen G. Krantz. *Function theory of one complex variable*, volume 40 of *Graduate Studies in Mathematics*. American mathematical Society, Providence, Rhode Island, third edition, 2006; Einar Hille. *Analytic Function Theory*. Ginn, New York, 1962. 2 Volumes; and Lars V. Ahlfors. *Complex Analysis: An Introduction of the Theory of Analytic Functions of One Complex Variable*. McGraw-Hill Book Co., New York, third edition, 1978

Eberhard Freitag and Rolf Busam. *Complex Analysis*. Springer, Berlin, Heidelberg, 2005

<sup>3</sup> Klaus Jänich. *Funktionentheorie. Eine Einführung*. Springer, Berlin, Heidelberg, sixth edition, 2008. DOI: 10.1007/978-3-540-35015-6. URL [10.1007/978-3-540-35015-6](https://doi.org/10.1007/978-3-540-35015-6); and Dietmar A. Salamon. *Funktionentheorie*. Birkhäuser, Basel, 2012. DOI: 10.1007/978-

ability of polynomials into linear factors, follows!

If not mentioned otherwise, it is assumed that the *Riemann surface*, representing a “deformed version” of the complex plane for functional purposes, is simply connected. Simple connectedness means that the Riemann surface is path-connected so that every path between two points can be continuously transformed, staying within the domain, into any other path while preserving the two endpoints between the paths. In particular, suppose that there are no “holes” in the Riemann surface; it is not “punctured.”

Furthermore, let  $i$  be the *imaginary unit* with the property that  $i^2 = -1$  is the solution of the equation  $x^2 + 1 = 0$ . With the introduction of imaginary numbers we can guarantee that all quadratic equations have two roots (i.e., solutions).

By combining imaginary and real numbers, any *complex number* can be defined to be some linear combination of the real unit number “1” with the imaginary unit number  $i$  that is,  $z = 1 \times (\Re z) + i \times (\Im z)$ , with the real valued factors  $(\Re z)$  and  $(\Im z)$ , respectively. By this definition, a complex number  $z$  can be decomposed into real numbers  $x$ ,  $y$ ,  $r$  and  $\varphi$  such that

$$z \stackrel{\text{def}}{=} \Re z + i \Im z = x + iy = r e^{i\varphi}, \quad (8.1)$$

with  $x = r \cos \varphi$  and  $y = r \sin \varphi$ , where Euler’s formula

$$e^{i\varphi} = \cos \varphi + i \sin \varphi \quad (8.2)$$

has been used. If  $z = \Re z$  we call  $z$  a real number. If  $z = i \Im z$  we call  $z$  a purely imaginary number.

The *modulus* or *absolute value* of a complex number  $z$  is defined by

$$|z| \stackrel{\text{def}}{=} \sqrt{(\Re z)^2 + (\Im z)^2}. \quad (8.3)$$

Many rules of classical arithmetic can be carried over to complex arithmetic<sup>4</sup>. Note, however, that, for instance,  $\sqrt{a}\sqrt{b} = \sqrt{ab}$  is only valid if at least one factor  $a$  or  $b$  is positive; hence  $-1 = i^2 = \sqrt{i}\sqrt{i} = \sqrt{-1}\sqrt{-1} \neq \sqrt{(-1)^2} = 1$ . More generally, for two arbitrary numbers,  $u$  and  $v$ ,  $\sqrt{u}\sqrt{v}$  is not always equal to  $\sqrt{uv}$ .

For many mathematicians *Euler’s identity*

$$e^{i\pi} = -1, \text{ or } e^{i\pi} + 1 = 0, \quad (8.4)$$

is the “most beautiful” theorem<sup>5</sup>.

Euler’s formula (8.2) can be used to derive *de Moivre’s formula* for integer  $n$  (for non-integer  $n$  the formula is multi-valued for different arguments  $\varphi$ ):

$$e^{in\varphi} = (\cos \varphi + i \sin \varphi)^n = \cos(n\varphi) + i \sin(n\varphi). \quad (8.5)$$

It is quite suggestive to consider the complex numbers  $z$ , which are linear combinations of the real and the imaginary unit, in the *complex plane*

<sup>4</sup> Tom M. Apostol. *Mathematical Analysis: A Modern Approach to Advanced Calculus*. Addison-Wesley Series in Mathematics. Addison-Wesley, Reading, MA, second edition, 1974. ISBN 0-201-00288-4; and Eberhard Freitag and Rolf Busam. *Funktionentheorie 1*. Springer, Berlin, Heidelberg, fourth edition, 1993, 1995, 2000, 2006. English translation in

Eberhard Freitag and Rolf Busam. *Complex Analysis*. Springer, Berlin, Heidelberg, 2005

Nevertheless,  $\sqrt{|u|}\sqrt{|v|} = \sqrt{|uv|}$ .

<sup>5</sup> David Wells. Which is the most beautiful? *The Mathematical Intelligencer*, 10:30–31, 1988. ISSN 0343-6993. DOI: 10.1007/BF03023741. URL <http://dx.doi.org/10.1007/BF03023741>

$\mathbb{C} = \mathbb{R} \times \mathbb{R}$  as a geometric representation of complex numbers. Thereby, the real and the imaginary unit are identified with the (orthonormal) basis vectors of the *standard (Cartesian) basis*; that is, with the tuples

$$\begin{aligned} 1 &\equiv (1, 0), \\ i &\equiv (0, 1). \end{aligned} \quad (8.6)$$

The addition and multiplication of two complex numbers represented by  $(x, y)$  and  $(u, v)$  with  $x, y, u, v \in \mathbb{R}$  are then defined by

$$\begin{aligned} (x, y) + (u, v) &= (x + u, y + v), \\ (x, y) \cdot (u, v) &= (xu - yv, xv + yu), \end{aligned} \quad (8.7)$$

and the neutral elements for addition and multiplication are  $(0, 0)$  and  $(1, 0)$ , respectively.

We shall also consider the *extended plane*  $\bar{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$  consisting of the entire complex plane  $\mathbb{C}$  together with the point “ $\infty$ ” representing infinity. Thereby,  $\infty$  is introduced as an ideal element, completing the one-to-one (bijective) mapping  $w = \frac{1}{z}$ , which otherwise would have no image at  $z = 0$ , and no pre-image (argument) at  $w = 0$ .

### 8.1 Differentiable, holomorphic (analytic) function

Consider the function  $f(z)$  on the domain  $G \subset \text{Domain}(f)$ .

$f$  is called *differentiable* at the point  $z_0$  if the differential quotient

$$\left. \frac{df}{dz} \right|_{z_0} = f'(z) \Big|_{z_0} = \left. \frac{\partial f}{\partial x} \right|_{z_0} = \left. \frac{1}{i} \frac{\partial f}{\partial y} \right|_{z_0} \quad (8.8)$$

exists.

If  $f$  is differentiable in the domain  $G$  it is called *holomorphic*, or, used synonymously, *analytic* in the domain  $G$ .

### 8.2 Cauchy-Riemann equations

The function  $f(z) = u(z) + i v(z)$  (where  $u$  and  $v$  are real valued functions) is analytic or holomorphic if and only if  $(a_b = \partial a / \partial b)$

$$u_x = v_y, \quad u_y = -v_x \quad . \quad (8.9)$$

For a proof, differentiate along the real, and then along the complex axis, taking

$$\begin{aligned} f'(z) &= \lim_{x \rightarrow 0} \frac{f(z+x) - f(z)}{x} = \frac{\partial f}{\partial x} = \frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x}, \\ \text{and } f'(z) &= \lim_{y \rightarrow 0} \frac{f(z+iy) - f(z)}{iy} = \frac{\partial f}{\partial iy} = -i \frac{\partial f}{\partial y} = -i \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \end{aligned} \quad (8.10)$$

For  $f$  to be analytic, both partial derivatives have to be identical, and thus  $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial iy}$ , or

$$\frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} = -i \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y}. \quad (8.11)$$

By comparing the real and imaginary parts of this equation, one obtains the two real Cauchy-Riemann equations

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y}, \\ \frac{\partial v}{\partial x} &= -\frac{\partial u}{\partial y}. \end{aligned} \quad (8.12)$$

### 8.3 Definition analytical function

If  $f$  is analytic in  $G$ , all derivatives of  $f$  exist, and all mixed derivatives are independent on the order of differentiations. Then the Cauchy-Riemann equations imply that

$$\begin{aligned} \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \right) &= \frac{\partial}{\partial x} \left( \frac{\partial v}{\partial y} \right) = \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial x} \right) = -\frac{\partial}{\partial y} \left( \frac{\partial u}{\partial y} \right), \\ \text{and } \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial y} \right) &= \frac{\partial}{\partial y} \left( \frac{\partial u}{\partial x} \right) = \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial y} \right) = -\frac{\partial}{\partial x} \left( \frac{\partial v}{\partial x} \right), \end{aligned} \quad (8.13)$$

and thus

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u = 0, \text{ and } \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) v = 0. \quad (8.14)$$

If  $f = u + iv$  is analytic in  $G$ , then the lines of constant  $u$  and  $v$  are orthogonal.

The tangential vectors of the lines of constant  $u$  and  $v$  in the two-dimensional complex plane are defined by the two-dimensional nabla operator  $\nabla u(x, y)$  and  $\nabla v(x, y)$ . Since, by the Cauchy-Riemann equations  $u_x = v_y$  and  $u_y = -v_x$

$$\nabla u(x, y) \cdot \nabla v(x, y) = \begin{pmatrix} u_x \\ u_y \end{pmatrix} \cdot \begin{pmatrix} v_x \\ v_y \end{pmatrix} = u_x v_x + u_y v_y = u_x v_x + (-v_x) u_x = 0 \quad (8.15)$$

these tangential vectors are normal.

$f$  is *angle (shape) preserving conformal* if and only if it is holomorphic and its derivative is everywhere non-zero.

Consider an analytic function  $f$  and an arbitrary path  $C$  in the complex plane of the arguments parameterized by  $z(t)$ ,  $t \in \mathbb{R}$ . The image of  $C$  associated with  $f$  is  $f(C) = C' : f(z(t))$ ,  $t \in \mathbb{R}$ .

The tangent vector of  $C'$  in  $t = 0$  and  $z_0 = z(0)$  is

$$\left. \frac{d}{dt} f(z(t)) \right|_{t=0} = \left. \frac{d}{dz} f(z) \right|_{z_0} \left. \frac{d}{dt} z(t) \right|_{t=0} = \lambda_0 e^{i\varphi_0} \left. \frac{d}{dt} z(t) \right|_{t=0}. \quad (8.16)$$

Note that the first term  $\left. \frac{d}{dz} f(z) \right|_{z_0}$  is independent of the curve  $C$  and only depends on  $z_0$ . Therefore, it can be written as a product of a squeeze (stretch)  $\lambda_0$  and a rotation  $e^{i\varphi_0}$ . This is independent of the curve; hence two curves  $C_1$  and  $C_2$  passing through  $z_0$  yield the same transformation of the image  $\lambda_0 e^{i\varphi_0}$ .

#### 8.4 Cauchy's integral theorem

If  $f$  is analytic on  $G$  and on its borders  $\partial G$ , then any closed line integral of  $f$  vanishes

$$\oint_{\partial G} f(z) dz = 0 \quad . \quad (8.17)$$

No proof is given here.

In particular,  $\oint_{C \subset \partial G} f(z) dz$  is independent of the particular curve, and only depends on the initial and the end points.

For a proof, subtract two line integral which follow arbitrary paths  $C_1$  and  $C_2$  to a common initial and end point, and which have the same integral kernel. Then reverse the integration direction of one of the line integrals. According to Cauchy's integral theorem the resulting integral over the closed loop has to vanish.

Often it is useful to parameterize a contour integral by some form of

$$\int_C f(z) dz = \int_a^b f(z(t)) \frac{dz(t)}{dt} dt. \quad (8.18)$$

Let  $f(z) = 1/z$  and  $C : z(\varphi) = R e^{i\varphi}$ , with  $R > 0$  and  $-\pi < \varphi \leq \pi$ . Then

$$\begin{aligned} \oint_{|z|=R} f(z) dz &= \int_{-\pi}^{\pi} f(z(\varphi)) \frac{dz(\varphi)}{d\varphi} d\varphi \\ &= \int_{-\pi}^{\pi} \frac{1}{R e^{i\varphi}} R i e^{i\varphi} d\varphi \\ &= \int_{-\pi}^{\pi} i d\varphi \\ &= 2\pi i \end{aligned} \quad (8.19)$$

is independent of  $R$ .

#### 8.5 Cauchy's integral formula

If  $f$  is analytic on  $G$  and on its borders  $\partial G$ , then

$$f(z_0) = \frac{1}{2\pi i} \oint_{\partial G} \frac{f(z)}{z - z_0} dz \quad . \quad (8.20)$$

No proof is given here.

Note that because of Cauchy's integral formula, analytic functions have an integral representation. This might appear as not very exciting; alas it has far-reaching consequences, because analytic functions have integral

representation, they have higher derivatives, which also have integral representation. And, as a result, if a function has one complex derivative, then it has infinitely many complex derivatives. This statement can be expressed formally precisely by the generalized Cauchy's integral formula or, by another term, Cauchy's differentiation formula states that if  $f$  is analytic on  $G$  and on its borders  $\partial G$ , then

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_{\partial G} \frac{f(z)}{(z - z_0)^{n+1}} dz. \quad (8.21)$$

No proof is given here.

Cauchy's integral formula presents a powerful method to compute integrals. Consider the following examples.

(i) First, let us calculate

$$\oint_{|z|=3} \frac{3z+2}{z(z+1)^3} dz.$$

The kernel has two poles at  $z = 0$  and  $z = -1$  which are both inside the domain of the contour defined by  $|z| = 3$ . By using Cauchy's integral formula we obtain for "small"  $\epsilon$

$$\begin{aligned} & \oint_{|z|=3} \frac{3z+2}{z(z+1)^3} dz \\ &= \oint_{|z|=\epsilon} \frac{3z+2}{z(z+1)^3} dz + \oint_{|z+1|=\epsilon} \frac{3z+2}{z(z+1)^3} dz \\ &= \oint_{|z|=\epsilon} \frac{3z+2}{(z+1)^3} \frac{1}{z} dz + \oint_{|z+1|=\epsilon} \frac{3z+2}{z} \frac{1}{(z+1)^3} dz \\ &= \frac{2\pi i}{0!} \left[ \left[ \frac{d^0}{dz^0} \right] \frac{3z+2}{(z+1)^3} \right]_{z=0} + \frac{2\pi i}{2!} \left[ \frac{d^2}{dz^2} \frac{3z+2}{z} \right]_{z=-1} \quad (8.22) \\ &= \frac{2\pi i}{0!} \frac{3z+2}{(z+1)^3} \Big|_{z=0} + \frac{2\pi i}{2!} \frac{d^2}{dz^2} \frac{3z+2}{z} \Big|_{z=-1} \\ &= 4\pi i - 4\pi i \\ &= 0. \end{aligned}$$

(ii) Consider

$$\begin{aligned} & \oint_{|z|=3} \frac{e^{2z}}{(z+1)^4} dz \\ &= \frac{2\pi i}{3!} \frac{3!}{2\pi i} \oint_{|z|=3} \frac{e^{2z}}{(z - (-1))^{3+1}} dz \\ &= \frac{2\pi i}{3!} \frac{d^3}{dz^3} \Big|_{z=-1} e^{2z} \quad (8.23) \\ &= \frac{2\pi i}{3!} 2^3 \Big|_{z=-1} e^{2z} \\ &= \frac{8\pi i e^{-2}}{3}. \end{aligned}$$

Suppose  $g(z)$  is a function with a pole of order  $n$  at the point  $z_0$ ; that is

$$g(z) = \frac{f(z)}{(z - z_0)^n} \quad (8.24)$$

where  $f(z)$  is an analytic function. Then,

$$\oint_{\partial G} g(z) dz = \frac{2\pi i}{(n-1)!} f^{(n-1)}(z_0) \quad (8.25)$$

### 8.6 Series representation of complex differentiable functions

As a consequence of Cauchy's (generalized) integral formula, analytic functions have power series representations.

For the sake of a proof, we shall recast the denominator  $z - z_0$  in Cauchy's integral formula (8.20) as a geometric series as follows (we shall assume that  $|z_0 - a| < |z - a|$ )

$$\begin{aligned} \frac{1}{z - z_0} &= \frac{1}{(z - a) - (z_0 - a)} \\ &= \frac{1}{(z - a)} \left[ \frac{1}{1 - \frac{z_0 - a}{z - a}} \right] \\ &= \frac{1}{(z - a)} \left[ \sum_{n=0}^{\infty} \frac{(z_0 - a)^n}{(z - a)^n} \right] \\ &= \sum_{n=0}^{\infty} \frac{(z_0 - a)^n}{(z - a)^{n+1}}. \end{aligned} \quad (8.26)$$

By substituting this in Cauchy's integral formula (8.20) and using Cauchy's generalized integral formula (8.21) yields an expansion of the analytical function  $f$  around  $z_0$  by a power series

$$\begin{aligned} f(z_0) &= \frac{1}{2\pi i} \oint_{\partial G} \frac{f(z)}{z - z_0} dz \\ &= \frac{1}{2\pi i} \oint_{\partial G} f(z) \sum_{n=0}^{\infty} \frac{(z_0 - a)^n}{(z - a)^{n+1}} dz \\ &= \sum_{n=0}^{\infty} (z_0 - a)^n \frac{1}{2\pi i} \oint_{\partial G} \frac{f(z)}{(z - a)^{n+1}} dz \\ &= \sum_{n=0}^{\infty} \frac{f^{(n)}(z_0)}{n!} (z_0 - a)^n. \end{aligned} \quad (8.27)$$

### 8.7 Laurent series

Every function  $f$  which is analytic in a concentric region  $R_1 < |z - z_0| < R_2$  can in this region be uniquely written as a *Laurent series*

$$f(z) = \sum_{k=-\infty}^{\infty} (z - z_0)^k a_k \quad (8.28)$$



The coefficients  $a_k$  are (the closed contour  $C$  must be in the concentric region)

$$a_k = \frac{1}{2\pi i} \oint_C (\chi - z_0)^{-k-1} f(\chi) d\chi \quad (8.29)$$

The coefficient

$$\text{Res}(f(z_0)) = a_{-1} = \frac{1}{2\pi i} \oint_C f(\chi) d\chi \quad (8.30)$$

is called the *residue*, denoted by “Res.”

For a proof, as in Eqs. (8.26) we shall recast  $(a - b)^{-1}$  for  $|a| > |b|$  as a geometric series

$$\begin{aligned} \frac{1}{a-b} &= \frac{1}{a} \left( \frac{1}{1-\frac{b}{a}} \right) = \frac{1}{a} \left( \sum_{n=0}^{\infty} \frac{b^n}{a^n} \right) = \sum_{n=0}^{\infty} \frac{b^n}{a^{n+1}} \\ [\text{substitution } n+1 \rightarrow -k, n \rightarrow -k-1, k \rightarrow -n-1] &= \sum_{k=-1}^{-\infty} \frac{a^k}{b^{k+1}}, \end{aligned} \quad (8.31)$$

and, for  $|a| < |b|$ ,

$$\begin{aligned} \frac{1}{a-b} &= -\frac{1}{b-a} = -\sum_{n=0}^{\infty} \frac{a^n}{b^{n+1}} \\ [\text{substitution } n+1 \rightarrow -k, n \rightarrow -k-1, k \rightarrow -n-1] &= -\sum_{k=-1}^{-\infty} \frac{b^k}{a^{k+1}}. \end{aligned} \quad (8.32)$$

Furthermore since  $a+b = a-(-b)$ , we obtain, for  $|a| > |b|$ ,

$$\frac{1}{a+b} = \sum_{n=0}^{\infty} (-1)^n \frac{b^n}{a^{n+1}} = \sum_{k=-1}^{-\infty} (-1)^{-k-1} \frac{a^k}{b^{k+1}} = -\sum_{k=-1}^{-\infty} (-1)^k \frac{a^k}{b^{k+1}}, \quad (8.33)$$

and, for  $|a| < |b|$ ,

$$\begin{aligned} \frac{1}{a+b} &= -\sum_{n=0}^{\infty} (-1)^{n+1} \frac{a^n}{b^{n+1}} = \sum_{n=0}^{\infty} (-1)^n \frac{a^n}{b^{n+1}} \\ &= \sum_{k=-1}^{-\infty} (-1)^{-k-1} \frac{b^k}{a^{k+1}} = -\sum_{k=-1}^{-\infty} (-1)^k \frac{b^k}{a^{k+1}}. \end{aligned} \quad (8.34)$$

Suppose that some function  $f(z)$  is analytic in an annulus bounded by the radius  $r_1$  and  $r_2 > r_1$ . By substituting this in Cauchy's integral formula (8.20) for an annulus bounded by the radius  $r_1$  and  $r_2 > r_1$  (note that the orientations of the boundaries with respect to the annulus are opposite, rendering a relative factor “ $-1$ ”) and using Cauchy's generalized integral formula (8.21) yields an expansion of the analytical function  $f$  around  $z_0$  by the Laurent series for a point  $a$  on the annulus; that is, for a path containing the point  $z$  around a circle with radius  $r_1$ ,  $|z - a| < |z_0 - a|$ ; likewise, for a path containing the point  $z$  around a circle with radius

$$r_2 > a > r_1, |z - a| > |z_0 - a|,$$

$$\begin{aligned} f(z_0) &= \frac{1}{2\pi i} \oint_{r_1} \frac{f(z)}{z - z_0} dz - \frac{1}{2\pi i} \oint_{r_2} \frac{f(z)}{z - z_0} dz \\ &= \frac{1}{2\pi i} \left[ \oint_{r_1} f(z) \sum_{n=0}^{\infty} \frac{(z_0 - a)^n}{(z - a)^{n+1}} dz + \oint_{r_2} f(z) \sum_{n=-1}^{-\infty} \frac{(z_0 - a)^n}{(z - a)^{n+1}} dz \right] \\ &= \frac{1}{2\pi i} \left[ \sum_{n=0}^{\infty} (z_0 - a)^n \oint_{r_1} \frac{f(z)}{(z - a)^{n+1}} dz + \sum_{n=-1}^{-\infty} (z_0 - a)^n \oint_{r_2} \frac{f(z)}{(z - a)^{n+1}} dz \right] \\ &= \sum_{n=-\infty}^{\infty} (z_0 - a)^n \left[ \frac{1}{2\pi i} \oint_{r_1 \leq r \leq r_2} \frac{f(z)}{(z - a)^{n+1}} dz \right]. \end{aligned} \quad (8.35)$$

Suppose that  $g(z)$  is a function with a pole of order  $n$  at the point  $z_0$ ; that is  $g(z) = h(z)/(z - z_0)^n$ , where  $h(z)$  is an analytic function. Then the terms  $k \leq -(n + 1)$  vanish in the Laurent series. This follows from Cauchy's integral formula

$$a_k = \frac{1}{2\pi i} \oint_c (\chi - z_0)^{-k-n-1} h(\chi) d\chi = 0 \quad (8.36)$$

for  $-k - n - 1 \geq 0$ .

Note that, if  $f$  has a simple pole (pole of order 1) at  $z_0$ , then it can be rewritten into  $f(z) = g(z)/(z - z_0)$  for some analytic function  $g(z) = (z - z_0)f(z)$  that remains after the singularity has been “split” from  $f$ . Cauchy's integral formula (8.20), and the residue can be rewritten as

$$a_{-1} = \frac{1}{2\pi i} \oint_{\partial G} \frac{g(z)}{z - z_0} dz = g(z_0). \quad (8.37)$$

For poles of higher order, the generalized Cauchy integral formula (8.21) can be used.

## 8.8 Residue theorem

Suppose  $f$  is analytic on a simply connected open subset  $G$  with the exception of finitely many (or denumerably many) points  $z_i$ . Then,

$$\oint_{\partial G} f(z) dz = 2\pi i \sum_{z_i} \text{Res } f(z_i) \quad (8.38)$$

No proof is given here.

The residue theorem presents a powerful tool for calculating integrals, both real and complex. Let us first mention a rather general case of a situation often used. Suppose we are interested in the integral

$$I = \int_{-\infty}^{\infty} R(x) dx$$

with rational kernel  $R$ ; that is,  $R(x) = P(x)/Q(x)$ , where  $P(x)$  and  $Q(x)$  are polynomials (or can at least be bounded by a polynomial) with no

common root (and therefore factor). Suppose further that the degrees of the polynomial is

$$\deg P(x) \leq \deg Q(x) - 2.$$

This condition is needed to assure that the additional upper or lower path we want to add when completing the contour does not contribute; that is, vanishes.

Now first let us analytically continue  $R(x)$  to the complex plane  $R(z)$ ; that is,

$$I = \int_{-\infty}^{\infty} R(x) dx = \int_{-\infty}^{\infty} R(z) dz.$$

Next let us close the contour by adding a (vanishing) path integral

$$\int_{\curvearrowright} R(z) dz = 0$$

in the upper (lower) complex plane

$$I = \int_{-\infty}^{\infty} R(z) dz + \int_{\curvearrowright} R(z) dz = \oint_{-\infty \& \curvearrowright} R(z) dz.$$

The added integral vanishes because it can be approximated by

$$\left| \int_{\curvearrowright} R(z) dz \right| \leq \lim_{r \rightarrow \infty} \left( \frac{\text{const.}}{r^2} \pi r \right) = 0.$$

With the contour closed the residue theorem can be applied for an evaluation of  $I$ ; that is,

$$I = 2\pi i \sum_{z_i} \text{Res} R(z_i)$$

for all singularities  $z_i$  in the region enclosed by “ $\rightarrow \& \curvearrowright$ .”

Let us consider some examples.

(i) Consider

$$I = \int_{-\infty}^{\infty} \frac{dx}{x^2 + 1}.$$

The analytic continuation of the kernel and the addition with vanishing a semicircle “far away” closing the integration path in the *upper*

complex half-plane of  $z$  yields

$$\begin{aligned}
 I &= \int_{-\infty}^{\infty} \frac{dx}{x^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{z^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{z^2 + 1} + \int_{\gamma} \frac{dz}{z^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{(z+i)(z-i)} + \int_{\gamma} \frac{dz}{(z+i)(z-i)} \\
 &= \oint \frac{1}{(z-i)} f(z) dz \text{ with } f(z) = \frac{1}{(z+i)} \\
 &= 2\pi i \operatorname{Res} \left( \frac{1}{(z+i)(z-i)} \right) \Big|_{z=i} \\
 &= 2\pi i f(i) \\
 &= 2\pi i \frac{1}{(2i)} \\
 &= \pi.
 \end{aligned} \tag{8.39}$$

Here, Eq. (8.37) has been used. Closing the integration path in the *lower* complex half-plane of  $z$  yields (note that in this case the contour integral is negative because of the path orientation)

$$\begin{aligned}
 I &= \int_{-\infty}^{\infty} \frac{dx}{x^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{z^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{z^2 + 1} + \int_{\text{lower path}} \frac{dz}{z^2 + 1} \\
 &= \int_{-\infty}^{\infty} \frac{dz}{(z+i)(z-i)} + \int_{\text{lower path}} \frac{dz}{(z+i)(z-i)} \\
 &= \oint \frac{1}{(z+i)} f(z) dz \text{ with } f(z) = \frac{1}{(z-i)} \\
 &= -2\pi i \operatorname{Res} \left( \frac{1}{(z+i)(z-i)} \right) \Big|_{z=-i} \\
 &= -2\pi i f(-i) \\
 &= 2\pi i \frac{1}{(2i)} \\
 &= \pi.
 \end{aligned} \tag{8.40}$$

(ii) Consider

$$F(p) = \int_{-\infty}^{\infty} \frac{e^{ipx}}{x^2 + a^2} dx$$

with  $a \neq 0$ .

The analytic continuation of the kernel yields

$$F(p) = \int_{-\infty}^{\infty} \frac{e^{ipz}}{z^2 + a^2} dz = \int_{-\infty}^{\infty} \frac{e^{ipz}}{(z-ia)(z+ia)} dz.$$

Suppose first that  $p > 0$ . Then, if  $z = x + iy$ ,  $e^{ipz} = e^{ipx}e^{-py} \rightarrow 0$  for  $z \rightarrow \infty$  in the *upper* half plane. Hence, we can close the contour in the upper half plane and obtain  $F(p)$  with the help of the residue theorem.

If  $a > 0$  only the pole at  $z = +ia$  is enclosed in the contour; thus we obtain

$$\begin{aligned} F(p) &= 2\pi i \operatorname{Res} \frac{e^{ipz}}{(z+ia)} \Big|_{z=+ia} \\ &= 2\pi i \frac{e^{i^2 pa}}{2ia} \\ &= \frac{\pi}{a} e^{-pa}. \end{aligned} \quad (8.41)$$

If  $a < 0$  only the pole at  $z = -ia$  is enclosed in the contour; thus we obtain

$$\begin{aligned} F(p) &= 2\pi i \operatorname{Res} \frac{e^{ipz}}{(z-ia)} \Big|_{z=-ia} \\ &= 2\pi i \frac{e^{-i^2 pa}}{-2ia} \\ &= \frac{\pi}{-a} e^{-i^2 pa} \\ &= \frac{\pi}{-a} e^{pa}. \end{aligned} \quad (8.42)$$

Hence, for  $a \neq 0$ ,

$$F(p) = \frac{\pi}{|a|} e^{-|pa|}. \quad (8.43)$$

For  $p < 0$  a very similar consideration, taking the *lower* path for continuation – and thus acquiring a minus sign because of the “clockwork” orientation of the path as compared to its interior – yields

$$F(p) = \frac{\pi}{|a|} e^{-|pa|}. \quad (8.44)$$

- (iii) If some function  $f(z)$  can be expanded into a Taylor series or Laurent series, the residue can be directly obtained by the coefficient of the  $\frac{1}{z}$  term. For instance, let  $f(z) = e^{\frac{1}{z}}$  and  $C : z(\varphi) = Re^{i\varphi}$ , with  $R = 1$  and  $-\pi < \varphi \leq \pi$ . This function is singular only in the origin  $z = 0$ , but this is an *essential singularity* near which the function exhibits extreme behavior. Nevertheless,  $f(z) = e^{\frac{1}{z}}$  can be expanded into a Laurent series

$$f(z) = e^{\frac{1}{z}} = \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{1}{z}\right)^l$$

around this singularity. The residue can be found by using the series expansion of  $f(z)$ ; that is, by *comparing* its coefficient of the  $1/z$  term.

Hence,  $\operatorname{Res} \left( e^{\frac{1}{z}} \right) \Big|_{z=0}$  is the coefficient 1 of the  $1/z$  term. Thus,

$$\oint_{|z|=1} e^{\frac{1}{z}} dz = 2\pi i \operatorname{Res} \left( e^{\frac{1}{z}} \right) \Big|_{z=0} = 2\pi i. \quad (8.45)$$

For  $f(z) = e^{-\frac{1}{z}}$ , a similar argument yields  $\text{Res} \left( e^{-\frac{1}{z}} \right) \Big|_{z=0} = -1$  and thus  $\oint_{|z|=1} e^{-\frac{1}{z}} dz = -2\pi i$ .

An alternative attempt to compute the residue, with  $z = e^{i\varphi}$ , yields

$$\begin{aligned}
 a_{-1} &= \text{Res} \left( e^{\pm \frac{1}{z}} \right) \Big|_{z=0} = \frac{1}{2\pi i} \oint_C e^{\pm \frac{1}{z}} dz \\
 &= \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{\pm \frac{1}{e^{i\varphi}}} \frac{dz(\varphi)}{d\varphi} d\varphi \\
 &= \pm \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{\pm \frac{1}{e^{i\varphi}}} i e^{\pm i\varphi} d\varphi \quad (8.46) \\
 &= \pm \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{\pm e^{\mp i\varphi}} e^{\pm i\varphi} d\varphi \\
 &= \pm \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{\pm e^{\mp i\varphi} \pm i\varphi} d\varphi.
 \end{aligned}$$

### 8.9 Multi-valued relationships, branch points and branch cuts

Suppose that the Riemann surface of is *not* simply connected.

Suppose further that  $f$  is a multi-valued function (or multifunction).

An argument  $z$  of the function  $f$  is called *branch point* if there is a closed curve  $C_z$  around  $z$  whose image  $f(C_z)$  is an open curve. That is, the multi-function  $f$  is discontinuous in  $z$ . Intuitively speaking, branch points are the points where the various sheets of a multifunction come together.

A *branch cut* is a curve (with ends possibly open, closed, or half-open) in the complex plane across which an analytic multifunction is discontinuous. Branch cuts are often taken as lines.

### 8.10 Riemann surface

Suppose  $f(z)$  is a multifunction. Then the various  $z$ -surfaces on which  $f(z)$  is uniquely defined, together with their connections through branch points and branch cuts, constitute the Riemann surface of  $f$ . The required leafs are called *Riemann sheet*.

A point  $z$  of the function  $f(z)$  is called a *branch point of order  $n$*  if through it and through the associated cut(s)  $n + 1$  Riemann sheets are connected.

### 8.11 Some special functional classes

The requirement that a function is holomorphic (analytic, differentiable) puts some stringent conditions on its type, form, and on its behaviour. For instance, let  $z_0 \in G$  the limit of a sequence  $\{z_n\} \in G$ ,  $z_n \neq z_0$ . Then it can be shown that, if two analytic functions  $f$  and  $g$  on the domain  $G$  coincide in the points  $z_n$ , then they coincide on the entire domain  $G$ .

### 8.11.1 Entire function

An function is said to be an *entire function* if it is defined and differentiable (holomorphic, analytic) in the entire *finite complex plane*  $\mathbb{C}$ .

An entire function may be either a *rational function*  $f(z) = P(z)/Q(z)$  which can be written as the ratio of two polynomial functions  $P(z)$  and  $Q(z)$ , or it may be a *transcendental function* such as  $e^z$  or  $\sin z$ .

The *Weierstrass factorization theorem* states that an entire function can be represented by a (possibly infinite<sup>6</sup>) product involving its zeroes [i.e., the points  $z_k$  at which the function vanishes  $f(z_k) = 0$ ]. For example (for a proof, see Eq. (6.2) of <sup>7</sup>),

$$\sin z = z \prod_{k=1}^{\infty} \left[ 1 - \left( \frac{z}{\pi k} \right)^2 \right]. \quad (8.47)$$

### 8.11.2 Liouville's theorem for bounded entire function

*Liouville's theorem* states that a bounded (i.e., its absolute square is finite everywhere in  $\mathbb{C}$ ) entire function which is defined at infinity is a constant. Conversely, a nonconstant entire function cannot be bounded.

For a proof, consider the integral representation of the derivative  $f'(z)$  of some bounded entire function  $f(z) < C$  (suppose the bound is  $C$ ) obtained through Cauchy's integral formula (8.21), taken along a circular path with arbitrarily large radius  $r$  of length  $2\pi r$  in the limit of infinite radius; that is,

$$\begin{aligned} |f'(z_0)| &= \left| \frac{1}{2\pi i} \oint_{\partial G} \frac{f(z)}{(z - z_0)^2} dz \right| \\ &< \frac{1}{2\pi i} \oint_{\partial G} \frac{|f(z)|}{(z - z_0)^2} dz < \frac{1}{2\pi i} 2\pi r \frac{C}{r^2} = \frac{C}{r} \xrightarrow{r \rightarrow \infty} 0. \end{aligned} \quad (8.48)$$

As a result,  $f'(z_0) = 0$  and thus  $f = A \in \mathbb{C}$ .

A *generalized Liouville theorem* states that if  $f : \mathbb{C} \rightarrow \mathbb{C}$  is an entire function and if for some real number  $c$  and some positive integer  $k$  it holds that  $|f(z)| \leq c|z|^k$  for all  $z$  with  $|z| > 1$ , then  $f$  is a polynomial in  $z$  of degree at most  $k$ .

No proof<sup>8</sup> is presented here. This theorem is needed for an investigation into the general form of the Fuchsian differential equation on page 211.

### 8.11.3 Picard's theorem

*Picard's theorem* states that any entire function that misses two or more points  $f : \mathbb{C} \mapsto \mathbb{C} - \{z_1, z_2, \dots\}$  is constant. Conversely, any nonconstant entire function covers the entire complex plane  $\mathbb{C}$  except a single point.

An example for a nonconstant entire function is  $e^z$  which never reaches the point 0.

<sup>6</sup> Theodore W. Gamelin. *Complex Analysis*. Springer, New York, NY, 2001

<sup>7</sup> J. B. Conway. *Functions of Complex Variables. Volume I*. Springer, New York, NY, 1973

It may (wrongly) appear that  $\sin z$  is nonconstant and bounded. However it is only bounded on the real axis; indeed,  $\sin iy = (1/2)(e^y + e^{-y}) \rightarrow \infty$  for  $y \rightarrow \infty$ .

<sup>8</sup> Robert E. Greene and Stephen G. Krantz. *Function theory of one complex variable*, volume 40 of *Graduate Studies in Mathematics*. American mathematical Society, Providence, Rhode Island, third edition, 2006

#### 8.11.4 Meromorphic function

If  $f$  has no singularities other than poles in the domain  $G$  it is called *meromorphic* in the domain  $G$ .

We state without proof (e.g., Theorem 8.5.1 of<sup>9</sup>) that a function  $f$  which is meromorphic in the extended plane is a rational function  $f(z) = P(z)/Q(z)$  which can be written as the ratio of two polynomial functions  $P(z)$  and  $Q(z)$ .

<sup>9</sup> Einar Hille. *Analytic Function Theory*. Ginn, New York, 1962. 2 Volumes

#### 8.12 Fundamental theorem of algebra

The *factor theorem* states that a polynomial  $P(z)$  in  $z$  of degree  $k$  has a factor  $z - z_0$  if and only if  $P(z_0) = 0$ , and can thus be written as  $P(z) = (z - z_0)Q(z)$ , where  $Q(z)$  is a polynomial in  $z$  of degree  $k - 1$ . Hence, by iteration,

$$P(z) = \alpha \prod_{i=1}^k (z - z_i), \quad (8.49)$$

where  $\alpha \in \mathbb{C}$ .

No proof is presented here.

The *fundamental theorem of algebra* states that every polynomial (with arbitrary complex coefficients) has a root [i.e. solution of  $f(z) = 0$ ] in the complex plane. Therefore, by the factor theorem, the number of roots of a polynomial, up to multiplicity, equals its degree.

Again, no proof is presented here.

<https://www.dpmms.cam.ac.uk/~wtg10/falg.html>





## Brief review of Fourier transforms

### 9.0.1 Functional spaces

That complex continuous waveforms or functions are comprised of a number of harmonics seems to be an idea at least as old as the Pythagoreans. In physical terms, Fourier analysis<sup>1</sup> attempts to decompose a function into its constituent frequencies, known as a frequency spectrum. Thereby the goal is the expansion of periodic and aperiodic functions into sine and cosine functions. Fourier's observation or conjecture is, informally speaking, that any "suitable" function  $f(x)$  can be expressed as a possibly infinite sum (i.e. linear combination), of sines and cosines of the form

$$f(x) = \sum_{k=-\infty}^{\infty} [A_k \cos(Ckx) + B_k \sin(Ckx)]. \quad (9.1)$$

Moreover, it is conjectured that any "suitable" function  $f(x)$  can be expressed as a possibly infinite sum (i.e. linear combination), of exponentials; that is,

$$f(x) = \sum_{k=-\infty}^{\infty} D_k e^{ikx}. \quad (9.2)$$

More generally, it is conjectured that any "suitable" function  $f(x)$  can be expressed as a possibly infinite sum (i.e. linear combination), of other (possibly orthonormal) functions  $g_k(x)$ ; that is,

$$f(x) = \sum_{k=-\infty}^{\infty} \gamma_k g_k(x). \quad (9.3)$$

The bigger picture can then be viewed in terms of *functional (vector) spaces*: these are spanned by the elementary functions  $g_k$ , which serve as elements of a *functional basis* of a possibly infinite-dimensional vector space. Suppose, in further analogy to the set of all such functions  $\mathfrak{G} = \bigcup_k g_k(x)$  to the (Cartesian) standard basis, we can consider these elementary functions  $g_k$  to be *orthonormal* in the sense of a *generalized functional scalar product* [cf. also Section 14.5 on page 231; in particular Eq. (14.89)]

$$\langle g_k | g_l \rangle = \int_a^b g_k(x) g_l(x) dx = \delta_{kl}. \quad (9.4)$$

<sup>1</sup> T. W. Körner. *Fourier Analysis*. Cambridge University Press, Cambridge, UK, 1988; Kenneth B. Howell. *Principles of Fourier analysis*. Chapman & Hall/CRC, Boca Raton, London, New York, Washington, D.C., 2001; and Russell Herman. *Introduction to Fourier and Complex Analysis with Applications to the Spectral Analysis of Signals*. University of North Carolina Wilmington, Wilmington, NC, 2010. URL <http://people.uncw.edu/hermanr/mat367/FCABook/Book2010/FTCA-book.pdf>. Creative Commons Attribution-NoncommercialShare Alike 3.0 United States License

One could arrange the coefficients  $\gamma_k$  into a tuple (an ordered list of elements)  $(\gamma_1, \gamma_2, \dots)$  and consider them as components or coordinates of a vector with respect to the linear orthonormal functional basis  $\mathfrak{G}$ .

### 9.0.2 Fourier series

Suppose that a function  $f(x)$  is periodic in the interval  $[-\frac{L}{2}, \frac{L}{2}]$  with period  $L$ . (Alternatively, the function may be only defined in this interval.) A function  $f(x)$  is *periodic* if there exist a period  $L \in \mathbb{R}$  such that, for all  $x$  in the domain of  $f$ ,

$$f(L+x) = f(x). \quad (9.5)$$

Then, under certain “mild” conditions – that is,  $f$  must be piecewise continuous and have only a finite number of maxima and minima –  $f$  can be decomposed into a *Fourier series*

$$\begin{aligned} f(x) &= \frac{a_0}{2} + \sum_{k=1}^{\infty} \left[ a_k \cos\left(\frac{2\pi}{L} kx\right) + b_k \sin\left(\frac{2\pi}{L} kx\right) \right], \text{ with} \\ a_k &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cos\left(\frac{2\pi}{L} kx\right) dx \text{ for } k \geq 0 \\ b_k &= \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \sin\left(\frac{2\pi}{L} kx\right) dx \text{ for } k > 0. \end{aligned} \quad (9.6)$$

For a (heuristic) proof, consider the Fourier conjecture (9.1), and compute the coefficients  $A_k$ ,  $B_k$ , and  $C$ .

First, observe that we have assumed that  $f$  is periodic in the interval  $[-\frac{L}{2}, \frac{L}{2}]$  with period  $L$ . This should be reflected in the sine and cosine terms of (9.1), which themselves are periodic functions in the interval  $[-\pi, \pi]$  with period  $2\pi$ . Thus in order to map the functional period of  $f$  into the sines and cosines, we can “stretch/shrink”  $L$  into  $2\pi$ ; that is,  $C$  in Eq. (9.1) is identified with

$$C = \frac{2\pi}{L}. \quad (9.7)$$

Thus we obtain

$$f(x) = \sum_{k=-\infty}^{\infty} \left[ A_k \cos\left(\frac{2\pi}{L} kx\right) + B_k \sin\left(\frac{2\pi}{L} kx\right) \right]. \quad (9.8)$$

Now use the following properties: (i) for  $k = 0$ ,  $\cos(0) = 1$  and  $\sin(0) = 0$ . Thus, by comparing the coefficient  $a_0$  in (9.6) with  $A_0$  in (9.1) we obtain  $A_0 = \frac{a_0}{2}$ .

(ii) Since  $\cos(x) = \cos(-x)$  is an *even function* of  $x$ , we can rearrange the summation by combining identical functions  $\cos(-\frac{2\pi}{L} kx) = \cos(\frac{2\pi}{L} kx)$ , thus obtaining  $a_k = A_{-k} + A_k$  for  $k > 0$ .

(iii) Since  $\sin(x) = -\sin(-x)$  is an *odd function* of  $x$ , we can rearrange the summation by combining identical functions  $\sin(-\frac{2\pi}{L} kx) = -\sin(\frac{2\pi}{L} kx)$ , thus obtaining  $b_k = -B_{-k} + B_k$  for  $k > 0$ .

Having obtained the same form of the Fourier series of  $f(x)$  as exposed in (9.6), we now turn to the derivation of the coefficients  $a_k$  and  $b_k$ .  $a_0$  can

For proofs and additional information see §8.1 in

Kenneth B. Howell. *Principles of Fourier analysis*. Chapman & Hall/CRC, Boca Raton, London, New York, Washington, D.C., 2001

be derived by just considering the functional scalar product exposed in Eq. (9.4) of  $f(x)$  with the constant identity function  $g(x) = 1$ ; that is,

$$\begin{aligned}\langle g | f \rangle &= \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) dx \\ &= \int_{-\frac{L}{2}}^{\frac{L}{2}} \left\{ \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right)] \right\} dx \\ &= a_0 \frac{L}{2},\end{aligned}\quad (9.9)$$

and hence

$$a_0 = \frac{2}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) dx \quad (9.10)$$

In a very similar manner, the other coefficients can be computed by considering  $\langle \cos\left(\frac{2\pi}{L} kx\right) | f(x) \rangle$ ,  $\langle \sin\left(\frac{2\pi}{L} kx\right) | f(x) \rangle$  and exploiting the *orthogonality relations for sines and cosines*

$$\begin{aligned}\int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi}{L} kx\right) \cos\left(\frac{2\pi}{L} lx\right) dx &= 0, \\ \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos\left(\frac{2\pi}{L} kx\right) \cos\left(\frac{2\pi}{L} lx\right) dx &= \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin\left(\frac{2\pi}{L} kx\right) \sin\left(\frac{2\pi}{L} lx\right) dx = \frac{L}{2} \delta_{kl}.\end{aligned}\quad (9.11)$$

For the sake of an example, let us compute the Fourier series of

$$f(x) = |x| = \begin{cases} -x, & \text{for } -\pi \leq x < 0, \\ +x, & \text{for } 0 \leq x \leq \pi. \end{cases}$$

First observe that  $L = 2\pi$ , and that  $f(x) = f(-x)$ ; that is,  $f$  is an *even* function of  $x$ ; hence  $b_n = 0$ , and the coefficients  $a_n$  can be obtained by considering only the integration between 0 and  $\pi$ .

For  $n = 0$ ,

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} dx f(x) = \frac{2}{\pi} \int_0^{\pi} x dx = \pi.$$

For  $n > 0$ ,

$$\begin{aligned}a_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) dx = \frac{2}{\pi} \int_0^{\pi} x \cos(nx) dx = \\ &= \frac{2}{\pi} \left[ \frac{\sin(nx)}{n} x \Big|_0^{\pi} - \int_0^{\pi} \frac{\sin(nx)}{n} dx \right] = \frac{2}{\pi} \frac{\cos(nx)}{n^2} \Big|_0^{\pi} = \\ &= \frac{2}{\pi} \frac{\cos(n\pi) - 1}{n^2} = -\frac{4}{\pi n^2} \sin^2 \frac{n\pi}{2} = \begin{cases} 0 & \text{for even } n \\ -\frac{4}{\pi n^2} & \text{for odd } n \end{cases}\end{aligned}$$

Thus,

$$\begin{aligned}f(x) &= \frac{\pi}{2} - \frac{4}{\pi} \left( \cos x + \frac{\cos 3x}{9} + \frac{\cos 5x}{25} + \cdots \right) = \\ &= \frac{\pi}{2} - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\cos[(2n+1)x]}{(2n+1)^2}.\end{aligned}$$

One could arrange the coefficients  $(a_0, a_1, b_1, a_2, b_2, \dots)$  into a tuple (an ordered list of elements) and consider them as components or coordinates of a vector spanned by the linear independent sine and cosine functions which serve as a basis of an infinite dimensional vector space.

### 9.0.3 Exponential Fourier series

Suppose again that a function is periodic in the interval  $[-\frac{L}{2}, \frac{L}{2}]$  with period  $L$ . Then, under certain “mild” conditions – that is,  $f$  must be piecewise continuous and have only a finite number of maxima and minima –  $f$  can be decomposed into an *exponential Fourier series*

$$\begin{aligned} f(x) &= \sum_{k=-\infty}^{\infty} c_k e^{ikx}, \text{ with} \\ c_k &= \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x') e^{-ikx'} dx'. \end{aligned} \quad (9.12)$$

The exponential form of the Fourier series can be derived from the Fourier series (9.6) by Euler’s formula (8.2), in particular,  $e^{ik\varphi} = \cos(k\varphi) + i \sin(k\varphi)$ , and thus

$$\cos(k\varphi) = \frac{1}{2} (e^{ik\varphi} + e^{-ik\varphi}), \text{ as well as } \sin(k\varphi) = \frac{1}{2i} (e^{ik\varphi} - e^{-ik\varphi}).$$

By comparing the coefficients of (9.6) with the coefficients of (9.12), we obtain

$$\begin{aligned} a_k &= c_k + c_{-k} \text{ for } k \geq 0, \\ b_k &= i(c_k - c_{-k}) \text{ for } k > 0, \end{aligned} \quad (9.13)$$

or

$$c_k = \begin{cases} \frac{1}{2}(a_k - i b_k) & \text{for } k > 0, \\ \frac{a_0}{2} & \text{for } k = 0, \\ \frac{1}{2}(a_{-k} + i b_{-k}) & \text{for } k < 0. \end{cases} \quad (9.14)$$

Eqs. (9.12) can be combined into

$$f(x) = \frac{1}{L} \sum_{k=-\infty}^{\infty} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x') e^{-ik(x'-x)} dx'. \quad (9.15)$$

### 9.0.4 Fourier transformation

Suppose we define  $\Delta k = 2\pi/L$ , or  $1/L = \Delta k/2\pi$ . Then Eq. (9.15) can be rewritten as

$$f(x) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x') e^{-ik(x'-x)} dx' \Delta k. \quad (9.16)$$

Now, in the “aperiodic” limit  $L \rightarrow \infty$  we obtain the *Fourier transformation* and the *Fourier inversion*  $\mathcal{F}^{-1}[\mathcal{F}[f(x)]] = \mathcal{F}[\mathcal{F}^{-1}[f(x)]] = f(x)$  by

$$\begin{aligned} f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x') e^{-ik(x'-x)} dx' dk, \text{ whereby} \\ \mathcal{F}^{-1}[\tilde{f}(k)] &= f(x) = \alpha \int_{-\infty}^{\infty} \tilde{f}(k) e^{\pm ikx} dk, \text{ and} \\ \mathcal{F}[f(x)] &= \tilde{f}(k) = \beta \int_{-\infty}^{\infty} f(x') e^{\mp ikx'} dx'. \end{aligned} \quad (9.17)$$

$\mathcal{F}[f(x)] = \tilde{f}(k)$  is called the *Fourier transform* of  $f(x)$ . Per convention, either one of the two sign pairs  $+-$  or  $-+$  must be chosen. The factors  $\alpha$  and  $\beta$  must be chosen such that

$$\alpha\beta = \frac{1}{2\pi}; \quad (9.18)$$

that is, the factorization can be “spread evenly among  $\alpha$  and  $\beta$ ,” such that  $\alpha = \beta = 1/\sqrt{2\pi}$ , or “unevenly,” such as, for instance,  $\alpha = 1$  and  $\beta = 1/2\pi$ , or  $\alpha = 1/2\pi$  and  $\beta = 1$ .

Most generally, the Fourier transformations can be rewritten (change of integration constant), with arbitrary  $A, B \in \mathbb{R}$ , as

$$\begin{aligned} \mathcal{F}^{-1}[\tilde{f}(k)](x) &= f(x) = B \int_{-\infty}^{\infty} \tilde{f}(k) e^{iAkx} dk, \text{ and} \\ \mathcal{F}[f(x)](k) &= \tilde{f}(k) = \frac{A}{2\pi B} \int_{-\infty}^{\infty} f(x') e^{-iAkx'} dx'. \end{aligned} \quad (9.19)$$

The choice  $A = 2\pi$  and  $B = 1$  renders a very symmetric form of (9.19); more precisely,

$$\begin{aligned} \mathcal{F}^{-1}[\tilde{f}(k)](x) &= f(x) = \int_{-\infty}^{\infty} \tilde{f}(k) e^{2\pi i k x} dk, \text{ and} \\ \mathcal{F}[f(x)](k) &= \tilde{f}(k) = \int_{-\infty}^{\infty} f(x') e^{-2\pi i k x'} dx'. \end{aligned} \quad (9.20)$$

For the sake of an example, assume  $A = 2\pi$  and  $B = 1$  in Eq. (9.19), therefore starting with (9.20), and consider the Fourier transform of the *Gaussian function*

$$\varphi(x) = e^{-\pi x^2}. \quad (9.21)$$

As a hint, notice that  $e^{-t^2}$  is analytic in the region  $0 \leq \text{Im } t \leq \sqrt{\pi}k$ ; also, as will be shown in Eqs. (10.18), the *Gaussian integral* is

$$\int_{-\infty}^{\infty} e^{-t^2} dt = \sqrt{\pi}. \quad (9.22)$$

With  $A = 2\pi$  and  $B = 1$  in Eq. (9.19), the Fourier transform of the Gaussian function is

$$\begin{aligned} \mathcal{F}[\varphi(x)](k) &= \tilde{\varphi}(k) = \int_{-\infty}^{\infty} e^{-\pi x^2} e^{-2\pi i k x} dx \\ &\quad \text{[completing the exponent]} \\ &= \int_{-\infty}^{\infty} e^{-\pi k^2} e^{-\pi(x+ik)^2} dx \end{aligned} \quad (9.23)$$

The variable transformation  $t = \sqrt{\pi}(x + ik)$  yields  $dt/dx = \sqrt{\pi}$ ; thus  $dx = dt/\sqrt{\pi}$ , and

$$\mathcal{F}[\varphi(x)](k) = \tilde{\varphi}(k) = \frac{e^{-\pi k^2}}{\sqrt{\pi}} \int_{-\infty+i\sqrt{\pi}k}^{+\infty+i\sqrt{\pi}k} e^{-t^2} dt \quad (9.24)$$

Let us rewrite the integration (9.24) into the Gaussian integral by considering the closed path whose “left and right pieces vanish;” moreover,

$$\oint_{\mathcal{C}} dt e^{-t^2} = \int_{+\infty}^{-\infty} e^{-t^2} dt + \int_{-\infty+i\sqrt{\pi}k}^{+\infty+i\sqrt{\pi}k} e^{-t^2} dt = 0, \quad (9.25)$$

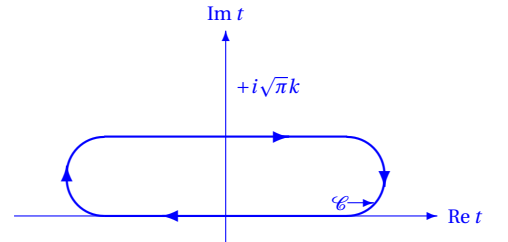


Figure 9.1: Integration path to compute the Fourier transform of the Gaussian.

because  $e^{-t^2}$  is analytic in the region  $0 \leq \text{Im } t \leq \sqrt{\pi}k$ . Thus, by substituting

$$\int_{-\infty+i\sqrt{\pi}k}^{+\infty+i\sqrt{\pi}k} e^{-t^2} dt = \int_{-\infty}^{+\infty} e^{-t^2} dt, \quad (9.26)$$

in (9.24) and by insertion of the value  $\sqrt{\pi}$  for the *Gaussian integral*, as shown in Eq. (10.18), we finally obtain

$$\mathcal{F}[\varphi(x)](k) = \tilde{\varphi}(k) = \frac{e^{-\pi k^2}}{\sqrt{\pi}} \underbrace{\int_{-\infty}^{+\infty} e^{-t^2} dt}_{\sqrt{\pi}} = e^{-\pi k^2}. \quad (9.27)$$

A very similar calculation yields

$$\mathcal{F}^{-1}[\varphi(k)](x) = \varphi(x) = e^{-\pi x^2}. \quad (9.28)$$

Eqs. (9.27) and (9.28) establish the fact that the Gaussian function  $\varphi(x) = e^{-\pi x^2}$  defined in (9.21) is an *eigenfunction* of the Fourier transformations  $\mathcal{F}$  and  $\mathcal{F}^{-1}$  with associated eigenvalue 1.

With a slightly different definition the Gaussian function  $f(x) = e^{-x^2/2}$  is also an eigenfunction of the operator

$$\mathcal{H} = -\frac{d^2}{dx^2} + x^2 \quad (9.29)$$

corresponding to a harmonic oscillator. The resulting eigenvalue equation is

$$\mathcal{H}f(x) = \left[ -\frac{d^2}{dx^2} + x^2 \right] f(x) = \left[ -\frac{d}{dx}(-x) + x^2 \right] f(x) = f(x); \quad (9.30)$$

with eigenvalue 1.

Instead of going too much into the details here, it may suffice to say that the *Hermite functions*

$$h_n(x) = \pi^{-1/4} (2^n n!)^{-1/2} \left( \frac{d}{dx} - x \right)^n e^{-x^2/2} = \pi^{-1/4} (2^n n!)^{-1/2} H_n(x) e^{-x^2/2} \quad (9.31)$$

are all eigenfunctions of the Fourier transform with the eigenvalue  $i^n \sqrt{2\pi}$ .

The polynomial  $H_n(x)$  of degree  $n$  is called *Hermite polynomial*. Hermite functions form a complete system, so that any function  $g$  (with  $\int |g(x)|^2 dx < \infty$ ) has a *Hermite expansion*

$$g(x) = \sum_{k=0}^{\infty} \langle g, h_k \rangle h_k(x). \quad (9.32)$$

This is an example of an *eigenfunction expansion*.

See Sect. 6.3 in

Robert Strichartz. *A Guide to Distribution Theory and Fourier Transforms*. CRC Press, Boca Roton, Florida, USA, 1994. ISBN 0849382734

## Distributions as generalized functions

### 10.1 Heuristically coping with discontinuities

What follows are “recipes” and a “cooking course” for some “dishes” Heaviside, Dirac and others have enjoyed “eating,” alas without being able to “explain their digestion” (cf. the citation by Heaviside on page 4).

Insofar theoretical physics is natural philosophy, the question arises if physical entities need to be smooth and continuous – in particular, if physical functions need to be *smooth* (i.e., in  $C^\infty$ ), having derivatives of all orders<sup>1</sup> (such as polynomials, trigonometric and exponential functions) – as “nature abhors sudden discontinuities,” or if we are willing to allow and conceptualize singularities of different sorts. Other, entirely different, scenarios are discrete<sup>2</sup> computer-generated universes<sup>3</sup>. This little course is no place for preference and judgments regarding these matters. Let me just point out that contemporary mathematical physics is not only leaning toward, but appears to be deeply committed to discontinuities; both in classical and quantized field theories dealing with “point charges,” as well as in general relativity, the (nonquantized field theoretical) geometrodynamics of gravitation, dealing with singularities such as “black holes” or “initial singularities” of various sorts.

Discontinuities were introduced quite naturally as electromagnetic pulses, which can, for instance be described with the *Heaviside function*  $H(t)$  representing vanishing, zero field strength until time  $t = 0$ , when suddenly a constant electrical field is “switched on eternally.” It is quite natural to ask what the derivative of the (infinite pulse) function  $H(t)$  might be. — At this point the reader is kindly ask to stop reading for a moment and contemplate on what kind of function that might be.

Heuristically, if we call this derivative the (*Dirac*) *delta function*  $\delta$  defined by  $\delta(t) = \frac{dH(t)}{dt}$ , we can assure ourselves of two of its properties (i) “ $\delta(t) = 0$  for  $t \neq 0$ ,” as well as as the antiderivative of the Heaviside function, yielding (ii) “ $\int_{-\infty}^{\infty} \delta(t) dt = \int_{-\infty}^{\infty} \frac{dH(t)}{dt} dt = H(\infty) - H(-\infty) = 1 - 0 = 1$ .”

Indeed, we could follow a pattern of “growing discontinuity,” reachable by ever higher and higher derivatives of the absolute value (or modulus);

<sup>1</sup> William F Trench. Introduction to real analysis. Free Hyperlinked Edition 2.01, 2012. URL [http://ramanujan.math.trinity.edu/wtrench/texts/TRENCH\\_REAL\\_ANALYSIS.PDF](http://ramanujan.math.trinity.edu/wtrench/texts/TRENCH_REAL_ANALYSIS.PDF)

<sup>2</sup> Konrad Zuse. Discrete mathematics and Rechnender Raum. 1994. URL <http://www.zib.de/PaperWeb/abstracts/TR-94-10/>; and Konrad Zuse. *Rechnender Raum*. Friedrich Vieweg & Sohn, Braunschweig, 1969

<sup>3</sup> Edward Fredkin. Digital mechanics. an informational process based on reversible universal cellular automata. *Physica*, D45:254–270, 1990. DOI: 10.1016/0167-2789(90)90186-S. URL [http://dx.doi.org/10.1016/0167-2789\(90\)90186-S](http://dx.doi.org/10.1016/0167-2789(90)90186-S); T. Toffoli. The role of the observer in uniform systems. In George J. Klir, editor, *Applied General Systems Research, Recent Developments and Trends*, pages 395–400. Plenum Press, New York, London, 1978; and Karl Svozil. Computational universes. *Chaos, Solitons & Fractals*, 25(4):845–859, 2006a. DOI: 10.1016/j.chaos.2004.11.055. URL <http://dx.doi.org/10.1016/j.chaos.2004.11.055>

This heuristic definition of the Dirac delta function  $\delta_y(x) = \delta(x, y) = \delta(x - y)$  with a discontinuity at  $y$  is not unlike the discrete Kronecker symbol  $\delta_{ij}$ , as (i)  $\delta_{ij} = 0$  for  $i \neq j$ , as well as (ii) “ $\sum_{i=-\infty}^{\infty} \delta_{ij} = \sum_{i=-\infty}^{\infty} \delta_{ij} = 1$ ,” We may even define the Kronecker symbol  $\delta_{ij}$  as the difference quotient of some “discrete Heaviside function”  $H_{ij} = 1$  for  $i \geq j$ , and  $H_{i,j} = 0$  else:  $\delta_{ij} = H_{ij} - H_{(i-1)j} = 1$  only for  $i = j$ ; else it vanishes.



that is, we shall pursue the path sketched by

$$|x| \xrightarrow{\frac{d}{dx}} \text{sgn}(x), H(x) \xrightarrow{\frac{d}{dx}} \delta(x) \xrightarrow{\frac{d^n}{dx^n}} \delta^{(n)}(x).$$

Objects like  $|x|$ ,  $H(t)$  or  $\delta(t)$  may be heuristically understandable as “functions” not unlike the regular analytic functions; alas their  $n$ th derivatives cannot be straightforwardly defined. In order to cope with a formally precised definition and derivation of (infinite) pulse functions and to achieve this goal, a theory of *generalized functions*, or, used synonymously, *distributions* has been developed. In what follows we shall develop the theory of distributions; always keeping in mind the assumptions regarding (dis)continuities that make necessary this part of calculus.

Thereby, we shall “pair” these generalized functions  $F$  with suitable “good” test functions  $\varphi$ ; integrate over these pairs, and thereby obtain a linear continuous functional  $F[\varphi]$ , also denoted by  $\langle F, \varphi \rangle$ . A further strategy then is to “transfer” or “shift” operations on and transformations of  $F$  – such as differentiations or Fourier transformations, but also multiplications with polynomials or other smooth functions – to the test function  $\varphi$  according to *adjoint identities*

$$\langle \mathbf{T}F, \varphi \rangle = \langle F, \mathbf{S}\varphi \rangle. \quad (10.1)$$

For example, for  $n$ -fold differentiation,

$$\mathbf{S} = (-1)^n \mathbf{T} = (-1)^n \frac{d^{(n)}}{dx^{(n)}}, \quad (10.2)$$

and for the Fourier transformation,

$$\mathbf{S} = \mathbf{T} = \mathcal{F}. \quad (10.3)$$

For some (smooth) functional multiplier  $g(x) \in C^\infty$ ,

$$\mathbf{S} = \mathbf{T} = g(x). \quad (10.4)$$

One more issue is the problem of the meaning and existence of *weak solutions* (also called generalized solutions) of differential equations for which, if interpreted in terms of regular functions, the derivatives may not all exist.

Take, for example, the wave equation in one spatial dimension  $\frac{\partial^2}{\partial t^2} u(x, t) = c^2 \frac{\partial^2}{\partial x^2} u(x, t)$ . It has a solution of the form <sup>4</sup>  $u(x, t) = f(x - ct) + g(x + ct)$ , where  $f$  and  $g$  characterize a travelling “shape” of inert, unchanged form. There is no obvious physical reason why the pulse shape function  $f$  or  $g$  should be differentiable, alas if it is not, then  $u$  is not differentiable either. What if we, for instance, set  $g = 0$ , and identify  $f(x - ct)$  with the Heaviside infinite pulse function  $H(x - ct)$ ?

See Sect. 2.3 in

Robert Strichartz. *A Guide to Distribution Theory and Fourier Transforms*. CRC Press, Boca Roton, Florida, USA, 1994. ISBN 0849382734

<sup>4</sup> Asim O. Barut.  $e = -\hbar\omega$ . *Physics Letters A*, 143(8):349–352, 1990. ISSN 0375-9601. DOI: 10.1016/0375-9601(90)90369-Y. URL [http://dx.doi.org/10.1016/0375-9601\(90\)90369-Y](http://dx.doi.org/10.1016/0375-9601(90)90369-Y)

## 10.2 General distribution

Suppose we have some “function”  $F(x)$ ; that is,  $F(x)$  could be either a regular analytical function, such as  $F(x) = x$ , or some other, “weirder function,” such as the Dirac delta function, or the derivative of the Heaviside (unit step) function, which might be “highly discontinuous.” As an *Ansatz*, we may associate with this “function”  $F(x)$  a *distribution*, or, used synonymously, a *generalized function*  $F[\varphi]$  or  $\langle F, \varphi \rangle$  which in the “weak sense” is defined as a *continuous linear functional* by integrating  $F(x)$  together with some “good” *test function*  $\varphi$  as follows<sup>5</sup>:

$$F(x) \longleftrightarrow \langle F, \varphi \rangle \equiv F[\varphi] = \int_{-\infty}^{\infty} F(x)\varphi(x)dx. \quad (10.5)$$

We say that  $F[\varphi]$  or  $\langle F, \varphi \rangle$  is the distribution *associated with* or *induced by*  $F(x)$ .

One interpretation of  $F[\varphi] \equiv \langle F, \varphi \rangle$  is that  $F$  stands for a sort of “measurement device,” and  $\varphi$  represents some “system to be measured;” then  $F[\varphi] \equiv \langle F, \varphi \rangle$  is the “outcome” or “measurement result.”

Thereby, it completely suffices to say what  $F$  “does to” some test function  $\varphi$ ; there is nothing more to it.

For example, the Dirac Delta function  $\delta(x)$  is completely characterised by

$$\delta(x) \longleftrightarrow \delta[\varphi] \equiv \langle \delta, \varphi \rangle = \varphi(0);$$

likewise, the shifted Dirac Delta function  $\delta_y(x) \equiv \delta(x - y)$  is completely characterised by

$$\delta_y(x) \equiv \delta(x - y) \longleftrightarrow \delta_y[\varphi] \equiv \langle \delta_y, \varphi \rangle = \varphi(y).$$

Many other (regular) functions which are usually not integrable in the interval  $(-\infty, +\infty)$  will, through the pairing with a “suitable” or “good” test function  $\varphi$ , induce a distribution.

For example, take

$$1 \longleftrightarrow 1[\varphi] \equiv \langle 1, \varphi \rangle = \int_{-\infty}^{\infty} \varphi(x)dx,$$

or

$$x \longleftrightarrow x[\varphi] \equiv \langle x, \varphi \rangle = \int_{-\infty}^{\infty} x\varphi(x)dx,$$

or

$$e^{2\pi i ax} \longleftrightarrow e^{2\pi i ax}[\varphi] \equiv \langle e^{2\pi i ax}, \varphi \rangle = \int_{-\infty}^{\infty} e^{2\pi i ax}\varphi(x)dx.$$

### 10.2.1 Duality

Sometimes,  $F[\varphi] \equiv \langle F, \varphi \rangle$  is also written in a scalar product notation; that is,  $F[\varphi] = \langle F | \varphi \rangle$ . This emphasizes the pairing aspect of  $F[\varphi] \equiv \langle F, \varphi \rangle$ . It can

A nice video on “Setting Up the Fourier Transform of a Distribution” by Professor Dr. Brad G. Osgood - Stanford is available via URLs <http://www.academicearth.org/lectures/setting-up-fourier-transform-of-distribution>

<sup>5</sup> Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin

also be shown that the set of all distributions  $F$  is the *dual space* of the set of test functions  $\varphi$ .

### 10.2.2 Linearity

Recall that a *linear* functional is some mathematical entity which maps a function or another mathematical object into scalars in a linear manner; that is, as the integral is linear, we obtain

$$F[c_1\varphi_1 + c_2\varphi_2] = c_1F[\varphi_1] + c_2F[\varphi_2]; \quad (10.6)$$

or, in the bracket notation,

$$\langle F, c_1\varphi_1 + c_2\varphi_2 \rangle = c_1\langle F, \varphi_1 \rangle + c_2\langle F, \varphi_2 \rangle. \quad (10.7)$$

This linearity is guaranteed by integration.

### 10.2.3 Continuity

One way of expressing *continuity* is the following:

$$\text{if } \varphi_n \xrightarrow{n \rightarrow \infty} \varphi, \text{ then } F[\varphi_n] \xrightarrow{n \rightarrow \infty} F[\varphi], \quad (10.8)$$

or, in the bracket notation,

$$\text{if } \varphi_n \xrightarrow{n \rightarrow \infty} \varphi, \text{ then } \langle F, \varphi_n \rangle \xrightarrow{n \rightarrow \infty} \langle F, \varphi \rangle. \quad (10.9)$$

## 10.3 Test functions

### 10.3.1 Desiderata on test functions

By invoking test functions, we would like to be able to differentiate distributions very much like ordinary functions. We would also like to transfer differentiations to the functional context. How can this be implemented in terms of possible “good” properties we require from the behaviour of test functions, in accord with our wishes?

Consider the partial integration obtained from  $(uv)' = u'v + uv'$ ; thus  $\int (uv)' = \int u'v + \int uv'$ , and finally  $\int u'v = \int (uv)' - \int uv'$ , thereby effectively allowing us to “shift” or “transfer” the differentiation of the original function to the test function. By identifying  $u$  with the generalized function  $g$  (such as, for instance  $\delta$ ), and  $v$  with the test function  $\varphi$ , respectively, we obtain

$$\begin{aligned} \langle g', \varphi \rangle &\equiv g'[\varphi] = \int_{-\infty}^{\infty} g'(x)\varphi(x)dx \\ &= g(x)\varphi(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} g(x)\varphi'(x)dx \\ &= \underbrace{g(\infty)\varphi(\infty)}_{\text{should vanish}} - \underbrace{g(-\infty)\varphi(-\infty)}_{\text{should vanish}} - \int_{-\infty}^{\infty} g(x)\varphi'(x)dx \\ &= -g[\varphi'] \equiv -\langle g, \varphi' \rangle. \end{aligned} \quad (10.10)$$

We can justify the two main requirements of “good” test functions, at least for a wide variety of purposes:

1. that they “sufficiently” vanish at infinity – that can, for instance, be achieved by requiring that their support (the set of arguments  $x$  where  $g(x) \neq 0$ ) is finite; and
2. that they are continuously differentiable – indeed, by induction, that they are arbitrarily often differentiable.

In what follows we shall enumerate three types of suitable test functions satisfying these *desiderata*. One should, however, bear in mind that the class of “good” test functions depends on the distribution. Take, for example, the Dirac delta function  $\delta(x)$ . It is so “concentrated” that any (infinitely often) differentiable – even constant – function  $f(x)$  defined “around  $x = 0$ ” can serve as a “good” test function (with respect to  $\delta$ ), as  $f(x)$  only evaluated at  $x = 0$ ; that is,  $\delta[f] = f(0)$ . This is again an indication of the *duality* between distributions on the one hand, and their test functions on the other hand.

### 10.3.2 Test function class I

Recall that we require<sup>6</sup> our test functions  $\varphi$  to be infinitely often differentiable. Furthermore, in order to get rid of terms at infinity “in a straightforward, simple way,” suppose that their support is compact. Compact support means that  $\varphi(x)$  does not vanish only at a finite, bounded region of  $x$ . Such a “good” test function is, for instance,

$$\varphi_{\sigma,a}(x) = \begin{cases} e^{-\frac{1}{1-(x-a)/\sigma)^2}} & \text{for } |\frac{x-a}{\sigma}| < 1, \\ 0 & \text{else.} \end{cases} \quad (10.11)$$

In order to show that  $\varphi_{\sigma,a}$  is a suitable test function, we have to prove its infinite differentiability, as well as the compactness of its support  $M_{\varphi_{\sigma,a}}$ . Let

$$\varphi_{\sigma,a}(x) := \varphi\left(\frac{x-a}{\sigma}\right)$$

and thus

$$\varphi(x) = \begin{cases} e^{-\frac{1}{1-x^2}} & \text{for } |x| < 1 \\ 0 & \text{for } |x| \geq 1 \end{cases}$$

This function is drawn in Fig. 10.1.

First, note, by definition, the support  $M_\varphi = (-1, 1)$ , because  $\varphi(x)$  vanishes outside  $(-1, 1)$ .

Second, consider the differentiability of  $\varphi(x)$ ; that is  $\varphi \in C^\infty(\mathbb{R})$ ? Note that  $\varphi^{(0)} = \varphi$  is continuous; and that  $\varphi^{(n)}$  is of the form

$$\varphi^{(n)}(x) = \begin{cases} \frac{P_n(x)}{(x^2-1)^{2n}} e^{\frac{1}{x^2-1}} & \text{for } |x| < 1 \\ 0 & \text{for } |x| \geq 1, \end{cases}$$

<sup>6</sup> Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin

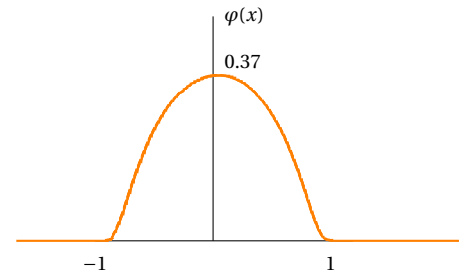


Figure 10.1: Plot of a test function  $\varphi(x)$ .

where  $P_n(x)$  is a finite polynomial in  $x$  ( $\varphi(u) = e^u \Rightarrow \varphi'(u) = \frac{d\varphi}{du} \frac{du}{dx^2} \frac{dx^2}{dx} = \varphi(u) \left( -\frac{1}{(x^2-1)^2} \right) 2x$  etc.) and  $[x = 1 - \varepsilon] \Rightarrow x^2 = 1 - 2\varepsilon + \varepsilon^2 \Rightarrow x^2 - 1 = \varepsilon(\varepsilon - 2)$

$$\begin{aligned} \lim_{x \uparrow 1} \varphi^{(n)}(x) &= \lim_{\varepsilon \downarrow 0} \frac{P_n(1 - \varepsilon)}{\varepsilon^{2n}(\varepsilon - 2)^{2n}} e^{\frac{1}{\varepsilon(\varepsilon-2)}} = \\ &= \lim_{\varepsilon \downarrow 0} \frac{P_n(1)}{\varepsilon^{2n} 2^{2n}} e^{-\frac{1}{2\varepsilon}} = \left[ \varepsilon = \frac{1}{R} \right] = \lim_{R \rightarrow \infty} \frac{P_n(1)}{2^{2n}} R^{2n} e^{-\frac{R}{2}} = 0, \end{aligned}$$

because the power  $e^{-x}$  of  $e$  decreases stronger than any polynomial  $x^n$ .

Note that the complex continuation  $\varphi(z)$  is not an analytic function and cannot be expanded as a Taylor series on the entire complex plane  $\mathbb{C}$  although it is infinitely often differentiable on the real axis; that is, although  $\varphi \in C^\infty(\mathbb{R})$ . This can be seen from a uniqueness theorem of complex analysis. Let  $B \subseteq \mathbb{C}$  be a domain, and let  $z_0 \in B$  the limit of a sequence  $\{z_n\} \in B$ ,  $z_n \neq z_0$ . Then it can be shown that, if two analytic functions  $f$  and  $g$  on  $B$  coincide in the points  $z_n$ , then they coincide on the entire domain  $B$ .

Now, take  $B = \mathbb{R}$  and the vanishing analytic function  $f$ ; that is,  $f(x) = 0$ .  $f(x)$  coincides with  $\varphi(x)$  only in  $\mathbb{R} - M_\varphi$ . As a result,  $\varphi$  cannot be analytic. Indeed,  $\varphi_{\sigma, \bar{a}}(x)$  diverges at  $x = a \pm \sigma$ . Hence  $\varphi(x)$  cannot be Taylor expanded, and

$$C^\infty(\mathbb{R}^k) \not\stackrel{\text{analytic function}}{\Longleftarrow}$$

### 10.3.3 Test function class II

Other “good” test functions are <sup>7</sup>

$$\{\phi_{c,d}(x)\}^{\frac{1}{n}} \quad (10.12)$$

obtained by choosing  $n \in \mathbb{N} - 0$  and  $-\infty \leq c < d \leq \infty$  and by defining

$$\phi_{c,d}(x) = \begin{cases} e^{-\left(\frac{1}{x-c} + \frac{1}{d-x}\right)} & \text{for } c < x < d, \\ 0 & \text{else.} \end{cases} \quad (10.13)$$

If  $\varphi(x)$  is a “good” test function, then

$$x^\alpha P_n(x) \varphi(x) \quad (10.14)$$

with any Polynomial  $P_n(x)$ , and, in particular,  $x^n \varphi(x)$  also is a “good” test function.

### 10.3.4 Test function class III: Tempered distributions and Fourier transforms

A particular class of “good” test functions – having the property that they vanish “sufficiently fast” for large arguments, but are nonzero at any finite argument – are capable of rendering Fourier transforms of generalized functions. Such generalized functions are called *tempered distributions*.

<sup>7</sup> Laurent Schwartz. *Introduction to the Theory of Distributions*. University of Toronto Press, Toronto, 1952. collected and written by Israel Halperin

One example of a test function yielding tempered distribution is the *Gaussian function*

$$\varphi(x) = e^{-\pi x^2}. \quad (10.15)$$

We can multiply the Gaussian function with polynomials (or take its derivatives) and thereby obtain a particular class of test functions inducing tempered distributions.

The Gaussian function is normalized such that

$$\begin{aligned} \int_{-\infty}^{\infty} \varphi(x) dx &= \int_{-\infty}^{\infty} e^{-\pi x^2} dx \\ \text{[variable substitution } x &= \frac{t}{\sqrt{\pi}}, dx = \frac{dt}{\sqrt{\pi}}] \\ &= \int_{-\infty}^{\infty} e^{-\pi \left(\frac{t}{\sqrt{\pi}}\right)^2} d\left(\frac{t}{\sqrt{\pi}}\right) \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-t^2} dt \\ &= \frac{1}{\sqrt{\pi}} \sqrt{\pi} = 1. \end{aligned} \quad (10.16)$$

In this evaluation, we have used the *Gaussian integral*

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}, \quad (10.17)$$

which can be obtained by considering its square and transforming into polar coordinates  $r, \theta$ ; that is,

$$\begin{aligned} I^2 &= \left( \int_{-\infty}^{\infty} e^{-x^2} dx \right) \left( \int_{-\infty}^{\infty} e^{-y^2} dy \right) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy \\ &= \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r d\theta dr \\ &= \int_0^{2\pi} d\theta \int_0^{\infty} e^{-r^2} r dr \\ &= 2\pi \int_0^{\infty} e^{-r^2} r dr \\ &\quad \left[ u = r^2, \frac{du}{dr} = 2r, dr = \frac{du}{2r} \right] \\ &= \pi \int_0^{\infty} e^{-u} du \\ &= \pi \left( -e^{-u} \Big|_0^{\infty} \right) \\ &= \pi \left( -e^{-\infty} + e^0 \right) \\ &= \pi. \end{aligned} \quad (10.18)$$

The Gaussian test function (10.15) has the advantage that, as has been shown in (9.27), with a certain kind of definition for the Fourier transform, namely  $A = 2\pi$  and  $B = 1$  in Eq. (9.19), its functional form does not change

under Fourier transforms. More explicitly, as derived in Eqs. (9.27) and (9.28),

$$\mathcal{F}[\varphi(x)](k) = \tilde{\varphi}(k) = \int_{-\infty}^{\infty} e^{-\pi x^2} e^{-2\pi i k x} dx = e^{-\pi k^2}. \quad (10.19)$$

Just as for differentiation discussed later it is possible to “shift” or “transfer” the Fourier transformation from the distribution to the test function as follows. Suppose we are interested in the Fourier transform  $\mathcal{F}[F]$  of some distribution  $F$ . Then, with the convention  $A = 2\pi$  and  $B = 1$  adopted in Eq. (9.19), we must consider

$$\begin{aligned} \langle \mathcal{F}[F], \varphi \rangle &\equiv \mathcal{F}[F][\varphi] = \int_{-\infty}^{\infty} \mathcal{F}[F](x) \varphi(x) dx \\ &= \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} F(y) e^{-2\pi i x y} dy \right] \varphi(x) dx \\ &= \int_{-\infty}^{\infty} F(y) \left[ \int_{-\infty}^{\infty} \varphi(x) e^{-2\pi i x y} dx \right] dy \\ &= \int_{-\infty}^{\infty} F(y) \mathcal{F}[\varphi](y) dy \\ &= \langle F, \mathcal{F}[\varphi] \rangle \equiv F[\mathcal{F}[\varphi]]. \end{aligned} \quad (10.20)$$

in the same way we obtain the *Fourier inversion* for distributions

$$\langle \mathcal{F}^{-1}[\mathcal{F}[F]], \varphi \rangle = \langle \mathcal{F}[\mathcal{F}^{-1}[F]], \varphi \rangle = \langle F, \varphi \rangle. \quad (10.21)$$

Note that, in the case of test functions with compact support – say,  $\hat{\varphi}(x) = 0$  for  $|x| > a > 0$  and finite  $a$  – if the order of integrals is exchanged, the “new test function”

$$\mathcal{F}[\hat{\varphi}](y) = \int_{-\infty}^{\infty} \hat{\varphi}(x) e^{-2\pi i x y} dx \int_{-a}^a \hat{\varphi}(x) e^{-2\pi i x y} dx \quad (10.22)$$

obtained through a Fourier transform of  $\hat{\varphi}(x)$ , does not necessarily inherit a compact support from  $\hat{\varphi}(x)$ ; in particular,  $\mathcal{F}[\hat{\varphi}](y)$  may not necessarily vanish [i.e.  $\mathcal{F}[\hat{\varphi}](y) = 0$ ] for  $|y| > a > 0$ .

Let us, with these conventions, compute the Fourier transform of the tempered Dirac delta distribution. Note that, by the very definition of the Dirac delta distribution,

$$\langle \mathcal{F}[\delta], \varphi \rangle = \langle \delta, \mathcal{F}[\varphi] \rangle = \mathcal{F}[\varphi](0) = \int_{-\infty}^{\infty} e^{-2\pi i x 0} \varphi(x) dx = \int_{-\infty}^{\infty} 1 \varphi(x) dx = \langle 1, \varphi \rangle. \quad (10.23)$$

Thus we may identify  $\mathcal{F}[\delta]$  with 1; that is,

$$\mathcal{F}[\delta] = 1. \quad (10.24)$$

This is an extreme example of an *infinitely concentrated* object whose Fourier transform is *infinitely spread out*.

A very similar calculation renders the tempered distribution associated with the Fourier transform of the shifted Dirac delta distribution

$$\mathcal{F}[\delta_y] = e^{-2\pi i x y}. \quad (10.25)$$

Alas we shall pursue a different, more conventional, approach, sketched in Section 10.5.

### 10.3.5 Test function class IV: $C^\infty$

If the generalized functions are “sufficiently concentrated” so that they themselves guarantee that the terms  $g(\infty)\varphi(\infty)$  as well as  $g(-\infty)\varphi(-\infty)$  in Eq. (10.10) to vanish, we may just require the test functions to be infinitely differentiable – and thus in  $C^\infty$  – for the sake of making possible a transfer of differentiation. (Indeed, if we are willing to sacrifice even infinite differentiability, we can widen this class of test functions even more.) We may, for instance, employ constant functions such as  $\varphi(x) = 1$  as test functions, thus giving meaning to, for instance,  $\langle \delta, 1 \rangle = \int_{-\infty}^{\infty} \delta(x) dx$ , or  $\langle f(x)\delta, 1 \rangle = \langle f(0)\delta, 1 \rangle = f(0) \int_{-\infty}^{\infty} \delta(x) dx$ .

## 10.4 Derivative of distributions

Equipped with “good” test functions which have a finite support and are infinitely often (or at least sufficiently often) differentiable, we can now give meaning to the transferral of differential quotients from the objects entering the integral towards the test function by *partial integration*. First note again that  $(uv)' = u'v + uv'$  and thus  $\int (uv)' = \int u'v + \int uv'$  and finally  $\int u'v = \int (uv)' - \int uv'$ . Hence, by identifying  $u$  with  $g$ , and  $v$  with the test function  $\varphi$ , we obtain

$$\begin{aligned} \langle F', \varphi \rangle &\equiv F'[\varphi] = \int_{-\infty}^{\infty} \left( \frac{d}{dx} q(x) \right) \varphi(x) dx \\ &= q(x)\varphi(x) \Big|_{x=-\infty}^{\infty} - \int_{-\infty}^{\infty} q(x) \left( \frac{d}{dx} \varphi(x) \right) dx \\ &= - \int_{-\infty}^{\infty} q(x) \left( \frac{d}{dx} \varphi(x) \right) dx \\ &= -F[\varphi'] \equiv -\langle F, \varphi' \rangle. \end{aligned} \quad (10.26)$$

By induction we obtain

$$\left\langle \frac{d^n}{dx^n} F, \varphi \right\rangle \langle F^{(n)}, \varphi \rangle \equiv F^{(n)}[\varphi] = (-1)^n F[\varphi^{(n)}] = (-1)^n \langle F, \varphi^{(n)} \rangle. \quad (10.27)$$

For the sake of a further example using *adjoint identities*, swapping products and differentiations forth and back in the  $F$ - $\varphi$  pairing, let us compute  $g(x)\delta'(x)$  where  $g \in C^\infty$ ; that is

$$\begin{aligned} \langle g\delta', \varphi \rangle &= \langle \delta', g\varphi \rangle \\ &= -\langle \delta, (g\varphi)' \rangle \\ &= -\langle \delta, g\varphi' + g'\varphi \rangle \\ &= -g(0)\varphi'(0) - g'(0)\varphi(0) \\ &= \langle g(0)\delta' - g'(0)\delta, \varphi \rangle. \end{aligned} \quad (10.28)$$



Therefore,

$$g(x)\delta'(x) = g(0)\delta'(x) - g'(0)\delta(x). \quad (10.29)$$

## 10.5 Fourier transform of distributions

We mention without proof that, if  $\{f_n(x)\}$  is a sequence of functions converging, for  $n \rightarrow \infty$  toward a function  $f$  in the functional sense (i.e. *via* integration of  $f_n$  and  $f$  with “good” test functions), then the Fourier transform  $\tilde{f}$  of  $f$  can be defined by<sup>8</sup>

$$\mathcal{F}[f(x)] = \tilde{f}(k) = \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} f_n(x) e^{-ikx} dx. \quad (10.30)$$

While this represents a method to calculate Fourier transforms of distributions, there are other, more direct ways of obtaining them. These were mentioned earlier. In what follows, we shall enumerate the Fourier transform of some species, mostly by complex analysis.

## 10.6 Dirac delta function

Historically, the Heaviside step function, which will be discussed later – was first used for the description of electromagnetic pulses. In the days when Dirac developed quantum mechanics there was a need to define “singular scalar products” such as “ $\langle x | y \rangle = \delta(x - y)$ ,” with some generalization of the Kronecker delta function  $\delta_{ij}$  which is zero whenever  $x \neq y$  and “large enough” needle shaped (see Fig. 10.2) to yield unity when integrated over the entire reals; that is, “ $\int_{-\infty}^{\infty} \langle x | y \rangle dy = \int_{-\infty}^{\infty} \delta(x - y) dy = 1$ .”

### 10.6.1 Delta sequence

One of the first attempts to formalize these objects with “large discontinuities” was in terms of functional limits. Take, for instance, the *delta sequence* which is a sequence of strongly peaked functions for which in some limit the sequences  $\{f_n(x - y)\}$  with, for instance,

$$\delta_n(x - y) = \begin{cases} n & \text{for } y - \frac{1}{2n} < x < y + \frac{1}{2n} \\ 0 & \text{else} \end{cases} \quad (10.31)$$

become the delta function  $\delta(x - y)$ . That is, in the functional sense

$$\lim_{n \rightarrow \infty} \delta_n(x - y) = \delta(x - y). \quad (10.32)$$

Note that the area of this particular  $\delta_n(x - y)$  above the  $x$ -axes is independent of  $n$ , since its width is  $1/n$  and the height is  $n$ .

In an *ad hoc* sense, other delta sequences can be enumerated as follows. They all converge towards the delta function in the sense of linear

<sup>8</sup> M. J. Lighthill. *Introduction to Fourier Analysis and Generalized Functions*. Cambridge University Press, Cambridge, 1958; Kenneth B. Howell. *Principles of Fourier analysis*. Chapman & Hall/CRC, Boca Raton, London, New York, Washington, D.C., 2001; and B.L. Burrows and D.J. Colwell. The Fourier transform of the unit step function. *International Journal of Mathematical Education in Science and Technology*, 21(4):629–635, 1990. DOI: 10.1080/0020739900210418. URL <http://dx.doi.org/10.1080/0020739900210418>

functionals (i.e. when integrated over a test function).

$$\delta_n(x) = \frac{n}{\sqrt{\pi}} e^{-n^2 x^2}, \quad (10.33)$$

$$= \frac{1}{\pi} \frac{\sin(nx)}{x}, \quad (10.34)$$

$$= (1 \mp i) \left( \frac{n}{2\pi} \right)^{\frac{1}{2}} e^{\pm i n x^2} \quad (10.35)$$

$$= \frac{1}{\pi x} \frac{e^{inx} - e^{-inx}}{2i}, \quad (10.36)$$

$$= \frac{1}{\pi} \frac{n e^{-x^2}}{1 + n^2 x^2}, \quad (10.37)$$

$$= \frac{1}{2\pi} \int_{-n}^n e^{ixt} dt = \frac{1}{2\pi i x} e^{ixt} \Big|_{-n}^n, \quad (10.38)$$

$$= \frac{1}{2\pi} \frac{\sin \left[ \left( n + \frac{1}{2} \right) x \right]}{\sin \left( \frac{1}{2} x \right)}, \quad (10.39)$$

$$= \frac{1}{\pi} \frac{n}{1 + n^2 x^2}, \quad (10.40)$$

$$= \frac{n}{\pi} \left( \frac{\sin(nx)}{nx} \right)^2. \quad (10.41)$$

Other commonly used limit forms of the  $\delta$ -function are the Gaussian, Lorentzian, and Dirichlet forms

$$\delta_\epsilon(x) = \frac{1}{\sqrt{\pi}\epsilon} e^{-\frac{x^2}{\epsilon^2}}, \quad (10.42)$$

$$= \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2} = \frac{1}{2\pi i} \left( \frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon} \right), \quad (10.43)$$

$$= \frac{1}{\pi} \frac{\sin\left(\frac{x}{\epsilon}\right)}{x}, \quad (10.44)$$

respectively. Note that (10.42) corresponds to (10.33), (10.43) corresponds to (10.40) with  $\epsilon = n^{-1}$ , and (10.44) corresponds to (10.34). Again, the limit

$$\delta(x) = \lim_{\epsilon \rightarrow 0} \delta_\epsilon(x) \quad (10.45)$$

has to be understood in the functional sense (see below).

Naturally, such “needle shaped functions” were viewed suspiciously by many mathematicians at first, but later they embraced these types of functions<sup>9</sup> by developing a theory of *functional analysis* or *distributions*.

### 10.6.2 $\delta[\varphi]$ distribution

In particular, the  $\delta$  function maps to

$$\int_{-\infty}^{\infty} \delta(x-y) \varphi(x) dx = \varphi(y). \quad (10.46)$$

A common way of expressing this is by writing

$$\delta(x-y) \longleftrightarrow \delta_y[\varphi] = \varphi(y). \quad (10.47)$$

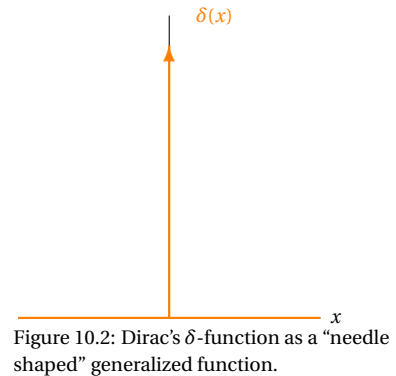


Figure 10.2: Dirac's  $\delta$ -function as a “needle shaped” generalized function.

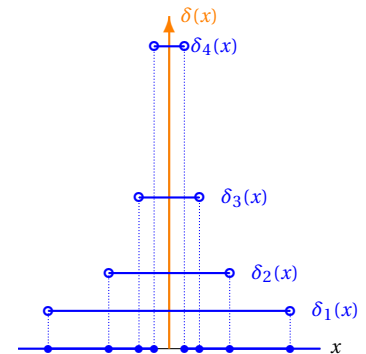


Figure 10.3: Delta sequence approximating Dirac's  $\delta$ -function as a more and more “needle shaped” generalized function.

<sup>9</sup> I. M. Gel'fand and G. E. Shilov. *Generalized Functions. Vol. 1: Properties and Operations*. Academic Press, New York,

For  $y = 0$ , we just obtain

$$\delta(x) \longleftrightarrow \delta[\varphi] \stackrel{\text{def}}{=} \delta_0[\varphi] = \varphi(0). \quad (10.48)$$

Let us proof that the sequence  $\{\delta_n\}$  with

$$\delta_n(x-y) = \begin{cases} n & \text{for } y - \frac{1}{2n} < x < y + \frac{1}{2n} \\ 0 & \text{else} \end{cases}$$

defined in Eq. (10.31) and depicted in Fig. 10.3 is a delta sequence; that is, if, for large  $n$ , it converges to  $\delta$  in a functional sense. In order to verify this claim, we have to integrate  $\delta_n(x)$  with “good” test functions  $\varphi(x)$  and take the limit  $n \rightarrow \infty$ ; if the result is  $\varphi(0)$ , then we can identify  $\delta_n(x)$  in this limit with  $\delta(x)$  (in the functional sense). Since  $\delta_n(x)$  is uniform convergent, we can exchange the limit with the integration; thus

$$\begin{aligned} & \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} \delta_n(x-y) \varphi(x) dx \\ & \quad \text{[variable transformation:} \\ & \quad \quad x' = x - y, x = x' + y \\ & \quad \quad dx' = dx, -\infty \leq x' \leq \infty] \\ &= \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} \delta_n(x') \varphi(x' + y) dx' \\ &= \lim_{n \rightarrow \infty} \int_{-\frac{1}{2n}}^{\frac{1}{2n}} n \varphi(x' + y) dx' \\ & \quad \text{[variable transformation:} \\ & \quad \quad u = 2nx', x' = \frac{u}{2n}, \\ & \quad \quad du = 2n dx', -1 \leq u \leq 1] \\ &= \lim_{n \rightarrow \infty} \int_{-1}^1 n \varphi\left(\frac{u}{2n} + y\right) \frac{du}{2n} \\ &= \lim_{n \rightarrow \infty} \frac{1}{2} \int_{-1}^1 \varphi\left(\frac{u}{2n} + y\right) du \\ &= \frac{1}{2} \int_{-1}^1 \lim_{n \rightarrow \infty} \varphi\left(\frac{u}{2n} + y\right) du \\ & \quad = \frac{1}{2} \varphi(y) \int_{-1}^1 du \\ & \quad = \varphi(y). \end{aligned} \quad (10.49)$$

Hence, in the functional sense, this limit yields the  $\delta$ -function. Thus we obtain

$$\lim_{n \rightarrow \infty} \delta_n[\varphi] = \delta[\varphi] = \varphi(0).$$

### 10.6.3 Useful formulæ involving $\delta$

The following formulae are sometimes enumerated without proofs.

$$\delta(x) = \delta(-x) \quad (10.50)$$

For a proof, note that  $\varphi(x)\delta(-x) = \varphi(0)\delta(-x)$ , and that, in particular, with the substitution  $x \rightarrow -x$ ,

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(-x)\varphi(x)dx &= \varphi(0) \int_{\infty}^{-\infty} \delta(-(-x))d(-x) \\ &= -\varphi(0) \int_{\infty}^{-\infty} \delta(x)dx = \varphi(0) \int_{-\infty}^{\infty} \delta(x)dx. \end{aligned} \quad (10.51)$$

$$\delta(x) = \lim_{\epsilon \rightarrow 0} \frac{H(x+\epsilon) - H(x)}{\epsilon} = \frac{d}{dx} H(x) \quad (10.52)$$

$$f(x)\delta(x-x_0) = f(x_0)\delta(x-x_0) \quad (10.53)$$

This results from a direct application of Eq. (10.4); that is,

$$f(x)\delta[\varphi] = \delta[f\varphi] = f(0)\varphi(0) = f(0)\delta[\varphi], \quad (10.54)$$

and

$$f(x)\delta_{x_0}[\varphi] = \delta_{x_0}[f\varphi] = f(x_0)\varphi(x_0) = f(x_0)\delta_{x_0}[\varphi]. \quad (10.55)$$

For a more explicit direct proof, note that

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)\varphi(x)dx = \int_{-\infty}^{\infty} \delta(x-x_0)(f(x)\varphi(x))dx = f(x_0)\varphi(x_0), \quad (10.56)$$

and hence  $f\delta_{x_0}[\varphi] = f(x_0)\delta_{x_0}[\varphi]$ .

For the  $\delta$  distribution with its “extreme concentration” at the origin, a “nonconcentrated test function” suffices; in particular, a constant test function such as  $\varphi(x) = 1$  is fine. This is the reason why test functions need not show up explicitly in expressions, and, in particular, integrals, containing  $\delta$ . Because, say, for suitable functions  $g(x)$  “well behaved” at the origin,

$$\begin{aligned} g(x)\delta(x-y)[1] &= g(x)\delta(x-y)[\varphi=1] \\ &= \int_{-\infty}^{\infty} g(x)\delta(x-y)[\varphi=1]dx = \int_{-\infty}^{\infty} g(x)\delta(x-y)1dx = g(y). \end{aligned} \quad (10.57)$$

$$x\delta(x) = 0 \quad (10.58)$$

For a proof consider

$$x\delta[\varphi] = \delta[x\varphi] = 0\varphi(0) = 0. \quad (10.59)$$

For  $a \neq 0$ ,

$$\delta(ax) = \frac{1}{|a|}\delta(x), \quad (10.60)$$

and, more generally,

$$\delta(a(x - x_0)) = \frac{1}{|a|} \delta(x - x_0) \quad (10.61)$$

For the sake of a proof, consider the case  $a > 0$  as well as  $x_0 = 0$  first:

$$\begin{aligned} & \int_{-\infty}^{\infty} \delta(ax) \varphi(x) dx \\ \text{[variable substitution } y = ax, x = \frac{y}{a}, dx = \frac{1}{a} dy] \\ &= \frac{1}{a} \int_{-\infty}^{\infty} \delta(y) \varphi\left(\frac{y}{a}\right) dy \\ &= \frac{1}{a} \varphi(0); \end{aligned} \quad (10.62)$$

and, second, the case  $a < 0$ :

$$\begin{aligned} & \int_{-\infty}^{\infty} \delta(ax) \varphi(x) dx \\ \text{[variable substitution } y = ax, x = \frac{y}{a}, dx = \frac{1}{a} dy] \\ &= \frac{1}{a} \int_{\infty}^{-\infty} \delta(y) \varphi\left(\frac{y}{a}\right) dy \\ &= -\frac{1}{a} \int_{-\infty}^{\infty} \delta(y) \varphi\left(\frac{y}{a}\right) dy \\ &= -\frac{1}{a} \varphi(0). \end{aligned} \quad (10.63)$$

In the case of  $x_0 \neq 0$  and  $\pm a > 0$ , we obtain

$$\begin{aligned} & \int_{-\infty}^{\infty} \delta(a(x - x_0)) \varphi(x) dx \\ \text{[variable substitution } y = a(x - x_0), x = \frac{y}{a} + x_0, dx = \frac{1}{a} dy] \\ &= \pm \frac{1}{a} \int_{-\infty}^{\infty} \delta(y) \varphi\left(\frac{y}{a} + x_0\right) dy \\ &= \frac{1}{|a|} \varphi(x_0). \end{aligned} \quad (10.64)$$

If there exists a simple singularity  $x_0$  of  $f(x)$  in the integration interval, then

$$\delta(f(x)) = \frac{1}{|f'(x_0)|} \delta(x - x_0). \quad (10.65)$$

More generally, if  $f$  has only simple roots and  $f'$  is nonzero there,

$$\delta(f(x)) = \sum_{x_i} \frac{\delta(x - x_i)}{|f'(x_i)|} \quad (10.66)$$

where the sum extends over all simple roots  $x_i$  in the integration interval.

In particular,

$$\delta(x^2 - x_0^2) = \frac{1}{2|x_0|} [\delta(x - x_0) + \delta(x + x_0)] \quad (10.67)$$

For a proof, note that, since  $f$  has only simple roots, it can be expanded around these roots by

$$f(x) \approx (x - x_0)f'(x_0)$$

with nonzero  $f'(x_0) \in \mathbb{R}$ . By identifying  $f'(x_0)$  with  $a$  in Eq. (10.60) we obtain Eq. (10.66).

$$\delta'(f(x)) = \sum_{i=0}^N \frac{f''(x_i)}{|f'(x_i)|^3} \delta(x - x_i) + \sum_{i=0}^N \frac{f'(x_i)}{|f'(x_i)|^3} \delta'(x - x_i) \quad (10.68)$$

$$|x|\delta(x^2) = \delta(x) \quad (10.69)$$

$$-x\delta'(x) = \delta(x), \quad (10.70)$$

which is a direct consequence of Eq. (10.29). More explicitly, we can write use partial integration and obtain

$$\begin{aligned} & \int_{-\infty}^{\infty} -x\delta'(x)\varphi(x)dx \\ &= -x\delta(x)|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \delta(x) \frac{d}{dx} (x\varphi(x)) dx \\ &= \int_{-\infty}^{\infty} \delta(x)x\varphi'(x)dx + \int_{-\infty}^{\infty} \delta(x)\varphi(x)dx \\ &= 0\varphi'(0) + \varphi(0) = \varphi(0). \end{aligned} \quad (10.71)$$

$$\delta^{(n)}(-x) = (-1)^n \delta^{(n)}(x), \quad (10.72)$$

where the index  $^{(n)}$  denotes  $n$ -fold differentiation, can be proven by

$$\begin{aligned} & \int_{-\infty}^{\infty} \delta^{(n)}(-x)\varphi(x)dx = (-1)^n \int_{-\infty}^{\infty} \delta(-x)\varphi^{(n)}(x)dx \\ &= (-1)^n \int_{-\infty}^{\infty} \delta(x)\varphi^{(n)}(x)dx = (-1)^n \int_{-\infty}^{\infty} \delta^{(n)}(x)\varphi(x)dx. \end{aligned} \quad (10.73)$$

$$x^{m+1}\delta^{(m)}(x) = 0, \quad (10.74)$$

where the index  $^{(m)}$  denotes  $m$ -fold differentiation;

$$x^2\delta'(x) = 0, \quad (10.75)$$

which is a consequence of Eq. (10.29).

More generally,

$$x^n \delta^{(m)}(x)[\varphi = 1] = \int_{-\infty}^{\infty} x^n \delta^{(m)}(x)dx = (-1)^n n! \delta_{nm}, \quad (10.76)$$

which can be demonstrated by considering

$$\begin{aligned}
 \langle x^n \delta^{(m)} | 1 \rangle &= \langle \delta^{(m)} | x^n \rangle \\
 &= (-1)^n \langle \delta | \frac{d^{(m)}}{dx^{(m)}} x^n \rangle \\
 &= (-1)^n n! \delta_{nm} \underbrace{\langle \delta | 1 \rangle}_1 \\
 &= (-1)^n n! \delta_{nm}.
 \end{aligned} \tag{10.77}$$

$$\frac{d^2}{dx^2} [xH(x)] = \frac{d}{dx} [H(x) + \underbrace{x\delta(x)}_0] = \frac{d}{dx} H(x) = \delta(x) \tag{10.78}$$

If  $\delta^3(\vec{r}) = \delta(x)\delta(y)\delta(z)$  with  $\vec{r} = (x, y, z)$ , then

$$\delta^3(\vec{r}) = \delta(x)\delta(y)\delta(z) = -\frac{1}{4\pi} \Delta \frac{1}{r} \tag{10.79}$$

$$\delta^3(\vec{r}) = -\frac{1}{4\pi} (\Delta + k^2) \frac{e^{ikr}}{r} \tag{10.80}$$

$$\delta^3(\vec{r}) = -\frac{1}{4\pi} (\Delta + k^2) \frac{\cos kr}{r} \tag{10.81}$$

In quantum field theory, phase space integrals of the form

$$\frac{1}{2E} = \int dp^0 H(p^0) \delta(p^2 - m^2) \tag{10.82}$$

if  $E = (\vec{p}^2 + m^2)^{(1/2)}$  are exploited.

#### 10.6.4 Fourier transform of $\delta$

The Fourier transform of the  $\delta$ -function can be obtained straightforwardly by insertion into Eq. (9.19); that is, with  $A = B = 1$

$$\begin{aligned}
 \mathcal{F}[\delta(x)] &= \tilde{\delta}(k) = \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx \\
 &= e^{-i0k} \int_{-\infty}^{\infty} \delta(x) dx \\
 &= 1, \text{ and thus} \\
 \mathcal{F}^{-1}[\tilde{\delta}(k)] &= \mathcal{F}^{-1}[1] = \delta(x) \\
 &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk \\
 &= \frac{1}{2\pi} \int_{-\infty}^{\infty} [\cos(kx) + i \sin(kx)] dk \\
 &= \frac{1}{\pi} \int_0^{\infty} \cos(kx) dk + \frac{i}{2\pi} \int_{-\infty}^{\infty} \sin(kx) dk \\
 &= \frac{1}{\pi} \int_0^{\infty} \cos(kx) dk.
 \end{aligned} \tag{10.83}$$

That is, the Fourier transform of the  $\delta$ -function is just a constant.  $\delta$ -spiked signals carry all frequencies in them. Note also that  $\mathcal{F}[\delta(x - y)] = e^{iky} \mathcal{F}[\delta(x)]$ .

From Eq. (10.83) we can compute

$$\begin{aligned}
 \mathcal{F}[1] &= \tilde{1}(k) = \int_{-\infty}^{\infty} e^{-ikx} dx \\
 &\text{[variable substitution } x \rightarrow -x] \\
 &= \int_{+\infty}^{-\infty} e^{-ik(-x)} d(-x) \\
 &= - \int_{+\infty}^{-\infty} e^{ikx} dx \\
 &= \int_{-\infty}^{+\infty} e^{ikx} dx \\
 &= 2\pi\delta(k).
 \end{aligned} \tag{10.84}$$

### 10.6.5 Eigenfunction expansion of $\delta$

The  $\delta$ -function can be expressed in terms of, or “decomposed” into, various *eigenfunction expansions*. We mention without proof<sup>10</sup> that, for  $0 < x, x_0 < L$ , two such expansions in terms of trigonometric functions are

$$\begin{aligned}
 \delta(x - x_0) &= \frac{2}{L} \sum_{k=1}^{\infty} \sin\left(\frac{\pi k x_0}{L}\right) \sin\left(\frac{\pi k x}{L}\right) \\
 &= \frac{1}{L} + \frac{2}{L} \sum_{k=1}^{\infty} \cos\left(\frac{\pi k x_0}{L}\right) \cos\left(\frac{\pi k x}{L}\right).
 \end{aligned} \tag{10.85}$$

This “decomposition of unity” is analogous to the expansion of the identity in terms of orthogonal projectors  $\mathbf{E}_i$  (for one-dimensional projectors,  $\mathbf{E}_i = |i\rangle\langle i|$ ) encountered in the spectral theorem 4.28.1.

Other decompositions are in terms of orthonormal (Legendre) polynomials (cf. Sect. 14.6 on page 232), or other functions of mathematical physics discussed later.

### 10.6.6 Delta function expansion

Just like “slowly varying” functions can be expanded into a Taylor series in terms of the power functions  $x^n$ , highly localized functions can be expanded in terms of derivatives of the  $\delta$ -function in the form<sup>11</sup>

$$\begin{aligned}
 f(x) &\sim f_0\delta(x) + f_1\delta'(x) + f_2\delta''(x) + \cdots + f_n\delta^{(n)}(x) + \cdots = \sum_{k=1}^{\infty} f_k\delta^{(k)}(x), \\
 \text{with } f_k &= \frac{(-1)^k}{k!} \int_{-\infty}^{\infty} f(y)y^k dy.
 \end{aligned} \tag{10.86}$$

The sign “ $\sim$ ” denotes the functional character of this “equation” (10.86).

<sup>10</sup> Dean G. Duffy. *Green's Functions with Applications*. Chapman and Hall/CRC, Boca Raton, 2001

<sup>11</sup> Ismo V. Lindell. Delta function expansions, complex delta functions and the steepest descent method. *American Journal of Physics*, 61(5):438–442, 1993. DOI: 10.1119/1.17238. URL <http://dx.doi.org/10.1119/1.17238>



The delta expansion (10.86) can be proven by considering a smooth function  $g(x)$ , and integrating over its expansion; that is,

$$\begin{aligned} & \int_{-\infty}^{\infty} g(x) f(x) dx \\ &= \int_{-\infty}^{\infty} g(x) [f_0 \delta(x) + f_1 \delta'(x) + f_2 \delta''(x) + \cdots + (-1)^n f_n \delta^{(n)}(x) + \cdots] dx \\ &= f_0 g(0) - f_1 g'(0) + f_2 g''(0) + \cdots + (-1)^n f_n g^{(n)}(0) + \cdots, \end{aligned} \quad (10.87)$$

and comparing the coefficients in (10.87) with the coefficients of the Taylor series expansion of  $g$  at  $x = 0$

$$\begin{aligned} \int_{-\infty}^{\infty} g(x) f(x) dx &= \int_{-\infty}^{\infty} \left[ g(0) + x g'(0) + \cdots + \frac{x^n}{n!} g^{(n)}(0) + \cdots \right] f(x) dx \\ &= g(0) \int_{-\infty}^{\infty} f(x) dx + g'(0) \int_{-\infty}^{\infty} x f(x) dx + \cdots + g^{(n)}(0) \int_{-\infty}^{\infty} \frac{x^n}{n!} f(x) dx + \cdots. \end{aligned} \quad (10.88)$$

## 10.7 Cauchy principal value

### 10.7.1 Definition

The (Cauchy) principal value  $\mathcal{P}$  (sometimes also denoted by p.v.) is a value associated with a (divergent) integral as follows:

$$\begin{aligned} \mathcal{P} \int_a^b f(x) dx &= \lim_{\varepsilon \rightarrow 0^+} \left[ \int_a^{c-\varepsilon} f(x) dx + \int_{c+\varepsilon}^b f(x) dx \right] \\ &= \lim_{\varepsilon \rightarrow 0^+} \int_{[a, c-\varepsilon] \cup [c+\varepsilon, b]} f(x) dx, \end{aligned} \quad (10.89)$$

if  $c$  is the “location” of a singularity of  $f(x)$ .

For example, the integral  $\int_{-1}^1 \frac{dx}{x}$  diverges, but

$$\begin{aligned} \mathcal{P} \int_{-1}^1 \frac{dx}{x} &= \lim_{\varepsilon \rightarrow 0^+} \left[ \int_{-1}^{-\varepsilon} \frac{dx}{x} + \int_{+\varepsilon}^1 \frac{dx}{x} \right] \\ &\text{[variable substitution } x \rightarrow -x \text{ in the first integral]} \\ &= \lim_{\varepsilon \rightarrow 0^+} \left[ \int_{+1}^{+\varepsilon} \frac{dx}{x} + \int_{+\varepsilon}^1 \frac{dx}{x} \right] \\ &= \lim_{\varepsilon \rightarrow 0^+} [\log \varepsilon - \log 1 + \log 1 - \log \varepsilon] = 0. \end{aligned} \quad (10.90)$$

### 10.7.2 Principle value and pole function $\frac{1}{x}$ distribution

The “standalone function”  $\frac{1}{x}$  does not define a distribution since it is not integrable in the vicinity of  $x = 0$ . This issue can be “alleviated” or “circumvented” by considering the principle value  $\mathcal{P} \frac{1}{x}$ . In this way the principle

value can be transferred to the context of distributions by defining a *principal value distribution* in a functional sense by

$$\begin{aligned}
 \mathcal{P}\left(\frac{1}{x}\right)[\varphi] &= \lim_{\varepsilon \rightarrow 0^+} \int_{|x| > \varepsilon} \frac{1}{x} \varphi(x) dx \\
 &= \lim_{\varepsilon \rightarrow 0^+} \left[ \int_{-\infty}^{-\varepsilon} \frac{1}{x} \varphi(x) dx + \int_{+\varepsilon}^{\infty} \frac{1}{x} \varphi(x) dx \right] \\
 &\quad \text{[variable substitution } x \rightarrow -x \text{ in the first integral]} \\
 &= \lim_{\varepsilon \rightarrow 0^+} \left[ \int_{+\infty}^{+\varepsilon} \frac{1}{x} \varphi(-x) dx + \int_{+\varepsilon}^{\infty} \frac{1}{x} \varphi(x) dx \right] \\
 &= \lim_{\varepsilon \rightarrow 0^+} \left[ - \int_{+\varepsilon}^{\infty} \frac{1}{x} \varphi(-x) dx + \int_{+\varepsilon}^{\infty} \frac{1}{x} \varphi(x) dx \right] \\
 &= \lim_{\varepsilon \rightarrow 0^+} \int_{\varepsilon}^{+\infty} \frac{\varphi(x) - \varphi(-x)}{x} dx \\
 &= \int_0^{+\infty} \frac{\varphi(x) - \varphi(-x)}{x} dx.
 \end{aligned} \tag{10.91}$$

In the functional sense,  $\frac{1}{x}[\varphi]$  can be interpreted as a principal value. That is,

$$\begin{aligned}
 \frac{1}{x}[\varphi] &= \int_{-\infty}^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= \int_{-\infty}^0 \frac{1}{x} \varphi(x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &\quad \text{[variable substitution } x \rightarrow -x, dx \rightarrow -dx \text{ in the first integral]} \\
 &= \int_{+\infty}^0 \frac{1}{(-x)} \varphi(-x) d(-x) + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= \int_{+\infty}^0 \frac{1}{x} \varphi(-x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= - \int_0^{\infty} \frac{1}{x} \varphi(-x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= \int_0^{\infty} \frac{\varphi(x) - \varphi(-x)}{x} dx \\
 &= \mathcal{P}\left(\frac{1}{x}\right)[\varphi],
 \end{aligned} \tag{10.92}$$

where in the last step the principle value distribution (10.91) has been used.

## 10.8 Absolute value distribution

The distribution associated with the absolute value  $|x|$  is defined by

$$|x|[\varphi] = \int_{-\infty}^{\infty} |x| \varphi(x) dx. \tag{10.93}$$

$|x|[\varphi]$  can be evaluated and represented as follows:

$$\begin{aligned}
 |x|[\varphi] &= \int_{-\infty}^{\infty} |x| \varphi(x) dx \\
 &= \int_{-\infty}^0 (-x) \varphi(x) dx + \int_0^{\infty} x \varphi(x) dx \\
 &= - \int_{-\infty}^0 x \varphi(x) dx + \int_0^{\infty} x \varphi(x) dx \\
 &\quad \text{[variable substitution } x \rightarrow -x, dx \rightarrow -dx \text{ in the first integral]} \quad (10.94) \\
 &= - \int_{+\infty}^0 x \varphi(-x) dx + \int_0^{\infty} x \varphi(x) dx \\
 &= \int_0^{\infty} x \varphi(-x) dx + \int_0^{\infty} x \varphi(x) dx \\
 &= \int_0^{\infty} x [\varphi(x) + \varphi(-x)] dx.
 \end{aligned}$$

## 10.9 Logarithm distribution

### 10.9.1 Definition

Let, for  $x \neq 0$ ,

$$\begin{aligned}
 \log|x|[\varphi] &= \int_{-\infty}^{\infty} \log|x| \varphi(x) dx \\
 &= \int_{-\infty}^0 \log(-x) \varphi(x) dx + \int_0^{\infty} \log x \varphi(x) dx \\
 &\quad \text{[variable substitution } x \rightarrow -x, dx \rightarrow -dx \text{ in the first integral]} \\
 &= \int_{+\infty}^0 \log(-(-x)) \varphi(-x) d(-x) + \int_0^{\infty} \log x \varphi(x) dx \quad (10.95) \\
 &= - \int_{+\infty}^0 \log x \varphi(-x) dx + \int_0^{\infty} \log x \varphi(x) dx \\
 &= \int_0^{\infty} \log x \varphi(-x) dx + \int_0^{\infty} \log x \varphi(x) dx \\
 &= \int_0^{\infty} \log x [\varphi(x) + \varphi(-x)] dx.
 \end{aligned}$$

### 10.9.2 Connection with pole function

Note that

$$\mathcal{P}\left(\frac{1}{x}\right)[\varphi] = \frac{d}{dx} \log|x|[\varphi], \quad (10.96)$$

and thus for the principal value of a pole of degree  $n$

$$\mathcal{P}\left(\frac{1}{x^n}\right)[\varphi] = \frac{(-1)^{n-1}}{(n-1)!} \frac{d^n}{dx^n} \log|x|[\varphi]. \quad (10.97)$$

For a proof of Eq. (10.96) consider the functional derivative  $\log' |x|[\varphi]$  of  $\log |x|[\varphi]$  by insertion into Eq. (10.95); that is

$$\begin{aligned}
 \log' |x|[\varphi] &= \int_{-\infty}^0 \frac{d \log(-x)}{dx} \varphi(x) dx + \int_0^{\infty} \frac{d \log x}{dx} \varphi(x) dx \\
 &= \int_{-\infty}^0 \left( -\frac{1}{(-x)} \right) \varphi(x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= \int_{-\infty}^0 \frac{1}{x} \varphi(x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &\quad \text{[variable substitution } x \rightarrow -x, dx \rightarrow -dx \text{ in the first integral]} \\
 &= \int_{+\infty}^0 \frac{1}{(-x)} \varphi(-x) d(-x) + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \quad (10.98) \\
 &= \int_{+\infty}^0 \frac{1}{x} \varphi(-x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= - \int_0^{\infty} \frac{1}{x} \varphi(-x) dx + \int_0^{\infty} \frac{1}{x} \varphi(x) dx \\
 &= \int_0^{\infty} \frac{\varphi(x) - \varphi(-x)}{x} dx \\
 &= \mathcal{D} \left( \frac{1}{x} \right) [\varphi].
 \end{aligned}$$

The more general Eq. (10.97) follows by direct differentiation.

### 10.10 Pole function $\frac{1}{x^n}$ distribution

For  $n \geq 2$ , the integral over  $\frac{1}{x^n}$  is undefined even if we take the principal value. Hence the direct route to an evaluation is blocked, and we have to take an indirect approach *via* derivatives of  $\frac{1}{x}$ <sup>12</sup>. Thus, let

$$\begin{aligned}
 \frac{1}{x^2} [\varphi] &= -\frac{d}{dx} \frac{1}{x} [\varphi] \\
 = \frac{1}{x} [\varphi'] &= \int_0^{\infty} \frac{1}{x} [\varphi'(x) - \varphi'(-x)] dx \quad (10.99) \\
 &= \mathcal{D} \left( \frac{1}{x} \right) [\varphi'].
 \end{aligned}$$

Also,

$$\begin{aligned}
 \frac{1}{x^3} [\varphi] &= -\frac{1}{2} \frac{d}{dx} \frac{1}{x^2} [\varphi] = \frac{1}{2} \frac{1}{x^2} [\varphi'] = \frac{1}{2x} [\varphi''] \\
 &= \frac{1}{2} \int_0^{\infty} \frac{1}{x} [\varphi''(x) - \varphi''(-x)] dx \quad (10.100) \\
 &= \frac{1}{2} \mathcal{D} \left( \frac{1}{x} \right) [\varphi''].
 \end{aligned}$$

<sup>12</sup> Thomas Sommer. Verallgemeinerte Funktionen. unpublished manuscript, 2012

More generally, for  $n > 1$ , by induction, using (10.99) as induction basis,

$$\begin{aligned}
 & \frac{1}{x^n} [\varphi] \\
 &= -\frac{1}{n-1} \frac{d}{dx} \frac{1}{x^{n-1}} [\varphi] = \frac{1}{n-1} \frac{1}{x^{n-1}} [\varphi'] \\
 &= -\left(\frac{1}{n-1}\right) \left(\frac{1}{n-2}\right) \frac{d}{dx} \frac{1}{x^{n-2}} [\varphi'] = \frac{1}{(n-1)(n-2)} \frac{1}{x^{n-2}} [\varphi''] \\
 &= \dots = \frac{1}{(n-1)!} \frac{1}{x} [\varphi^{(n-1)}] \\
 &= \frac{1}{(n-1)!} \int_0^\infty \frac{1}{x} [\varphi^{(n-1)}(x) - \varphi^{(n-1)}(-x)] dx \\
 &= \frac{1}{(n-1)!} \mathcal{P} \left( \frac{1}{x} \right) [\varphi^{(n-1)}].
 \end{aligned} \tag{10.101}$$

### 10.11 Pole function $\frac{1}{x \pm i\alpha}$ distribution

We are interested in the limit  $\alpha \rightarrow 0$  of  $\frac{1}{x+i\alpha}$ . Let  $\alpha > 0$ . Then,

$$\begin{aligned}
 \frac{1}{x+i\alpha} [\varphi] &= \int_{-\infty}^\infty \frac{1}{x+i\alpha} \varphi(x) dx \\
 &= \int_{-\infty}^\infty \frac{x-i\alpha}{(x+i\alpha)(x-i\alpha)} \varphi(x) dx \\
 &= \int_{-\infty}^\infty \frac{x-i\alpha}{x^2+\alpha^2} \varphi(x) dx \\
 &= \int_{-\infty}^\infty \frac{x}{x^2+\alpha^2} \varphi(x) dx - i\alpha \int_{-\infty}^\infty \frac{1}{x^2+\alpha^2} \varphi(x) dx.
 \end{aligned} \tag{10.102}$$

Let us treat the two summands of (10.102) separately. (i) Upon variable substitution  $x = \alpha y$ ,  $dx = \alpha dy$  in the second integral in (10.102) we obtain

$$\begin{aligned}
 \alpha \int_{-\infty}^\infty \frac{1}{x^2+\alpha^2} \varphi(x) dx &= \alpha \int_{-\infty}^\infty \frac{1}{\alpha^2 y^2 + \alpha^2} \varphi(\alpha y) \alpha dy \\
 &= \alpha^2 \int_{-\infty}^\infty \frac{1}{\alpha^2 (y^2+1)} \varphi(\alpha y) dy \\
 &= \int_{-\infty}^\infty \frac{1}{y^2+1} \varphi(\alpha y) dy
 \end{aligned} \tag{10.103}$$

In the limit  $\alpha \rightarrow 0$ , this is

$$\begin{aligned}
 \lim_{\alpha \rightarrow 0} \int_{-\infty}^\infty \frac{1}{y^2+1} \varphi(\alpha y) dy &= \varphi(0) \int_{-\infty}^\infty \frac{1}{y^2+1} dy \\
 &= \varphi(0) (\arctan y) \Big|_{y=-\infty}^{y=\infty} \\
 &= \pi \varphi(0) = \pi \delta[\varphi].
 \end{aligned} \tag{10.104}$$

(ii) The first integral in (10.102) is

$$\begin{aligned}
 & \int_{-\infty}^{\infty} \frac{x}{x^2 + \alpha^2} \varphi(x) dx \\
 &= \int_{-\infty}^0 \frac{x}{x^2 + \alpha^2} \varphi(x) dx + \int_0^{\infty} \frac{x}{x^2 + \alpha^2} \varphi(x) dx \\
 &= \int_{+\infty}^0 \frac{-x}{(-x)^2 + \alpha^2} \varphi(-x) d(-x) + \int_0^{\infty} \frac{x}{x^2 + \alpha^2} \varphi(x) dx \quad (10.105) \\
 &= - \int_0^{\infty} \frac{x}{x^2 + \alpha^2} \varphi(-x) dx + \int_0^{\infty} \frac{x}{x^2 + \alpha^2} \varphi(x) dx \\
 &= \int_0^{\infty} \frac{x}{x^2 + \alpha^2} [\varphi(x) - \varphi(-x)] dx.
 \end{aligned}$$

In the limit  $\alpha \rightarrow 0$ , this becomes

$$\begin{aligned}
 \lim_{\alpha \rightarrow 0} \int_0^{\infty} \frac{x}{x^2 + \alpha^2} [\varphi(x) - \varphi(-x)] dx &= \int_0^{\infty} \frac{\varphi(x) - \varphi(-x)}{x} dx \\
 &= \mathcal{P} \left( \frac{1}{x} \right) [\varphi], \quad (10.106)
 \end{aligned}$$

where in the last step the principle value distribution (10.91) has been used.

Putting all parts together, we obtain

$$\frac{1}{x + i0^+} [\varphi] = \lim_{\alpha \rightarrow 0} \frac{1}{x + i\alpha} [\varphi] = \mathcal{P} \left( \frac{1}{x} \right) [\varphi] - i\pi\delta[\varphi] = \left\{ \mathcal{P} \left( \frac{1}{x} \right) - i\pi\delta \right\} [\varphi]. \quad (10.107)$$

A very similar calculation yields

$$\frac{1}{x - i0^+} [\varphi] = \lim_{\alpha \rightarrow 0} \frac{1}{x - i\alpha} [\varphi] = \mathcal{P} \left( \frac{1}{x} \right) [\varphi] + i\pi\delta[\varphi] = \left\{ \mathcal{P} \left( \frac{1}{x} \right) + i\pi\delta \right\} [\varphi]. \quad (10.108)$$

These equations (10.107) and (10.108) are often called the *Sokhotsky formula*, also known as the *Plemelj formula*, or the *Plemelj-Sokhotsky formula*.

## 10.12 Heaviside step function

### 10.12.1 Ambiguities in definition

Let us now turn to some very common generalized functions; in particular to Heaviside's electromagnetic *infinite pulse function*. One of the possible definitions of the Heaviside step function  $H(x)$ , and maybe the most common one – they differ by the difference of the value(s) of  $H(0)$  at the origin  $x = 0$ , a difference which is irrelevant measure theoretically for “good” functions since it is only about an isolated point – is

$$H(x - x_0) = \begin{cases} 1 & \text{for } x \geq x_0 \\ 0 & \text{for } x < x_0 \end{cases} \quad (10.109)$$

The function is plotted in Fig. 10.4.

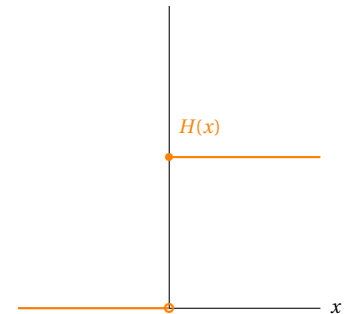


Figure 10.4: Plot of the Heaviside step function  $H(x)$ .

In the spirit of the above definition, it might have been more appropriate to define  $H(0) = \frac{1}{2}$ ; that is,

$$H(x - x_0) = \begin{cases} 1 & \text{for } x > x_0 \\ \frac{1}{2} & \text{for } x = x_0 \\ 0 & \text{for } x < x_0 \end{cases} \quad (10.110)$$

and, since this affects only an isolated point at  $x = 0$ , we may happily do so if we prefer.

It is also very common to define the Heaviside step function as the *antiderivative of the  $\delta$  function*; likewise the delta function is the derivative of the Heaviside step function; that is,

$$\begin{aligned} H(x - x_0) &= \int_{-\infty}^{x-x_0} \delta(t) dt, \\ \frac{d}{dx} H(x - x_0) &= \delta(x - x_0). \end{aligned} \quad (10.111)$$

The latter equation can – in the functional sense – be proven through

$$\begin{aligned} \langle H', \varphi \rangle &= -\langle H, \varphi' \rangle \\ &= -\int_{-\infty}^{\infty} H(x) \varphi'(x) dx \\ &= -\int_0^{\infty} \varphi'(x) dx \\ &= -\varphi(x) \Big|_{x=0}^{x=\infty} \\ &= -\underbrace{\varphi(\infty)}_{=0} + \varphi(0) \\ &= \langle \delta, \varphi \rangle \end{aligned} \quad (10.112)$$

for all test functions  $\varphi(x)$ . Hence we can – in the functional sense – identify  $\delta$  with  $H'$ . More explicitly, through integration by parts, we obtain

$$\begin{aligned} &\int_{-\infty}^{\infty} \left[ \frac{d}{dx} H(x - x_0) \right] \varphi(x) dx \\ &= H(x - x_0) \varphi(x) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} H(x - x_0) \left[ \frac{d}{dx} \varphi(x) \right] dx \\ &= \underbrace{H(\infty) \varphi(\infty)}_{\varphi(\infty)=0} - \underbrace{H(-\infty) \varphi(-\infty)}_{0^2=0} - \int_{x_0}^{\infty} \left[ \frac{d}{dx} \varphi(x) \right] dx \\ &= -\int_{x_0}^{\infty} \left[ \frac{d}{dx} \varphi(x) \right] dx \\ &= -\varphi(x) \Big|_{x=x_0}^{x=\infty} \\ &= -[\varphi(\infty) - \varphi(x_0)] \\ &= \varphi(x_0). \end{aligned} \quad (10.113)$$

### 10.12.2 Useful formulæ involving $H$

Some other formulæ involving the Heaviside step function are

$$H(\pm x) = \lim_{\epsilon \rightarrow 0^+} \frac{\mp i}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{ikx}}{k \mp i\epsilon} dk, \quad (10.114)$$

and

$$H(x) = \frac{1}{2} + \sum_{l=0}^{\infty} (-1)^l \frac{(2l)!(4l+3)}{2^{2l+2} l! (l+1)!} P_{2l+1}(x), \quad (10.115)$$

where  $P_{2l+1}(x)$  is a Legendre polynomial. Furthermore,

$$\delta(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} H\left(\frac{\epsilon}{2} - |x|\right). \quad (10.116)$$

An integral representation of  $H(x)$  is

$$H(x) = \lim_{\epsilon \downarrow 0^+} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t \pm i\epsilon} e^{\mp ixt} dt. \quad (10.117)$$

One commonly used limit form of the Heaviside step function is

$$H(x) = \lim_{\epsilon \rightarrow 0} H_{\epsilon}(x) = \lim_{\epsilon \rightarrow 0} \left[ \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \frac{x}{\epsilon} \right]. \quad (10.118)$$

respectively.

Another limit representation of the Heaviside function is in terms of the *Dirichlet's discontinuity factor*

$$\begin{aligned} H(x) &= \lim_{t \rightarrow \infty} H_t(x) \\ &= \frac{2}{\pi} \lim_{t \rightarrow \infty} \int_0^t \frac{\sin(kx)}{k} dk \\ &= \frac{2}{\pi} \int_0^{\infty} \frac{\sin(kx)}{x} dx. \end{aligned} \quad (10.119)$$

A proof uses a variant<sup>13</sup> of the *sine integral function*

$$\text{Si}(x) = \int_0^x \frac{\sin t}{t} dt \quad (10.120)$$

which in the limit of large argument converges towards the *Dirichlet integral* (no proof is given here)

$$\text{Si}(\infty) = \int_0^{\infty} \frac{\sin t}{t} dt = \frac{\pi}{2}. \quad (10.121)$$

In the Dirichlet integral (10.121), if we replace  $t$  with  $tx$  and substitute  $u$  for  $tx$  (hence, by identifying  $u = tx$  and  $du/dt = x$ , thus  $dt = du/x$ ), we arrive at

$$\int_0^{\infty} \frac{\sin(xt)}{t} dt = \int_0^{\pm\infty} \frac{\sin(u)}{u} du. \quad (10.122)$$

The  $\mp$  sign depends on whether  $k$  is positive or negative. The Dirichlet integral can be restored in its original form (10.121) by a further substitution  $u \rightarrow -u$  for negative  $k$ . Due to the odd function  $\sin$  this yields  $-\pi/2$  or  $+\pi/2$  for negative or positive  $k$ , respectively. The Dirichlet's discontinuity factor (10.119) is obtained by normalizing (10.122) to unity by multiplying it with  $2/\pi$ .

<sup>13</sup> Eli Maor. *Trigonometric Delights*. Princeton University Press, Princeton, 1998. URL <http://press.princeton.edu/books/maor/>



### 10.12.3 $H[\varphi]$ distribution

The distribution associated with the Heaviside function  $H(x)$  is defined by

$$H[\varphi] = \int_{-\infty}^{\infty} H(x)\varphi(x)dx. \quad (10.123)$$

$H[\varphi]$  can be evaluated and represented as follows:

$$\begin{aligned} H[\varphi] &= \int_{-\infty}^{\infty} H(x)\varphi(x)dx \\ &= \int_0^{\infty} \varphi(x)dx. \end{aligned} \quad (10.124)$$

### 10.12.4 Regularized regularized Heaviside function

In order to be able to define the distribution associated with the Heaviside function (and its Fourier transform), we sometimes consider the distribution of the *regularized Heaviside function*

$$H_\varepsilon(x) = H(x)e^{-\varepsilon x}, \quad (10.125)$$

with  $\varepsilon > 0$ , such that  $\lim_{\varepsilon \rightarrow 0^+} H_\varepsilon(x) = H(x)$ .

### 10.12.5 Fourier transform of Heaviside (unit step) function

The Fourier transform of the Heaviside (unit step) function cannot be directly obtained by insertion into Eq. (9.19), because the associated integrals do not exist. For a derivation of the Fourier transform of the Heaviside (unit step) function we shall thus use the regularized Heaviside function (10.125), and arrive at *Sokhotsky's formula* (also known as the *Plemelj's formula*, or the *Plemelj-Sokhotsky formula*)

$$\begin{aligned} \mathcal{F}[H(x)] &= \tilde{H}(k) = \int_{-\infty}^{\infty} H(x)e^{-ikx}dx \\ &= \pi\delta(k) - i\mathcal{P}\frac{1}{k} \\ &= -i\left(i\pi\delta(k) + \mathcal{P}\frac{1}{k}\right) \\ &= \lim_{\varepsilon \rightarrow 0^+} -\frac{i}{k - i\varepsilon} \end{aligned} \quad (10.126)$$

We shall compute the Fourier transform of the regularized Heaviside function  $H_\varepsilon(x) = H(x)e^{-\varepsilon x}$ , with  $\varepsilon > 0$ , of Eq. (10.125); that is <sup>14</sup>,

<sup>14</sup> Thomas Sommer. Verallgemeinerte Funktionen. unpublished manuscript, 2012

$$\begin{aligned}
\mathcal{F}[H_\varepsilon(x)] &= \mathcal{F}[H(x)e^{-\varepsilon x}] = \widetilde{H}_\varepsilon(k) \\
&= \int_{-\infty}^{\infty} H_\varepsilon(x) e^{-ikx} dx \\
&= \int_{-\infty}^{\infty} H(x) e^{-\varepsilon x} e^{-ikx} dx \\
&= \int_{-\infty}^{\infty} H(x) e^{-ikx + (-i)^2 \varepsilon x} dx \\
&= \int_{-\infty}^{\infty} H(x) e^{-i(k-i\varepsilon)x} dx \\
&= \int_0^{\infty} e^{-i(k-i\varepsilon)x} dx \\
&= \left[ -\frac{e^{-i(k-i\varepsilon)x}}{i(k-i\varepsilon)} \right]_{x=0}^{x=\infty} \\
&= \left[ -\frac{e^{-ik} e^{-\varepsilon} x}{i(k-i\varepsilon)} \right]_{x=0}^{x=\infty} \\
&= \left[ -\frac{e^{-ik\infty} e^{-\varepsilon\infty}}{i(k-i\varepsilon)} \right] - \left[ -\frac{e^{-ik0} e^{-\varepsilon0}}{i(k-i\varepsilon)} \right] \\
&= 0 - \frac{(-1)}{i(k-i\varepsilon)} = -\frac{i}{(k-i\varepsilon)}.
\end{aligned} \tag{10.127}$$

By using Sokhotsky's formula (10.108) we conclude that

$$\mathcal{F}[H(x)] = \mathcal{F}[H_{0+}(x)] = \lim_{\varepsilon \rightarrow 0^+} \mathcal{F}[H_\varepsilon(x)] = \pi\delta(k) - i\mathcal{P}\left(\frac{1}{k}\right). \tag{10.128}$$

### 10.13 The sign function

#### 10.13.1 Definition

The *sign function* is defined by

$$\text{sgn}(x - x_0) = \begin{cases} -1 & \text{for } x < x_0 \\ 0 & \text{for } x = x_0 \\ +1 & \text{for } x > x_0 \end{cases}. \tag{10.129}$$

It is plotted in Fig. 10.5.

#### 10.13.2 Connection to the Heaviside function

In terms of the Heaviside step function, in particular, with  $H(0) = \frac{1}{2}$  as in Eq. (10.110), the sign function can be written by “stretching” the former (the Heaviside step function) by a factor of two, and shifting it by one negative unit as follows

$$\begin{aligned}
\text{sgn}(x - x_0) &= 2H(x - x_0) - 1, \\
H(x - x_0) &= \frac{1}{2} [\text{sgn}(x - x_0) + 1]; \\
&\text{and also} \\
\text{sgn}(x - x_0) &= H(x - x_0) - H(x_0 - x).
\end{aligned} \tag{10.130}$$

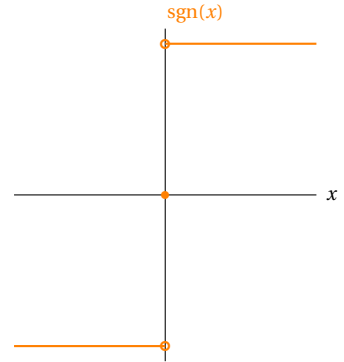


Figure 10.5: Plot of the sign function  $\text{sgn}(x)$ .

### 10.13.3 Sign sequence

The sequence of functions

$$\operatorname{sgn}_n(x - x_0) = \begin{cases} -e^{-\frac{x}{n}} & \text{for } x < x_0 \\ +e^{\frac{-x}{n}} & \text{for } x > x_0 \end{cases} \quad (10.131)$$

is a limiting sequence of  $\operatorname{sgn}(x - x_0) \stackrel{x \neq x_0}{=} \lim_{n \rightarrow \infty} \operatorname{sgn}_n(x - x_0)$ .

Note (without proof) that

$$\operatorname{sgn}(x) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\sin[(2n+1)x]}{(2n+1)} \quad (10.132)$$

$$= \frac{4}{\pi} \sum_{n=0}^{\infty} (-1)^n \frac{\cos[(2n+1)(x - \pi/2)]}{(2n+1)}, \quad -\pi < x < \pi. \quad (10.133)$$

### 10.13.4 Fourier transform of $\operatorname{sgn}$

Since the Fourier transform is linear, we may use the connection between the sign and the Heaviside functions  $\operatorname{sgn}(x) = 2H(x) - 1$ , Eq. (10.130), together with the Fourier transform of the Heaviside function  $\mathcal{F}[H(x)] = \pi\delta(k) - i\mathcal{P}\left(\frac{1}{k}\right)$ , Eq. (10.128) and the Dirac delta function  $\mathcal{F}[1] = 2\pi\delta(k)$ , Eq. (10.84), to compose and compute the Fourier transform of  $\operatorname{sgn}$ :

$$\begin{aligned} \mathcal{F}[\operatorname{sgn}(x)] &= \mathcal{F}[2H(x) - 1] = 2\mathcal{F}[H(x)] - \mathcal{F}[1] \\ &= 2 \left[ \pi\delta(k) - i\mathcal{P}\left(\frac{1}{k}\right) \right] - 2\pi\delta(k) \\ &= -2i\mathcal{P}\left(\frac{1}{k}\right). \end{aligned} \quad (10.134)$$

## 10.14 Absolute value function (or modulus)

### 10.14.1 Definition

The *absolute value* (or *modulus*) of  $x$  is defined by

$$|x - x_0| = \begin{cases} x - x_0 & \text{for } x > x_0 \\ 0 & \text{for } x = x_0 \\ x_0 - x & \text{for } x < x_0 \end{cases} \quad (10.135)$$

It is plotted in Fig. 10.6.

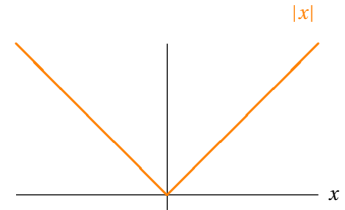


Figure 10.6: Plot of the absolute value  $|x|$ .

### 10.14.2 Connection of absolute value with sign and Heaviside functions

Its relationship to the sign function is twofold: on the one hand, there is

$$|x| = x \operatorname{sgn}(x), \quad (10.136)$$

and thus, for  $x \neq 0$ ,

$$\operatorname{sgn}(x) = \frac{|x|}{x} = \frac{x}{|x|}. \quad (10.137)$$

On the other hand, the derivative of the absolute value function is the sign function, at least up to a singular point at  $x = 0$ , and thus the absolute value function can be interpreted as the integral of the sign function (in the distributional sense); that is,

$$\frac{d|x|}{dx} = \begin{cases} 1 & \text{for } x > 0 \\ \text{undefined} & \text{for } x = 0 \\ -1 & \text{for } x < 0 \end{cases} \stackrel{x \neq 0}{=} \text{sgn}(x); \quad (10.138)$$

$$|x| = \int \text{sgn}(x) dx.$$

### 10.15 Some examples

Let us compute some concrete examples related to distributions.

1. For a start, let us prove that

$$\lim_{\epsilon \rightarrow 0} \frac{\epsilon \sin^2 \frac{x}{\epsilon}}{\pi x^2} = \delta(x). \quad (10.139)$$

As a hint, take  $\int_{-\infty}^{+\infty} \frac{\sin^2 x}{x^2} dx = \pi$ .

Let us prove this conjecture by integrating over a good test function  $\varphi$

$$\begin{aligned} & \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \frac{\epsilon \sin^2 \left( \frac{x}{\epsilon} \right)}{x^2} \varphi(x) dx \\ & [\text{variable substitution } y = \frac{x}{\epsilon}, \frac{dy}{dx} = \frac{1}{\epsilon}, dx = \epsilon dy] \\ & = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \varphi(\epsilon y) \frac{\epsilon^2 \sin^2(y)}{\epsilon^2 y^2} dy \quad (10.140) \\ & = \frac{1}{\pi} \varphi(0) \int_{-\infty}^{+\infty} \frac{\sin^2(y)}{y^2} dy \\ & = \varphi(0). \end{aligned}$$

Hence we can identify

$$\lim_{\epsilon \rightarrow 0} \frac{\epsilon \sin^2 \left( \frac{x}{\epsilon} \right)}{\pi x^2} = \delta(x). \quad (10.141)$$

2. In order to prove that  $\frac{1}{\pi} \frac{n e^{-x^2}}{1+n^2 x^2}$  is a  $\delta$ -sequence we proceed again by integrating over a good test function  $\varphi$ , and with the hint that  $\int_{-\infty}^{+\infty} dx/(1+x^2) = \pi$

$x^2) = \pi$  we obtain

$$\begin{aligned}
 & \lim_{n \rightarrow \infty} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{n e^{-x^2}}{1 + n^2 x^2} \varphi(x) dx \\
 & \text{[variable substitution } y = xn, x = \frac{y}{n}, \frac{dy}{dx} = n, dx = \frac{dy}{n}] \\
 & = \lim_{n \rightarrow \infty} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{n e^{-(\frac{y}{n})^2}}{1 + y^2} \varphi\left(\frac{y}{n}\right) \frac{dy}{n} \\
 & = \frac{1}{\pi} \int_{-\infty}^{+\infty} \lim_{n \rightarrow \infty} \left[ e^{-(\frac{y}{n})^2} \varphi\left(\frac{y}{n}\right) \right] \frac{1}{1 + y^2} dy \quad (10.142) \\
 & = \frac{1}{\pi} \int_{-\infty}^{+\infty} [e^0 \varphi(0)] \frac{1}{1 + y^2} dy \\
 & = \frac{\varphi(0)}{\pi} \int_{-\infty}^{+\infty} \frac{1}{1 + y^2} dy \\
 & = \frac{\varphi(0)}{\pi} \pi \\
 & = \varphi(0).
 \end{aligned}$$

Hence we can identify

$$\lim_{n \rightarrow \infty} \frac{1}{\pi} \frac{n e^{-x^2}}{1 + n^2 x^2} = \delta(x). \quad (10.143)$$

3. Let us prove that  $x^n \delta^{(n)}(x) = C \delta(x)$  and determine the constant  $C$ . We proceed again by integrating over a good test function  $\varphi$ . First note that if  $\varphi(x)$  is a good test function, then so is  $x^n \varphi(x)$ .

$$\begin{aligned}
 \int dx x^n \delta^{(n)}(x) \varphi(x) &= \int dx \delta^{(n)}(x) [x^n \varphi(x)] = \\
 &= (-1)^n \int dx \delta(x) [x^n \varphi(x)]^{(n)} = \\
 &= (-1)^n \int dx \delta(x) [n x^{n-1} \varphi(x) + x^n \varphi'(x)]^{(n-1)} = \\
 &\quad \dots \\
 &= (-1)^n \int dx \delta(x) \left[ \sum_{k=0}^n \binom{n}{k} (x^n)^{(k)} \varphi^{(n-k)}(x) \right] = \\
 &= (-1)^n \int dx \delta(x) [n! \varphi(x) + n \cdot n! x \varphi'(x) + \dots + x^n \varphi^{(n)}(x)] = \\
 &= (-1)^n n! \int dx \delta(x) \varphi(x);
 \end{aligned}$$

hence,  $C = (-1)^n n!$ . Note that  $\varphi(x)$  is a good test function then so is  $x^n \varphi(x)$ .

4. Let us simplify  $\int_{-\infty}^{\infty} \delta(x^2 - a^2) g(x) dx$ . First recall Eq. (10.66) stating that

$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|},$$

whenever  $x_i$  are simple roots of  $f(x)$ , and  $f'(x_i) \neq 0$ . In our case,  $f(x) = x^2 - a^2 = (x - a)(x + a)$ , and the roots are  $x = \pm a$ . Furthermore,

$$f'(x) = (x - a) + (x + a);$$

hence

$$|f'(a)| = 2|a|, \quad |f'(-a)| = |-2a| = 2|a|.$$

As a result,

$$\delta(x^2 - a^2) = \delta((x - a)(x + a)) = \frac{1}{|2a|} (\delta(x - a) + \delta(x + a)).$$

Taking this into account we finally obtain

$$\begin{aligned} & \int_{-\infty}^{+\infty} \delta(x^2 - a^2) g(x) dx \\ &= \int_{-\infty}^{+\infty} \frac{\delta(x - a) + \delta(x + a)}{2|a|} g(x) dx \\ &= \frac{g(a) + g(-a)}{2|a|}. \end{aligned} \quad (10.144)$$

5. Let us evaluate

$$I = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x_1^2 + x_2^2 + x_3^2 - R^2) d^3 x \quad (10.145)$$

for  $R \in \mathbb{R}, R > 0$ . We may, of course, remain in the standard Cartesian coordinate system and evaluate the integral by “brute force.” Alternatively, a more elegant way is to use the spherical symmetry of the problem and use spherical coordinates  $r, \Omega(\theta, \varphi)$  by rewriting  $I$  into

$$I = \int_{r, \Omega} r^2 \delta(r^2 - R^2) d\Omega dr. \quad (10.146)$$

As the integral kernel  $\delta(r^2 - R^2)$  just depends on the radial coordinate  $r$  the angular coordinates just integrate to  $4\pi$ . Next we make use of Eq. (10.66), eliminate the solution for  $r = -R$ , and obtain

$$\begin{aligned} I &= 4\pi \int_0^{\infty} r^2 \delta(r^2 - R^2) dr \\ &= 4\pi \int_0^{\infty} r^2 \frac{\delta(r + R) + \delta(r - R)}{2R} dr \\ &= 4\pi \int_0^{\infty} r^2 \frac{\delta(r - R)}{2R} dr \\ &= 2\pi R. \end{aligned} \quad (10.147)$$

6. Let us compute

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta(x^3 - y^2 + 2y) \delta(x + y) H(y - x - 6) f(x, y) dx dy. \quad (10.148)$$

First, in dealing with  $\delta(x+y)$ , we evaluate the  $y$  integration at  $x = -y$  or  $y = -x$ :

$$\int_{-\infty}^{\infty} \delta(x^3 - x^2 - 2x) H(-2x-6) f(x, -x) dx$$

Use of Eq. (10.66)

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i),$$

at the roots

$$\begin{aligned} x_1 &= 0 \\ x_{2,3} &= \frac{1 \pm \sqrt{1+8}}{2} = \frac{1 \pm 3}{2} = \begin{cases} 2 \\ -1 \end{cases} \end{aligned}$$

of the argument  $f(x) = x^3 - x^2 - 2x = x(x^2 - x - 2) = x(x-2)(x+1)$  of the remaining  $\delta$ -function, together with

$$f'(x) = \frac{d}{dx}(x^3 - x^2 - 2x) = 3x^2 - 2x - 2;$$

yields

$$\begin{aligned} & \int_{-\infty}^{\infty} dx \frac{\delta(x) + \delta(x-2) + \delta(x+1)}{|3x^2 - 2x - 2|} H(-2x-6) f(x, -x) = \\ &= \frac{1}{|-2|} \underbrace{H(-6)}_{=0} f(0, -0) + \frac{1}{|12-4-2|} \underbrace{H(-4-6)}_{=0} f(2, -2) + \\ &+ \frac{1}{|3+2-2|} \underbrace{H(2-6)}_{=0} f(-1, 1) \\ &= 0 \end{aligned}$$

7. When simplifying derivatives of generalized functions it is always useful to evaluate their properties – such as  $x\delta(x) = 0$ ,  $f(x)\delta(x-x_0) = f(x_0)\delta(x-x_0)$ , or  $\delta(-x) = \delta(x)$  – first and before proceeding with the next differentiation or evaluation. We shall present some applications of this “rule” next.

First, simplify

$$\left( \frac{d}{dx} - \omega \right) H(x) e^{\omega x} \quad (10.149)$$

as follows

$$\begin{aligned} & \frac{d}{dx} [H(x) e^{\omega x}] - \omega H(x) e^{\omega x} \\ &= \delta(x) e^{\omega x} + \omega H(x) e^{\omega x} - \omega H(x) e^{\omega x} \\ &= \delta(x) e^0 \\ &= \delta(x) \end{aligned} \quad (10.150)$$

8. Next, simplify

$$\left(\frac{d^2}{dx^2} + \omega^2\right) \frac{1}{\omega} H(x) \sin(\omega x) \quad (10.151)$$

as follows

$$\begin{aligned} & \frac{d^2}{dx^2} \left[ \frac{1}{\omega} H(x) \sin(\omega x) \right] + \omega H(x) \sin(\omega x) \\ &= \frac{1}{\omega} \frac{d}{dx} \left[ \underbrace{\delta(x) \sin(\omega x)}_{=0} + \omega H(x) \cos(\omega x) \right] + \omega H(x) \sin(\omega x) \\ &= \frac{1}{\omega} \left[ \omega \underbrace{\delta(x) \cos(\omega x)}_{\delta(x)} - \omega^2 H(x) \sin(\omega x) \right] + \omega H(x) \sin(\omega x) = \delta(x) \end{aligned} \quad (10.152)$$

9. Let us compute the  $n$ th derivative of

$$f(x) = \begin{cases} 0 & \text{for } x < 0, \\ x & \text{for } 0 \leq x \leq 1, \\ 0 & \text{for } x > 1. \end{cases} \quad (10.153)$$

As depicted in Fig. 10.7,  $f$  can be composed from two functions  $f(x) = f_2(x) \cdot f_1(x)$ ; and this composition can be done in at least two ways.

Decomposition (i)

$$\begin{aligned} f(x) &= x[H(x) - H(x-1)] = xH(x) - xH(x-1) \\ f'(x) &= H(x) + x\delta(x) - H(x-1) - x\delta(x-1) \end{aligned}$$

Because of  $x\delta(x-a) = a\delta(x-a)$ ,

$$\begin{aligned} f'(x) &= H(x) - H(x-1) - \delta(x-1) \\ f''(x) &= \delta(x) - \delta(x-1) - \delta'(x-1) \end{aligned}$$

and hence by induction

$$f^{(n)}(x) = \delta^{(n-2)}(x) - \delta^{(n-2)}(x-1) - \delta^{(n-1)}(x-1)$$

for  $n > 1$ .

Decomposition (ii)

$$\begin{aligned} f(x) &= xH(x)H(1-x) \\ f'(x) &= H(x)H(1-x) + \underbrace{x\delta(x)H(1-x)}_{=0} + \underbrace{xH(x)(-1)\delta(1-x)}_{-H(x)\delta(1-x)} = \\ &= H(x)H(1-x) - \delta(1-x) = [\delta(x) = \delta(-x)] = H(x)H(1-x) - \delta(x-1) \\ f''(x) &= \underbrace{\delta(x)H(1-x)}_{=\delta(x)} + \underbrace{(-1)H(x)\delta(1-x)}_{-\delta(1-x)} - \delta'(x-1) = \\ &= \delta(x) - \delta(x-1) - \delta'(x-1) \end{aligned}$$

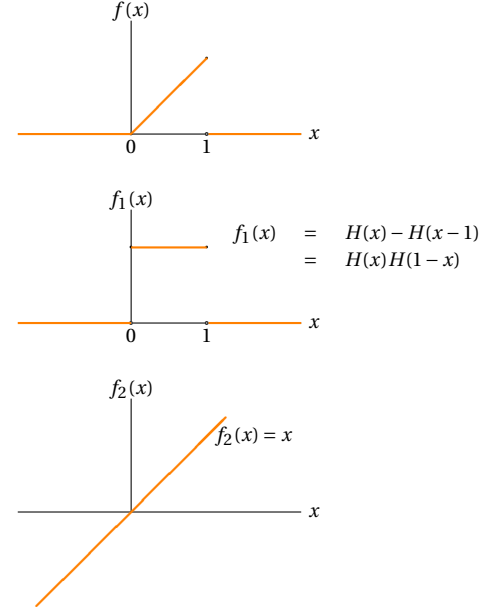


Figure 10.7: Composition of  $f(x)$



and hence by induction

$$f^{(n)}(x) = \delta^{(n-2)}(x) - \delta^{(n-2)}(x-1) - \delta^{(n-1)}(x-1)$$

for  $n > 1$ .

10. Let us compute the  $n$ th derivative of

$$f(x) = \begin{cases} |\sin x| & \text{for } -\pi \leq x \leq \pi, \\ 0 & \text{for } |x| > \pi. \end{cases} \quad (10.154)$$

$$f(x) = |\sin x| H(\pi + x) H(\pi - x)$$

$$|\sin x| = \sin x \operatorname{sgn}(\sin x) = \sin x \operatorname{sgn} x \quad \text{für } -\pi < x < \pi;$$

hence we start from

$$f(x) = \sin x \operatorname{sgn} x H(\pi + x) H(\pi - x),$$

Note that

$$\begin{aligned} \operatorname{sgn} x &= H(x) - H(-x), \\ (\operatorname{sgn} x)' &= H'(x) - H'(-x)(-1) = \delta(x) + \delta(-x) = \delta(x) + \delta(x) = 2\delta(x). \end{aligned}$$

$$\begin{aligned} f'(x) &= \cos x \operatorname{sgn} x H(\pi + x) H(\pi - x) + \sin x 2\delta(x) H(\pi + x) H(\pi - x) + \\ &\quad + \sin x \operatorname{sgn} x \delta(\pi + x) H(\pi - x) + \sin x \operatorname{sgn} x H(\pi + x) \delta(\pi - x)(-1) = \\ &= \cos x \operatorname{sgn} x H(\pi + x) H(\pi - x) \\ f''(x) &= -\sin x \operatorname{sgn} x H(\pi + x) H(\pi - x) + \cos x 2\delta(x) H(\pi + x) H(\pi - x) + \\ &\quad + \cos x \operatorname{sgn} x \delta(\pi + x) H(\pi - x) + \cos x \operatorname{sgn} x H(\pi + x) \delta(\pi - x)(-1) = \\ &= -\sin x \operatorname{sgn} x H(\pi + x) H(\pi - x) + 2\delta(x) + \delta(\pi + x) + \delta(\pi - x) \\ f'''(x) &= -\cos x \operatorname{sgn} x H(\pi + x) H(\pi - x) - \sin x 2\delta(x) H(\pi + x) H(\pi - x) - \\ &\quad - \sin x \operatorname{sgn} x \delta(\pi + x) H(\pi - x) - \sin x \operatorname{sgn} x H(\pi + x) \delta(\pi - x)(-1) + \\ &\quad + 2\delta'(x) + \delta'(\pi + x) - \delta'(\pi - x) = \\ &= -\cos x \operatorname{sgn} x H(\pi + x) H(\pi - x) + 2\delta'(x) + \delta'(\pi + x) - \delta'(\pi - x) \\ f^{(4)}(x) &= \sin x \operatorname{sgn} x H(\pi + x) H(\pi - x) - \cos x 2\delta(x) H(\pi + x) H(\pi - x) - \\ &\quad - \cos x \operatorname{sgn} x \delta(\pi + x) H(\pi - x) - \cos x \operatorname{sgn} x H(\pi + x) \delta(\pi - x)(-1) + \\ &\quad + 2\delta''(x) + \delta''(\pi + x) + \delta''(\pi - x) = \\ &= \sin x \operatorname{sgn} x H(\pi + x) H(\pi - x) - 2\delta(x) - \delta(\pi + x) - \delta(\pi - x) + \\ &\quad + 2\delta''(x) + \delta''(\pi + x) + \delta''(\pi - x); \end{aligned}$$

hence

$$\begin{aligned} f^{(4)} &= f(x) - 2\delta(x) + 2\delta''(x) - \delta(\pi + x) + \delta''(\pi + x) - \delta(\pi - x) + \delta''(\pi - x), \\ f^{(5)} &= f'(x) - 2\delta'(x) + 2\delta'''(x) - \delta'(\pi + x) + \delta'''(\pi + x) + \delta'(\pi - x) - \delta'''(\pi - x); \end{aligned}$$

and thus by induction

$$\begin{aligned}
 f^{(n)} &= f^{(n-4)}(x) - 2\delta^{(n-4)}(x) + 2\delta^{(n-2)}(x) - \delta^{(n-4)}(\pi+x) + \\
 &\quad + \delta^{(n-2)}(\pi+x) + (-1)^{n-1}\delta^{(n-4)}(\pi-x) + (-1)^n\delta^{(n-2)}(\pi-x) \\
 &\quad (n=4,5,6,\dots)
 \end{aligned}$$





# 11

## Green's function

This chapter marks the beginning of a series of chapters dealing with the solution to differential equations of theoretical physics. Very often, these differential equations are *linear*; that is, the “sought after” function  $\Psi(x)$ ,  $y(x)$ ,  $\phi(t)$  *et cetera* occur only as a polynomial of degree zero and one, and *not* of any higher degree, such as, for instance,  $[y(x)]^2$ .

### 11.1 Elegant way to solve linear differential equations

Green's functions present a very elegant way of solving linear differential equations of the form

$$\begin{aligned}\mathcal{L}_x y(x) &= f(x), \text{ with the differential operator} \\ \mathcal{L}_x &= a_n(x) \frac{d^n}{dx^n} + a_{n-1}(x) \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1(x) \frac{d}{dx} + a_0(x) \\ &= \sum_{j=0}^n a_j(x) \frac{d^j}{dx^j},\end{aligned}\tag{11.1}$$

where  $a_i(x)$ ,  $0 \leq i \leq n$  are functions of  $x$ . The idea is quite straightforward: if we are able to obtain the “inverse”  $G$  of the differential operator  $\mathcal{L}$  defined by

$$\mathcal{L}_x G(x, x') = \delta(x - x'),\tag{11.2}$$

with  $\delta$  representing Dirac's delta function, then the solution to the inhomogeneous differential equation (11.1) can be obtained by integrating  $G(x - x')$  alongside with the inhomogeneous term  $f(x')$ ; that is,

$$y(x) = \int_{-\infty}^{\infty} G(x, x') f(x') dx'.\tag{11.3}$$

This claim, as posted in Eq. (11.3), can be verified by explicitly applying the differential operator  $\mathcal{L}_x$  to the solution  $y(x)$ ,

$$\begin{aligned}
 & \mathcal{L}_x y(x) \\
 &= \mathcal{L}_x \int_{-\infty}^{\infty} G(x, x') f(x') dx' \\
 &= \int_{-\infty}^{\infty} \mathcal{L}_x G(x, x') f(x') dx' \\
 &= \int_{-\infty}^{\infty} \delta(x - x') f(x') dx' \\
 &= f(x).
 \end{aligned} \tag{11.4}$$

Let us check whether  $G(x, x') = H(x - x') \sinh(x - x')$  is a Green's function of the differential operator  $\mathcal{L}_x = \frac{d^2}{dx^2} - 1$ . In this case, all we have to do is to verify that  $\mathcal{L}_x$ , applied to  $G(x, x')$ , actually renders  $\delta(x - x')$ , as required by Eq. (11.2).

$$\begin{aligned}
 \mathcal{L}_x G(x, x') &= \delta(x - x') \\
 \left( \frac{d^2}{dx^2} - 1 \right) H(x - x') \sinh(x - x') &\stackrel{?}{=} \delta(x - x')
 \end{aligned}$$

Note that  $\frac{d}{dx} \sinh x = \cosh x$ ,  $\frac{d}{dx} \cosh x = \sinh x$ ; and hence

$$\begin{aligned}
 & \frac{d}{dx} \left( \underbrace{\delta(x - x') \sinh(x - x') + H(x - x') \cosh(x - x')}_{=0} \right) - H(x - x') \sinh(x - x') = \\
 & \delta(x - x') \cosh(x - x') + H(x - x') \sinh(x - x') - H(x - x') \sinh(x - x') = \delta(x - x').
 \end{aligned}$$

The solution (11.4) so obtained is *not unique*, as it is only a special solution to the inhomogeneous equation (11.1). The general solution to (11.1) can be found by adding the general solution  $y_0(x)$  of the corresponding *homogeneous* differential equation

$$\mathcal{L}_x y(x) = 0 \tag{11.5}$$

to one special solution – say, the one obtained in Eq. (11.4) through Green's function techniques.

Indeed, the most general solution

$$Y(x) = y(x) + y_0(x) \tag{11.6}$$

clearly is a solution of the inhomogeneous differential equation (11.4), as

$$\mathcal{L}_x Y(x) = \mathcal{L}_x y(x) + \mathcal{L}_x y_0(x) = f(x) + 0 = f(x). \tag{11.7}$$

Conversely, any two distinct special solutions  $y_1(x)$  and  $y_2(x)$  of the inhomogeneous differential equation (11.4) differ only by a function which is

a solution of the homogenous differential equation (11.5), because due to linearity of  $\mathcal{L}_x$ , their difference  $y_d(x) = y_1(x) - y_2(x)$  can be parameterized by some function in  $y_0$

$$\mathcal{L}_x[y_1(x) - y_2(x)] = \mathcal{L}_x y_1(x) + \mathcal{L}_x y_2(x) = f(x) - f(x) = 0. \quad (11.8)$$

From now on, we assume that the coefficients  $a_j(x) = a_j$  in Eq. (11.1) are constants, and thus *translational invariant*. Then the differential operator  $\mathcal{L}_x$ , as well as the entire *Ansatz* (11.2) for  $G(x, x')$ , is translation invariant, because derivatives are defined only by relative distances, and  $\delta(x - x')$  is translation invariant for the same reason. Hence,

$$G(x, x') = G(x - x'). \quad (11.9)$$

For such translation invariant systems, the Fourier analysis represents an excellent way of analyzing the situation.

Let us see why translational invariance of the coefficients  $a_j(x) = a_j(x + \xi) = a_j$  under the translation  $x \rightarrow x + \xi$  with arbitrary  $\xi$  – that is, independence of the coefficients  $a_j$  on the “coordinate” or “parameter”  $x$  – and thus of the Green's function, implies a simple form of the latter. Translational invariance of the Green's function really means

$$G(x + \xi, x' + \xi) = G(x, x'). \quad (11.10)$$

Now set  $\xi = -x'$ ; then we can define a new green's functions which just depends on one argument (instead of previously two), which is the difference of the old arguments

$$G(x - x', x' - x') = G(x - x', 0) \rightarrow G(x - x'). \quad (11.11)$$

What is important for applications is the possibility to adapt the solutions of some inhomogenous differential equation to boundary and initial value problems. In particular, a properly chosen  $G(x - x')$ , in its dependence on the parameter  $x$ , “inherits” some behaviour of the solution  $y(x)$ . Suppose, for instance, we would like to find solutions with  $y(x_i) = 0$  for some parameter values  $x_i$ ,  $i = 1, \dots, k$ . Then, the Green's function  $G$  must vanish there also

$$G(x_i - x') = 0 \text{ for } i = 1, \dots, k. \quad (11.12)$$

## 11.2 Finding Green's functions by spectral decompositions

It has been mentioned earlier (cf. Section 10.6.5 on page 161) that the  $\delta$ -function can be expressed in terms of various *eigenfunction expansions*. We shall make use of these expansions here <sup>1</sup>.

Suppose  $\psi_i(x)$  are *eigenfunctions* of the differential operator  $\mathcal{L}_x$ , and  $\lambda_i$  are the associated *eigenvalues*; that is,

$$\mathcal{L}_x \psi_i(x) = \lambda_i \psi_i(x). \quad (11.13)$$

<sup>1</sup> Dean G. Duffy. *Green's Functions with Applications*. Chapman and Hall/CRC, Boca Raton, 2001

Suppose further that  $\mathcal{L}_x$  is of degree  $n$ , and therefore (we assume without proof) that we know all (a complete set of) the  $n$  eigenfunctions  $\psi_1(x), \psi_2(x), \dots, \psi_n(x)$  of  $\mathcal{L}_x$ . In this case, orthogonality of the system of eigenfunctions holds, such that

$$\int_{-\infty}^{\infty} \psi_i(x) \overline{\psi_j(x)} dx = \delta_{ij}, \quad (11.14)$$

as well as completeness, such that,

$$\sum_{i=1}^n \psi_i(x) \overline{\psi_i(x')} = \delta(x - x'). \quad (11.15)$$

$\overline{\psi_i(x')}$  stands for the complex conjugate of  $\psi_i(x')$ . The sum in Eq. (11.15) stands for an integral in the case of continuous spectrum of  $\mathcal{L}_x$ . In this case, the Kronecker  $\delta_{ij}$  in (11.14) is replaced by the Dirac delta function  $\delta(k - k')$ . It has been mentioned earlier that the  $\delta$ -function can be expressed in terms of various *eigenfunction expansions*.

The Green's function of  $\mathcal{L}_x$  can be written as the spectral sum of the absolute squares of the eigenfunctions, divided by the eigenvalues  $\lambda_j$ ; that is,

$$G(x - x') = \sum_{j=1}^n \frac{\psi_j(x) \overline{\psi_j(x')}}{\lambda_j}. \quad (11.16)$$

For the sake of proof, apply the differential operator  $\mathcal{L}_x$  to the Green's function *Ansatz*  $G$  of Eq. (11.16) and verify that it satisfies Eq. (11.2):

$$\begin{aligned} & \mathcal{L}_x G(x - x') \\ &= \mathcal{L}_x \sum_{j=1}^n \frac{\psi_j(x) \overline{\psi_j(x')}}{\lambda_j} \\ &= \sum_{j=1}^n \frac{[\mathcal{L}_x \psi_j(x)] \overline{\psi_j(x')}}{\lambda_j} \\ &= \sum_{j=1}^n \frac{[\lambda_j \psi_j(x)] \overline{\psi_j(x')}}{\lambda_j} \\ &= \sum_{j=1}^n \psi_j(x) \overline{\psi_j(x')} \\ &= \delta(x - x'). \end{aligned} \quad (11.17)$$

For a demonstration of completeness of systems of eigenfunctions, consider, for instance, the differential equation corresponding to the harmonic vibration [please do not confuse this with the harmonic oscillator (9.29)]

$$\mathcal{L}_t \psi = \frac{d^2}{dt^2} \psi = k^2, \quad (11.18)$$

with  $k \in \mathbb{R}$ .

Without any boundary conditions the associated eigenfunctions are

$$\psi_\omega(t) = e^{-i\omega t}, \quad (11.19)$$

with  $0 \leq \omega \leq \infty$ , and with eigenvalue  $-\omega^2$ . Taking the complex conjugate and integrating over  $\omega$  yields [modulo a constant factor which depends on the choice of Fourier transform parameters; see also Eq. (10.84)]

$$\begin{aligned} & \int_{-\infty}^{\infty} \psi_{\omega}(t) \overline{\psi_{\omega}(t')} d\omega \\ &= \int_{-\infty}^{\infty} e^{-i\omega t} e^{i\omega t'} d\omega \\ &= \int_{-\infty}^{\infty} e^{-i\omega(t-t')} d\omega \\ &= \delta(t-t'). \end{aligned} \quad (11.20)$$

The associated Green's function is

$$G(t-t') = \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')}}{(-\omega^2)} d\omega. \quad (11.21)$$

The solution is obtained by integrating over the constant  $k^2$ ; that is,

$$\psi(t) = \int_{-\infty}^{\infty} G(t-t') k^2 dt' = - \int_{-\infty}^{\infty} \left( \frac{k}{\omega} \right)^2 e^{-i\omega(t-t')} d\omega dt'. \quad (11.22)$$

Note that if we are imposing boundary conditions; e.g.,  $\psi(0) = \psi(L) = 0$ , representing a string “fastened” at positions 0 and  $L$ , the eigenfunctions change to

$$\psi_k(t) = \sin(\omega_n t) = \sin\left(\frac{n\pi}{L} t\right), \quad (11.23)$$

with  $\omega_n = \frac{n\pi}{L}$  and  $n \in \mathbb{Z}$ . We can deduce orthogonality and completeness by listening to the orthogonality relations for sines (9.11).

For the sake of another example suppose, from the Euler-Bernoulli bending theory, we know (no proof is given here) that the equation for the quasistatic bending of slender, isotropic, homogeneous beams of constant cross-section under an applied transverse load  $q(x)$  is given by

$$\mathcal{L}_x y(x) = \frac{d^4}{dx^4} y(x) = q(x) \approx c, \quad (11.24)$$

with constant  $c \in \mathbb{R}$ . Let us further assume the boundary conditions

$$y(0) = y(L) = \frac{d^2}{dx^2} y(0) = \frac{d^2}{dx^2} y(L) = 0. \quad (11.25)$$

Also, we require that  $y(x)$  vanishes everywhere except inbetween 0 and  $L$ ; that is,  $y(x) = 0$  for  $x = (-\infty, 0)$  and for  $x = (L, \infty)$ . Then in accordance with these boundary conditions, the system of eigenfunctions  $\{\psi_j(x)\}$  of  $\mathcal{L}_x$  can be written as

$$\psi_j(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi j x}{L}\right) \quad (11.26)$$

for  $j = 1, 2, \dots$ . The associated eigenvalues

$$\lambda_j = \left(\frac{\pi j}{L}\right)^4$$



can be verified through explicit differentiation

$$\begin{aligned}
 \mathcal{L}_x \psi_j(x) &= \mathcal{L}_x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi j x}{L}\right) \\
 &= \mathcal{L}_x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi j x}{L}\right) \\
 &= \left(\frac{\pi j}{L}\right)^4 \sqrt{\frac{2}{L}} \sin\left(\frac{\pi j x}{L}\right) \\
 &= \left(\frac{\pi j}{L}\right)^4 \psi_j(x).
 \end{aligned} \tag{11.27}$$

The cosine functions which are also solutions of the Euler-Bernoulli equations (11.24) do not vanish at the origin  $x = 0$ .

Hence,

$$\begin{aligned}
 G(x-x')(x) &= \frac{2}{L} \sum_{j=1}^{\infty} \frac{\sin\left(\frac{\pi j x}{L}\right) \sin\left(\frac{\pi j x'}{L}\right)}{\left(\frac{\pi j}{L}\right)^4} \\
 &= \frac{2L^3}{\pi^4} \sum_{j=1}^{\infty} \frac{1}{j^4} \sin\left(\frac{\pi j x}{L}\right) \sin\left(\frac{\pi j x'}{L}\right)
 \end{aligned} \tag{11.28}$$

Finally we are in a good shape to calculate the solution explicitly by

$$\begin{aligned}
 y(x) &= \int_0^L G(x-x') g(x') dx' \\
 &\approx \int_0^L c \left[ \frac{2L^3}{\pi^4} \sum_{j=1}^{\infty} \frac{1}{j^4} \sin\left(\frac{\pi j x}{L}\right) \sin\left(\frac{\pi j x'}{L}\right) \right] dx' \\
 &\approx \frac{2cL^3}{\pi^4} \sum_{j=1}^{\infty} \frac{1}{j^4} \sin\left(\frac{\pi j x}{L}\right) \left[ \int_0^L \sin\left(\frac{\pi j x'}{L}\right) dx' \right] \\
 &\approx \frac{4cL^4}{\pi^5} \sum_{j=1}^{\infty} \frac{1}{j^5} \sin\left(\frac{\pi j x}{L}\right) \sin^2\left(\frac{\pi j}{2}\right)
 \end{aligned} \tag{11.29}$$

### 11.3 Finding Green's functions by Fourier analysis

If one is dealing with translation invariant systems of the form

$$\begin{aligned}
 \mathcal{L}_x y(x) &= f(x), \text{ with the differential operator} \\
 \mathcal{L}_x &= a_n \frac{d^n}{dx^n} + a_{n-1} \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1 \frac{d}{dx} + a_0 \\
 &= \sum_{j=0}^n a_j \frac{d^j}{dx^j},
 \end{aligned} \tag{11.30}$$

with constant coefficients  $a_j$ , then we can apply the following strategy using Fourier analysis to obtain the Green's function.

First, recall that, by Eq. (10.83) on page 160 the Fourier transform of the delta function  $\tilde{\delta}(k) = 1$  is just a constant; with our definition unity. Then,  $\delta$  can be written as

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk \quad (11.31)$$

Next, consider the Fourier transform of the Green's function

$$\tilde{G}(k) = \int_{-\infty}^{\infty} G(x) e^{-ikx} dx \quad (11.32)$$

and its back transform

$$G(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{G}(k) e^{ikx} dk. \quad (11.33)$$

Insertion of Eq. (11.33) into the Ansatz  $\mathcal{L}_x G(x - x') = \delta(x - x')$  yields

$$\begin{aligned} \mathcal{L}_x G(x) &= \mathcal{L}_x \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{G}(k) e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{G}(k) \left( \mathcal{L}_x e^{ikx} \right) dk \\ &= \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk. \end{aligned} \quad (11.34)$$

and thus, through comparison of the integral kernels,

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} [\tilde{G}(k) \mathcal{L}_x - 1] e^{ikx} dk &= 0, \\ \tilde{G}(k) \mathcal{L}_k - 1 &= 0, \\ \tilde{G}(k) &= (\mathcal{L}_k)^{-1}, \end{aligned} \quad (11.35)$$

where  $\mathcal{L}_k$  is obtained from  $\mathcal{L}_x$  by substituting every derivative  $\frac{d}{dx}$  in the latter by  $ik$  in the former. In that way, the Fourier transform  $\tilde{G}(k)$  is obtained as a polynomial of degree  $n$ , the same degree as the highest order of derivative in  $\mathcal{L}_x$ .

In order to obtain the Green's function  $G(x)$ , and to be able to integrate over it with the inhomogeneous term  $f(x)$ , we have to Fourier transform  $\tilde{G}(k)$  back to  $G(x)$ .

Then we have to make sure that the solution obeys the initial conditions, and, if necessary, we have to add solutions of the homogeneous equation  $\mathcal{L}_x G(x - x') = 0$ . That is all.

Let us consider a few examples for this procedure.

1. First, let us solve the differential operator  $y' - y = t$  on the interval  $[0, \infty)$  with the boundary conditions  $y(0) = 0$ .

We observe that the associated differential operator is given by

$$\mathcal{L}_t = \frac{d}{dt} - 1,$$

and the inhomogeneous term can be identified with  $f(t) = t$ .

We use the *Ansatz*  $G_1(t, t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}_1(k) e^{ik(t-t')} dk$ ; hence

$$\begin{aligned} \mathcal{L}_t G_1(t, t') &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}_1(k) \underbrace{\left( \frac{d}{dt} - 1 \right) e^{ik(t-t')}}_{= (ik-1)e^{ik(t-t')}} dk = \\ &= \delta(t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(t-t')} dk \end{aligned}$$

Now compare the kernels of the Fourier integrals of  $\mathcal{L}_t G_1$  and  $\delta$ :

$$\tilde{G}_1(k)(ik-1) = 1 \Rightarrow \tilde{G}_1(k) = \frac{1}{ik-1} = \frac{1}{i(k+i)}$$

$$G_1(t, t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{ik(t-t')}}{i(k+i)} dk$$

The paths in the upper and lower integration plain are drawn in Frig. 11.1.

The “closures” throught the respective half-circle paths vanish.

$$\begin{aligned} \text{residuum theorem: } G_1(t, t') &= 0 \quad \text{for } t > t' \\ G_1(t, t') &= -2\pi i \operatorname{Res} \left( \frac{1}{2\pi i} \frac{e^{ik(t-t')}}{(k+i)}; -i \right) = \\ &= -e^{t-t'} \quad \text{for } t < t'. \end{aligned}$$

Hence we obtain a Green's function for the inhomogeneous differential equation

$$G_1(t, t') = -H(t' - t)e^{t-t'}$$

However, this Green's function and its associated (special) solution does not obey the boundary conditions  $G_1(0, t') = -H(t')e^{-t'} \neq 0$  for  $t' \in [0, \infty)$ .

Therefore, we have to fit the Green's function by adding an appropriately weighted solution to the homogenous differential equation. The homogenous Green's function is found by

$$\mathcal{L}_t G_0(t, t') = 0,$$

and thus, in particular,

$$\frac{d}{dt} G_0 = G_0 \Rightarrow G_0 = ae^{t-t'}.$$

with the *Ansatz*

$$G(0, t') = G_1(0, t') + G_0(0, t'; a) = -H(t')e^{-t'} + ae^{-t'}$$

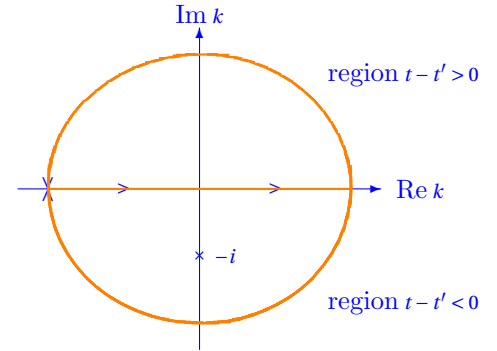


Figure 11.1: Plot of the two paths required for solving the Fourier integral.

for the general solution we can choose the constant coefficient  $a$  so that

$$G(0, t') = G_1(0, t') + G_0(0, t'; a) = -H(t')e^{-t'} + ae^{-t'} = 0$$

For  $a = 1$ , the Green's function and thus the solution obeys the boundary value conditions; that is,

$$G(t, t') = [1 - H(t' - t)]e^{t-t'}.$$

Since  $H(-x) = 1 - H(x)$ ,  $G(t, t')$  can be rewritten as

$$G(t, t') = H(t - t')e^{t-t'}.$$

In the final step we obtain the solution through integration of  $G$  over the inhomogeneous term  $t$ :

$$\begin{aligned} y(t) &= \int_0^\infty \underbrace{H(t-t')}_{=1 \text{ for } t' < t} e^{t-t'} t' dt' = \\ &= \int_0^t e^{t-t'} t' dt' = e^t \int_0^t t' e^{-t'} dt' = \\ &= e^t \left( -t' e^{-t'} \Big|_0^t - \int_0^t (-e^{-t'}) dt' \right) = \\ &= e^t \left[ (-te^{-t}) - e^{-t} \Big|_0^t \right] = e^t (-te^{-t} - e^{-t} + 1) = e^t - 1 - t. \end{aligned}$$

2. Next, let us solve the differential equation  $\frac{d^2 y}{dt^2} + y = \cos t$  on the interval  $t \in [0, \infty)$  with the boundary conditions  $y(0) = y'(0) = 0$ .

First, observe that

$$\mathcal{L} = \frac{d^2}{dt^2} + 1.$$

The Fourier *Ansatz* for the Green's function is

$$\begin{aligned} G_1(t, t') &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}(k) e^{ik(t-t')} dk \\ \mathcal{L} G_1 &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}(k) \left( \frac{d^2}{dt^2} + 1 \right) e^{ik(t-t')} dk = \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}(k) ((ik)^2 + 1) e^{ik(t-t')} dk = \\ &= \delta(t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ik(t-t')} dk = \end{aligned}$$

Hence

$$\tilde{G}(k)(1 - k^2) = 1$$

ant thus

$$\tilde{G}(k) = \frac{1}{(1-k^2)} = \frac{-1}{(k+1)(k-1)}$$

The Fourier transformation is

$$\begin{aligned} G_1(t, t') &= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{ik(t-t')}}{(k+1)(k-1)} dk = \\ &= -\frac{1}{2\pi} 2\pi i \left[ \operatorname{Res} \left( \frac{e^{ik(t-t')}}{(k+1)(k-1)}; k=1 \right) + \right. \\ &\quad \left. \operatorname{Res} \left( \frac{e^{ik(t-t')}}{(k+1)(k-1)}; k=-1 \right) \right] H(t-t') \end{aligned}$$

The path in the upper integration plain is drawn in Fig. 11.2.

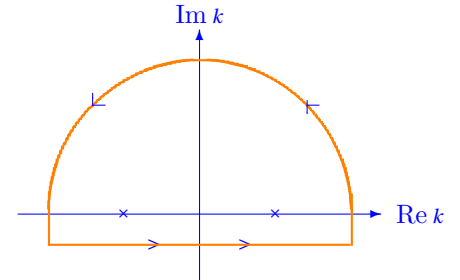


Figure 11.2: Plot of the path required for solving the Fourier integral.

$$\begin{aligned} G_1(t, t') &= -\frac{i}{2} \left( e^{i(t-t')} - e^{-i(t-t')} \right) H(t-t') = \\ &= \frac{e^{i(t-t')} - e^{-i(t-t')}}{2i} H(t-t') = \sin(t-t') H(t-t') \\ G_1(0, t') &= \sin(-t') H(-t') = 0 \quad \text{since } t' > 0 \\ G'_1(t, t') &= \cos(t-t') H(t-t') + \underbrace{\sin(t-t') \delta(t-t')}_{=0} \\ G'_1(0, t') &= \cos(-t') H(-t') = 0 \quad \text{as before.} \end{aligned}$$

$G_1$  already satisfies the boundary conditions; hence we do not need to find the Green's function  $G_0$  of the homogenous equation.

$$\begin{aligned} y(t) &= \int_0^\infty G(t, t') f(t') dt' = \int_0^\infty \sin(t-t') \underbrace{H(t-t')}_{=1 \text{ for } t > t'} \cos t' dt' = \\ &= \int_0^t \sin(t-t') \cos t' dt' = \int_0^t (\sin t \cos t' - \cos t \sin t') \cos t' dt' = \\ &= \int_0^t [\sin t (\cos t')^2 - \cos t \sin t' \cos t'] dt' = \\ &= \sin t \int_0^t (\cos t')^2 dt' - \cos t \int_0^t \sin t' \cos t' dt' = \\ &= \sin t \left[ \frac{1}{2} (t' + \sin t' \cos t') \right]_0^t - \cos t \left[ \frac{\sin^2 t'}{2} \right]_0^t = \\ &= \frac{t \sin t}{2} + \frac{\sin^2 t \cos t}{2} - \frac{\cos t \sin^2 t}{2} = \frac{t \sin t}{2}. \end{aligned}$$



*Part IV:*

*Differential equations*



# 12

## *Sturm-Liouville theory*

This is only a very brief “dive into Sturm-Liouville theory,” which has many fascinating aspects and connections to Fourier analysis, the special functions of mathematical physics, operator theory, and linear algebra<sup>1</sup>. In physics, many formalizations involve second order differential equations, which, in their most general form, can be written as<sup>2</sup>

$$\mathcal{L}_x y(x) = a_0(x)y(x) + a_1(x)\frac{d}{dx}y(x) + a_2(x)\frac{d^2}{dx^2}y(x) = f(x). \quad (12.1)$$

The differential operator is defined by

$$\mathcal{L}_x = a_0(x) + a_1(x)\frac{d}{dx} + a_2(x)\frac{d^2}{dx^2}. \quad (12.2)$$

The solutions  $y(x)$  are often subject to boundary conditions of various forms.

*Dirichlet boundary conditions* are of the form  $y(a) = y(b) = 0$  for some  $a, b$ .

*Neumann boundary conditions* are of the form  $y'(a) = y'(b) = 0$  for some  $a, b$ .

*Periodic boundary conditions* are of the form  $y(a) = y(b)$  and  $y'(a) = y'(b)$  for some  $a, b$ .

### 12.1 *Sturm-Liouville form*

Any second order differential equation of the general form (12.1) can be rewritten into a differential equation of the *Sturm-Liouville form*

$$\begin{aligned} \mathcal{L}_x y(x) &= \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] y(x) + q(x)y(x) = F(x), \\ &\text{with } p(x) = e^{\int \frac{a_1(x)}{a_2(x)} dx}, \\ q(x) &= p(x) \frac{a_0(x)}{a_2(x)} = \frac{a_0(x)}{a_2(x)} e^{\int \frac{a_1(x)}{a_2(x)} dx}, \\ F(x) &= p(x) \frac{f(x)}{a_2(x)} = \frac{f(x)}{a_2(x)} e^{\int \frac{a_1(x)}{a_2(x)} dx} \end{aligned} \quad (12.3)$$

<sup>1</sup> Garrett Birkhoff and Gian-Carlo Rota. *Ordinary Differential Equations*. John Wiley & Sons, New York, Chichester, Brisbane, Toronto, fourth edition, 1959, 1960, 1962, 1969, 1978, and 1989; M. A. Al-Gwaiz. *Sturm-Liouville Theory and its Applications*. Springer, London, 2008; and William Norrie Everitt. A catalogue of Sturm-Liouville differential equations. In Werner O. Amrein, Andreas M. Hinz, and David B. Pearson, editors, *Sturm-Liouville Theory, Past and Present*, pages 271–331. Birkhäuser Verlag, Basel, 2005. URL <http://www.math.niu.edu/SL2/papers/birk0.pdf>

<sup>2</sup> Russell Herman. *A Second Course in Ordinary Differential Equations: Dynamical Systems and Boundary Value Problems*. University of North Carolina Wilmington, Wilmington, NC, 2008. URL [http://people.uncw.edu/hermanr/mat463/ODEBook/Book/ODE\\_LargeFont.pdf](http://people.uncw.edu/hermanr/mat463/ODEBook/Book/ODE_LargeFont.pdf). Creative Commons Attribution-NoncommercialShare Alike 3.0 United States License



The associated differential operator

$$\begin{aligned}\mathcal{S}_x &= \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] + q(x) \\ &= p(x) \frac{d^2}{dx^2} + p'(x) \frac{d}{dx} + q(x)\end{aligned}\tag{12.4}$$

is called *Sturm-Liouville differential operator*.

For a proof, we insert  $p(x)$ ,  $q(x)$  and  $F(x)$  into the Sturm-Liouville form of Eq. (12.3) and compare it with Eq. (12.1).

$$\begin{aligned}\left\{ \frac{d}{dx} \left[ e^{\int \frac{a_1(x)}{a_2(x)} dx} \frac{d}{dx} \right] + \frac{a_0(x)}{a_2(x)} e^{\int \frac{a_1(x)}{a_2(x)} dx} \right\} y(x) &= \frac{f(x)}{a_2(x)} e^{\int \frac{a_1(x)}{a_2(x)} dx} \\ e^{\int \frac{a_1(x)}{a_2(x)} dx} \left\{ \frac{d^2}{dx^2} + \frac{a_1(x)}{a_2(x)} \frac{d}{dx} + \frac{a_0(x)}{a_2(x)} \right\} y(x) &= \frac{f(x)}{a_2(x)} e^{\int \frac{a_1(x)}{a_2(x)} dx} \\ \left\{ a_2(x) \frac{d^2}{dx^2} + a_1(x) \frac{d}{dx} + a_0(x) \right\} y(x) &= f(x).\end{aligned}\tag{12.5}$$

## 12.2 Sturm-Liouville eigenvalue problem

The Sturm-Liouville eigenvalue problem is given by the differential equation

$$\begin{aligned}\mathcal{S}_x \phi(x) &= -\lambda \rho(x) \phi(x), \text{ or} \\ \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] \phi(x) + [q(x) + \lambda \rho(x)] \phi(x) &= 0\end{aligned}\tag{12.6}$$

for  $x \in (a, b)$  and continuous  $p(x) > 0$ ,  $p'(x)$ ,  $q(x)$  and  $\rho(x) > 0$ .

We mention without proof (for proofs, see, for instance, Ref. <sup>3</sup>) that

- the eigenvalues  $\lambda$  turn out to be real, countable, and ordered, and that there is a smallest eigenvalue  $\lambda_1$  such that  $\lambda_1 < \lambda_2 < \lambda_3 < \dots$ ;
- for each eigenvalue  $\lambda_j$  there exists an eigenfunction  $\phi_j(x)$  with  $j - 1$  zeroes on  $(a, b)$ ;
- eigenfunctions corresponding to different eigenvalues are *orthogonal*, and can be normalized, with respect to the weight function  $\rho(x)$ ; that is,

$$\langle \phi_j | \phi_k \rangle = \int_a^b \phi_j(x) \phi_k(x) \rho(x) dx = \delta_{jk}\tag{12.7}$$

- the set of eigenfunctions is *complete*; that is, any piecewise smooth function can be represented by

$$\begin{aligned}f(x) &= \sum_{k=1}^{\infty} c_k \phi_k(x), \\ &\text{with} \\ c_k &= \frac{\langle f | \phi_k \rangle}{\langle \phi_k | \phi_k \rangle} = \langle f | \phi_k \rangle.\end{aligned}\tag{12.8}$$

<sup>3</sup> M. A. Al-Gwaiz. *Sturm-Liouville Theory and its Applications*. Springer, London, 2008

- the orthonormal (with respect to the weight  $\rho$ ) set  $\{\phi_j(x) \mid j \in \mathbb{N}\}$  is a *basis* of a Hilbert space with the inner product

$$\langle f \mid g \rangle = \int_a^b f(x)g(x)\rho(x)dx. \quad (12.9)$$

### 12.3 Adjoint and self-adjoint operators

In operator theory, just as in matrix theory, we can define an *adjoint operator* via the scalar product defined in Eq. (12.9). In this formalization, the Sturm-Liouville differential operator  $\mathcal{L}$  is self-adjoint.

Let us first define the *domain* of a differential operator  $\mathcal{L}$  as the set of all square integrable (with respect to the weight  $\rho(x)$ ) functions  $\varphi$  satisfying boundary conditions.

$$\int_a^b |\varphi(x)|^2 \rho(x) dx < \infty. \quad (12.10)$$

Then, the adjoint operator  $\mathcal{L}^\dagger$  is defined by satisfying

$$\begin{aligned} \langle \psi \mid \mathcal{L}\varphi \rangle &= \int_a^b \psi(x) [\mathcal{L}\varphi(x)] \rho(x) dx \\ &= \langle \mathcal{L}^\dagger \psi \mid \varphi \rangle = \int_a^b [\mathcal{L}^\dagger \psi(x)] \varphi(x) \rho(x) dx \end{aligned} \quad (12.11)$$

for all  $\psi(x)$  in the domain of  $\mathcal{L}^\dagger$  and  $\varphi(x)$  in the domain of  $\mathcal{L}$ .

Note that in the case of second order differential operators in the standard form (12.2) and with  $\rho(x) = 1$ , we can move the differential quotients and the entire differential operator in

$$\begin{aligned} \langle \psi \mid \mathcal{L}\varphi \rangle &= \int_a^b \psi(x) [\mathcal{L}_x \varphi(x)] \rho(x) dx \\ &= \int_a^b \psi(x) [a_2(x)\varphi''(x) + a_1(x)\varphi'(x) + a_0(x)\varphi(x)] dx \end{aligned} \quad (12.12)$$

from  $\varphi$  to  $\psi$  by one and two partial integrations.

Integrating the kernel  $a_1(x)\varphi'(x)$  by parts yields

$$\int_a^b \psi(x) a_1(x) \varphi'(x) dx = \psi(x) a_1(x) \varphi(x) \Big|_a^b - \int_a^b (\psi(x) a_1(x))' \varphi(x) dx. \quad (12.13)$$

Integrating the kernel  $a_2(x)\varphi''(x)$  by parts twice yields

$$\begin{aligned} \int_a^b \psi(x) a_2(x) \varphi''(x) dx &= \psi(x) a_2(x) \varphi'(x) \Big|_a^b - \int_a^b (\psi(x) a_2(x))' \varphi'(x) dx \\ &= \psi(x) a_2(x) \varphi'(x) \Big|_a^b - (\psi(x) a_2(x))' \varphi(x) \Big|_a^b + \int_a^b (\psi(x) a_2(x))'' \varphi(x) dx \\ &= \psi(x) a_2(x) \varphi'(x) - (\psi(x) a_2(x))' \varphi(x) \Big|_a^b + \int_a^b (\psi(x) a_2(x))'' \varphi(x) dx. \end{aligned} \quad (12.14)$$

Combining these two calculations yields

$$\begin{aligned}
 \langle \psi | \mathcal{L} \varphi \rangle &= \int_a^b \psi(x) [\mathcal{L}_x \varphi(x)] \rho(x) dx \\
 &= \int_a^b \psi(x) [a_2(x) \varphi''(x) + a_1(x) \varphi'(x) + a_0(x) \varphi(x)] dx \\
 &= \psi(x) a_1(x) \varphi(x) + \psi(x) a_2(x) \varphi'(x) - (\psi(x) a_2(x))' \varphi(x) \Big|_a^b \\
 &\quad + \int_a^b [(a_2(x) \psi(x))'' - (a_1(x) \psi(x))' + a_0(x) \psi(x)] \varphi(x) dx.
 \end{aligned} \tag{12.15}$$

If the terms with no integral vanish (because of boundary conditions or other reasons); that is, if

$$\psi(x) a_1(x) \varphi(x) + \psi(x) a_2(x) \varphi'(x) - (\psi(x) a_2(x))' \varphi(x) \Big|_a^b = 0,$$

then Eq. (12.15) reduces to

$$\langle \psi | \mathcal{L} \varphi \rangle = \int_a^b [(a_2(x) \psi(x))'' - (a_1(x) \psi(x))' + a_0(x) \psi(x)] \varphi(x) dx, \tag{12.16}$$

and we can identify the adjoint differential operator  $\mathcal{L}_x^\dagger$  with

$$\begin{aligned}
 \mathcal{L}_x^\dagger &= \frac{d^2}{dx^2} a_2(x) - \frac{d}{dx} a_1(x) + a_0(x) \\
 &= \frac{d}{dx} \left[ a_2(x) \frac{d}{dx} + a_2'(x) \right] - a_1'(x) - a_1(x) \frac{d}{dx} + a_0(x) \\
 &= a_2'(x) \frac{d}{dx} + a_2(x) \frac{d^2}{dx^2} + a_2''(x) + a_2'(x) \frac{d}{dx} - a_1'(x) - a_1(x) \frac{d}{dx} + a_0(x) \\
 &= a_2(x) \frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)] \frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x).
 \end{aligned} \tag{12.17}$$

If

$$\mathcal{L}_x^\dagger = \mathcal{L}_x, \tag{12.18}$$

the operator  $\mathcal{L}_x$  is called self-adjoint.

In order to prove that the Sturm-Liouville differential operator

$$\mathcal{S} = \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] + q(x) = p(x) \frac{d^2}{dx^2} + p'(x) \frac{d}{dx} + q(x) \tag{12.19}$$

from Eq. (12.4) is self-adjoint, we verify Eq. (12.17) with  $\mathcal{S}^\dagger$  taken from Eq. (12.16). Thereby, we identify  $a_2(x) = p(x)$ ,  $a_1(x) = p'(x)$ , and  $a_0(x) = q(x)$ ; hence

$$\begin{aligned}
 \mathcal{S}_x^\dagger &= a_2(x) \frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)] \frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x) \\
 &= p(x) \frac{d^2}{dx^2} + [2p'(x) - p'(x)] \frac{d}{dx} + p''(x) - p''(x) + q(x) \\
 &= p(x) \frac{d^2}{dx^2} + p'(x) \frac{d}{dx} q(x) \\
 &= \mathcal{S}_x.
 \end{aligned} \tag{12.20}$$

Alternatively we could argue from Eqs. (12.17) and (12.18), noting that a differential operator is self-adjoint if and only if

$$\begin{aligned}\mathcal{L}_x^\dagger &= a_2(x) \frac{d^2}{dx^2} - a_1(x) \frac{d}{dx} + a_0(x) \\ &= \mathcal{L}_x^\dagger = a_2(x) \frac{d^2}{dx^2} + [2a_2'(x) - a_1(x)] \frac{d}{dx} + a_2''(x) - a_1'(x) + a_0(x).\end{aligned}\quad (12.21)$$

By comparison of the coefficients,

$$\begin{aligned}a_2(x) &= a_2(x), \\ a_1(x) &= 2a_2'(x) - a_1(x), \\ a_0(x) &= a_2''(x) - a_1'(x) + a_0(x),\end{aligned}\quad (12.22)$$

and hence,

$$a_2'(x) = a_1(x), \quad (12.23)$$

which is exactly the form of the Sturm-Liouville differential operator.

#### 12.4 Sturm-Liouville transformation into Liouville normal form

Let, for  $x \in [a, b]$ ,

$$\begin{aligned}[\mathcal{S}_x + \lambda \rho(x)]y(x) &= 0, \\ \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] y(x) + [q(x) + \lambda \rho(x)]y(x) &= 0, \\ \left[ p(x) \frac{d^2}{dx^2} + p'(x) \frac{d}{dx} + q(x) + \lambda \rho(x) \right] y(x) &= 0, \\ \left[ \frac{d^2}{dx^2} + \frac{p'(x)}{p(x)} \frac{d}{dx} + \frac{q(x) + \lambda \rho(x)}{p(x)} \right] y(x) &= 0\end{aligned}\quad (12.24)$$

be a second order differential equation of the Sturm-Liouville form<sup>4</sup>.

This equation (12.24) can be written in the *Liouville normal form* containing no first order differentiation term

$$-\frac{d^2}{dt^2} w(t) + [\hat{q}(t) - \lambda] w(t) = 0, \text{ with } t \in [t(a), t(b)]. \quad (12.25)$$

It is obtained *via* the *Sturm-Liouville transformation*

$$\begin{aligned}\xi &= t(x) = \int_a^x \sqrt{\frac{\rho(s)}{p(s)}} ds, \\ w(t) &= \sqrt[4]{p(x(t))\rho(x(t))} y(x(t)),\end{aligned}\quad (12.26)$$

where

$$\hat{q}(t) = \frac{1}{\rho} \left[ -q - \sqrt[4]{p\rho} \left( p \left( \frac{1}{\sqrt[4]{p\rho}} \right)' \right)' \right]. \quad (12.27)$$

The apostrophe represents derivation with respect to  $x$ .

<sup>4</sup> Garrett Birkhoff and Gian-Carlo Rota. *Ordinary Differential Equations*. John Wiley & Sons, New York, Chichester, Brisbane, Toronto, fourth edition, 1959, 1960, 1962, 1969, 1978, and 1989

For the sake of an example, suppose we want to know the normalized eigenfunctions of

$$x^2 y'' + 3xy' + y = -\lambda y, \text{ with } x \in [1, 2] \quad (12.28)$$

with the boundary conditions  $y(1) = y(2) = 0$ .

The first thing we have to do is to transform this differential equation into its Sturm-Liouville form by identifying  $a_2(x) = x^2$ ,  $a_1(x) = 3x$ ,  $a_0 = 1$ ,  $\rho = 1$  such that  $f(x) = -\lambda y(x)$ ; and hence

$$p(x) = e^{\int \frac{3x}{x^2} dx} = e^{\int \frac{3}{x} dx} = e^{3 \log x} = x^3, \quad (12.29)$$

$$q(x) = p(x) \frac{1}{x^2} = x,$$

$$F(x) = p(x) \frac{\lambda y}{(-x^2)} = -\lambda xy, \text{ and hence } \rho(x) = x.$$

As a result we obtain the Sturm-Liouville form

$$\frac{1}{x} ((x^3 y')' + xy) = -\lambda y. \quad (12.30)$$

In the next step we apply the Sturm-Liouville transformation

$$\xi = t(x) = \int \sqrt{\frac{\rho(x)}{p(x)}} dx = \int \frac{dx}{x} = \log x,$$

$$w(t(x)) = \sqrt[4]{p(x(t))\rho(x(t))} y(x(t)) = \sqrt[4]{x^4} y(x(t)) = xy, \quad (12.31)$$

$$\hat{q}(t) = \frac{1}{x} \left[ -x - \sqrt[4]{x^4} \left( x^3 \left( \frac{1}{\sqrt[4]{x^4}} \right)' \right)' \right] = 0.$$

We now take the Ansatz  $y = \frac{1}{x} w(t(x)) = \frac{1}{x} w(\log x)$  and finally obtain the Liouville normal form

$$-w'' = \lambda w. \quad (12.32)$$

As an *Ansatz* for solving the Liouville normal form we use

$$w(\xi) = a \sin(\sqrt{\lambda} \xi) + b \cos(\sqrt{\lambda} \xi) \quad (12.33)$$

The boundary conditions translate into  $x = 1 \rightarrow \xi = 0$ , and  $x = 2 \rightarrow \xi = \log 2$ . From  $w(0) = 0$  we obtain  $b = 0$ . From  $w(\log 2) = a \sin(\sqrt{\lambda} \log 2) = 0$  we obtain  $\sqrt{\lambda_n} \log 2 = n\pi$ .

Thus the eigenvalues are

$$\lambda_n = \left( \frac{n\pi}{\log 2} \right)^2. \quad (12.34)$$

The associated eigenfunctions are

$$w_n(\xi) = a \sin \left[ \frac{n\pi}{\log 2} \xi \right], \quad (12.35)$$

and thus

$$y_n = \frac{1}{x} a \sin \left[ \frac{n\pi}{\log 2} \log x \right]. \quad (12.36)$$

We can check that they are orthonormal by inserting into Eq. (12.7) and verifying it; that is,

$$\int_1^2 \rho(x) y_n(x) y_m(x) dx = \delta_{nm}; \quad (12.37)$$

more explicitly,

$$\begin{aligned} & \int_1^2 dx x \left( \frac{1}{x^2} \right) a^2 \sin \left( n\pi \frac{\log x}{\log 2} \right) \sin \left( m\pi \frac{\log x}{\log 2} \right) \\ & \quad [\text{variable substitution } u = \frac{\log x}{\log 2} \\ & \quad \frac{du}{dx} = \frac{1}{\log 2} \frac{1}{x}, u = \frac{dx}{x \log 2}] \\ & = \int_{u=0}^{u=1} du \log 2 a^2 \sin(n\pi u) \sin(m\pi u) \\ & = \underbrace{a^2 \left( \frac{\log 2}{2} \right)}_{=1} \underbrace{2 \int_0^1 du \sin(n\pi u) \sin(m\pi u)}_{=\delta_{nm}} \\ & = \delta_{nm}. \end{aligned} \quad (12.38)$$

Finally, with  $a = \sqrt{\frac{2}{\log 2}}$  we obtain the solution

$$y_n = \sqrt{\frac{2}{\log 2}} \frac{1}{x} \sin \left( n\pi \frac{\log x}{\log 2} \right). \quad (12.39)$$

## 12.5 Varieties of Sturm-Liouville differential equations

A catalogue of Sturm-Liouville differential equations comprises the following *species*, among many others<sup>5</sup>. Some of these cases are tabellated as functions  $p$ ,  $q$ ,  $\lambda$  and  $\rho$  appearing in the general form of the Sturm-Liouville eigenvalue problem (12.6)

$$\begin{aligned} & \mathcal{L}_x \phi(x) = -\lambda \rho(x) \phi(x), \text{ or} \\ & \frac{d}{dx} \left[ p(x) \frac{d}{dx} \right] \phi(x) + [q(x) + \lambda \rho(x)] \phi(x) = 0 \end{aligned} \quad (12.40)$$

in Table 12.1.



<sup>5</sup> George B. Arfken and Hans J. Weber. *Mathematical Methods for Physicists*. Elsevier, Oxford, 6th edition, 2005. ISBN 0-12-059876-0; 0-12-088584-0; M. A. Al-Gwaiz. *Sturm-Liouville Theory and its Applications*. Springer, London, 2008; and William Norrie Everitt. A catalogue of Sturm-Liouville differential equations. In Werner O. Amrein, Andreas M. Hinz, and David B. Pearson, editors, *Sturm-Liouville Theory, Past and Present*, pages 271–331. Birkhäuser Verlag, Basel, 2005. URL <http://www.math.niu.edu/SL2/papers/birk0.pdf>

Equation	$p(x)$	$q(x)$	$-\lambda$	$\rho(x)$
Hypergeometric	$x^{\alpha+1}(1-x)^{\beta+1}$	0	$\mu$	$x^\alpha(1-x)^\beta$
Legendre	$1-x^2$	0	$l(l+1)$	1
Shifted Legendre	$x(1-x)$	0	$l(l+1)$	1
Associated Legendre	$1-x^2$	$-\frac{m^2}{1-x^2}$	$l(l+1)$	1
Chebyshev I	$\sqrt{1-x^2}$	0	$n^2$	$\frac{1}{\sqrt{1-x^2}}$
Shifted Chebyshev I	$\sqrt{x(1-x)}$	0	$n^2$	$\frac{1}{\sqrt{x(1-x)}}$
Chebyshev II	$(1-x^2)^{\frac{3}{2}}$	0	$n(n+2)$	$\sqrt{1-x^2}$
Ultraspherical (Gegenbauer)	$(1-x^2)^{\alpha+\frac{1}{2}}$	0	$n(n+2\alpha)$	$(1-x^2)^{\alpha-\frac{1}{2}}$
Bessel	$x$	$-\frac{n^2}{x}$	$a^2$	$x$
Laguerre	$xe^{-x}$	0	$\alpha$	$e^{-x}$
Associated Laguerre	$x^{k+1}e^{-x}$	0	$\alpha-k$	$x^k e^{-x}$
Hermite	$xe^{-x^2}$	0	$2\alpha$	$e^{-x}$
Fourier (harmonic oscillator)	1	0	$k^2$	1
Schrödinger (hydrogen atom)	1	$l(l+1)x^{-2}$	$\mu$	1

Table 12.1: Some varieties of differential equations expressible as Sturm-Liouville differential equations

## Separation of variables

This chapter deals with the ancient alchemic suspicion of “*solve et coagula*” that it is possible to solve a problem by splitting it up into partial problems, solving these issues separately; and consecutively joining together the partial solutions, thereby yielding the full answer to the problem – translated into the context of *partial differential equations*; that is, equations with derivatives of more than one variable. Thereby, solving the separate partial problems is not dissimilar to applying subprograms from some program library.

Already Descartes mentioned this sort of method in his *Discours de la méthode pour bien conduire sa raison et chercher la vérité dans les sciences* (English translation: *Discourse on the Method of Rightly Conducting One's Reason and of Seeking Truth*)<sup>1</sup> stating that (in a newer translation<sup>2</sup>)

*[Rule Five:] The whole method consists entirely in the ordering and arranging of the objects on which we must concentrate our mind's eye if we are to discover some truth. We shall be following this method exactly if we first reduce complicated and obscure propositions step by step to simpler ones, and then, starting with the intuition of the simplest ones of all, try to ascend through the same steps to a knowledge of all the rest. [Rule Thirteen:] If we perfectly understand a problem we must abstract it from every superfluous conception, reduce it to its simplest terms and, by means of an enumeration, divide it up into the smallest possible parts.*

The method of separation of variables is one among a couple of strategies to solve differential equations<sup>3</sup>, and it is a very important one in physics.

Separation of variables can be applied whenever we have no “mixtures of derivatives and functional dependencies;” more specifically, whenever the partial differential equation can be written as a sum

$$\begin{aligned}\mathcal{L}_{x,y}\psi(x,y) &= (\mathcal{L}_x + \mathcal{L}_y)\psi(x,y) = 0, \text{ or} \\ \mathcal{L}_x\psi(x,y) &= -\mathcal{L}_y\psi(x,y).\end{aligned}\tag{13.1}$$

Because in this case we may make a *multiplicative Ansatz*

$$\psi(x,y) = v(x)u(y).\tag{13.2}$$

For a counterexample see the Kochen-Specker theorem on page 80.

<sup>1</sup> Rene Descartes. *Discours de la méthode pour bien conduire sa raison et chercher la vérité dans les sciences* (*Discourse on the Method of Rightly Conducting One's Reason and of Seeking Truth*). 1637. URL <http://www.gutenberg.org/etext/59>

<sup>2</sup> Rene Descartes. *The Philosophical Writings of Descartes. Volume 1*. Cambridge University Press, Cambridge, 1985. translated by John Cottingham, Robert Stoothoff and Dugald Murdoch

<sup>3</sup> Lawrence C. Evans. *Partial differential equations. Graduate Studies in Mathematics, volume 19*. American Mathematical Society, Providence, Rhode Island, 1998; and Klaus Jänich. *Analysis für Physiker und Ingenieure. Funktionen-theorie, Differentialgleichungen, Spezielle Funktionen*. Springer, Berlin, Heidelberg, fourth edition, 2001. URL <http://www.springer.com/mathematics/analysis/book/978-3-540-41985-3>



Inserting (13.2) into (13) effectively separates the variable dependencies

$$\begin{aligned}\mathcal{L}_x v(x)u(y) &= -\mathcal{L}_y v(x)u(y), \\ u(y) [\mathcal{L}_x v(x)] &= -v(x) [\mathcal{L}_y u(y)], \\ \frac{1}{v(x)} \mathcal{L}_x v(x) &= -\frac{1}{u(y)} \mathcal{L}_y u(y) = a,\end{aligned}\tag{13.3}$$

with constant  $a$ , because  $\frac{\mathcal{L}_x v(x)}{v(x)}$  does not depend on  $x$ , and  $\frac{\mathcal{L}_y u(y)}{u(y)}$  does not depend on  $y$ . Therefore, neither side depends on  $x$  or  $y$ ; hence both sides are constants.

As a result, we can treat and integrate both sides separately; that is,

$$\begin{aligned}\frac{1}{v(x)} \mathcal{L}_x v(x) &= a, \\ \frac{1}{u(y)} \mathcal{L}_y u(y) &= -a,\end{aligned}\tag{13.4}$$

or

$$\begin{aligned}\mathcal{L}_x v(x) - av(x) &= 0, \\ \mathcal{L}_y u(y) + au(y) &= 0.\end{aligned}\tag{13.5}$$

This separation of variable *Ansatz* can be often used when the *Laplace operator*  $\Delta = \nabla \cdot \nabla$  is involved, since there the partial derivatives with respect to different variables occur in different summands.

The general solution is a linear combination (superposition) of the products of all the linear independent solutions – that is, the sum of the products of all separate (linear independent) solutions, weighted by an arbitrary scalar factor.

For the sake of demonstration, let us consider a few examples.

#### 1. Let us separate the homogenous Laplace differential equation

$$\Delta \Phi = \frac{1}{u^2 + v^2} \left( \frac{\partial^2 \Phi}{\partial u^2} + \frac{\partial^2 \Phi}{\partial v^2} \right) + \frac{\partial^2 \Phi}{\partial z^2} = 0\tag{13.6}$$

in parabolic cylinder coordinates  $(u, v, z)$  with  $\mathbf{x} = (\frac{1}{2}(u^2 - v^2), uv, z)$ .

The separation of variables *Ansatz* is

$$\Phi(u, v, z) = \Phi_1(u)\Phi_2(v)\Phi_3(z).$$

Then,

$$\begin{aligned}\frac{1}{u^2 + v^2} \left( \Phi_2 \Phi_3 \frac{\partial^2 \Phi_1}{\partial u^2} + \Phi_1 \Phi_3 \frac{\partial^2 \Phi_2}{\partial v^2} \right) + \Phi_1 \Phi_2 \frac{\partial^2 \Phi_3}{\partial z^2} &= 0 \\ \frac{1}{u^2 + v^2} \left( \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} \right) &= -\frac{\Phi_3''}{\Phi_3} = \lambda = \text{const.}\end{aligned}$$

$\lambda$  is constant because it does neither depend on  $u, v$  [because of the right hand side  $\Phi_3''(z)/\Phi_3(z)$ ], nor on  $z$  (because of the left hand side).

Furthermore,

$$\frac{\Phi_1''}{\Phi_1} - \lambda u^2 = -\frac{\Phi_2''}{\Phi_2} + \lambda v^2 = l^2 = \text{const.}$$

If we would just consider a single product of all general one parameter solutions we would run into the same problem as in the entangled case on page 37 – we could not cover all the solutions of the original equation.

with constant  $l$  for analogous reasons. The three resulting differential equations are

$$\begin{aligned}\Phi_1'' - (\lambda u^2 + l^2)\Phi_1 &= 0, \\ \Phi_2'' - (\lambda v^2 - l^2)\Phi_2 &= 0, \\ \Phi_3'' + \lambda\Phi_3 &= 0.\end{aligned}$$

2. Let us separate the homogenous (i) Laplace, (ii) wave, and (iii) diffusion equations, in elliptic cylinder coordinates  $(u, v, z)$  with  $\vec{x} = (a \cosh u \cos v, a \sinh u \sin v, z)$  and

$$\Delta = \frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left[ \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right] + \frac{\partial^2}{\partial z^2}.$$

*ad (i):*

Again the separation of variables *Ansatz* is  $\Phi(u, v, z) = \Phi_1(u)\Phi_2(v)\Phi_3(z)$ . Hence,

$$\begin{aligned}\frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \Phi_2\Phi_3 \frac{\partial^2 \Phi_1}{\partial u^2} + \Phi_1\Phi_3 \frac{\partial^2 \Phi_2}{\partial v^2} \right) &= -\Phi_1\Phi_2 \frac{\partial^2 \Phi}{\partial z^2}, \\ \frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} \right) &= -\frac{\Phi_3''}{\Phi_3} = k^2 = \text{const.} \implies \Phi_3'' + k^2\Phi_3 = 0 \\ \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} &= k^2 a^2 (\sinh^2 u + \sin^2 v), \\ \frac{\Phi_1''}{\Phi_1} - k^2 a^2 \sinh^2 u &= -\frac{\Phi_2''}{\Phi_2} + k^2 a^2 \sin^2 v = l^2, \\ &\quad (13.7)\end{aligned}$$

and finally,

$$\begin{aligned}\Phi_1'' - (k^2 a^2 \sinh^2 u + l^2)\Phi_1 &= 0, \\ \Phi_2'' - (k^2 a^2 \sin^2 v - l^2)\Phi_2 &= 0.\end{aligned}$$

*ad (ii):*

the wave equation is given by

$$\Delta\Phi = \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2}.$$

Hence,

$$\frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) \Phi + \frac{\partial^2 \Phi}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2}.$$

The separation of variables *Ansatz* is  $\Phi(u, v, z, t) = \Phi_1(u)\Phi_2(v)\Phi_3(z)T(t)$

$$\begin{aligned} \Rightarrow \frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} \right) + \frac{\Phi_3''}{\Phi_3} &= \frac{1}{c^2} \frac{T''}{T} = -\omega^2 = \text{const.}, \\ \frac{1}{c^2} \frac{T''}{T} &= -\omega^2 \Rightarrow T'' + c^2 \omega^2 T = 0, \\ \frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} \right) &= -\frac{\Phi_3''}{\Phi_3} - \omega^2 = k^2, \\ \Phi_3'' + (\omega^2 + k^2)\Phi_3 &= 0 \\ \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} &= k^2 a^2 (\sinh^2 u + \sin^2 v) \\ \frac{\Phi_1''}{\Phi_1} - a^2 k^2 \sinh^2 u &= -\frac{\Phi_2''}{\Phi_2} + a^2 k^2 \sin^2 v = l^2, \end{aligned} \quad (13.8)$$

and finally,

$$\begin{aligned} \Phi_1'' - (k^2 a^2 \sinh^2 u + l^2)\Phi_1 &= 0, \\ \Phi_2'' - (k^2 a^2 \sin^2 v - l^2)\Phi_2 &= 0. \end{aligned} \quad (13.9)$$

*ad (iii):*

The diffusion equation is  $\Delta\Phi = \frac{1}{D} \frac{\partial\Phi}{\partial t}$ .

The separation of variables *Ansatz* is  $\Phi(u, v, z, t) = \Phi_1(u)\Phi_2(v)\Phi_3(z)T(t)$ .

Let us take the result of (i), then

$$\begin{aligned} \frac{1}{a^2(\sinh^2 u + \sin^2 v)} \left( \frac{\Phi_1''}{\Phi_1} + \frac{\Phi_2''}{\Phi_2} \right) + \frac{\Phi_3''}{\Phi_3} &= \frac{1}{D} \frac{T'}{T} = -\alpha^2 = \text{const.} \\ T &= Ae^{-\alpha^2 D t} \end{aligned} \quad (13.10)$$

$$\Phi_3'' + (\alpha^2 + k^2)\Phi_3 = 0 \Rightarrow \Phi_3'' = -(\alpha^2 + k^2)\Phi_3 \Rightarrow \Phi_3 = Be^{i\sqrt{\alpha^2 + k^2} z}$$

and finally,

$$\begin{aligned} \Phi_1'' - (\alpha^2 k^2 \sinh^2 u + l^2)\Phi_1 &= 0 \\ \Phi_2'' - (\alpha^2 k^2 \sin^2 v - l^2)\Phi_2 &= 0. \end{aligned} \quad (13.11)$$



## Special functions of mathematical physics

This chapter follows several good approaches<sup>1</sup>. For reference, consider<sup>2</sup>.

Special functions often arise as solutions of differential equations; for instance as eigenfunctions of differential operators in quantum mechanics. Sometimes they occur after several *separation of variables* and substitution steps have transformed the physical problem into something manageable. For instance, we might start out with some linear partial differential equation like the wave equation, then separate the space from time coordinates, then separate the radial from the angular components, and finally separate the two angular parameters. After we have done that, we end up with several separate differential equations of the Liouville form; among them the Legendre differential equation leading us to the Legendre polynomials.

In what follows, a particular class of special functions will be considered. These functions are all special cases of the *hypergeometric function*, which is the solution of the *hypergeometric equation*. The hypergeometric function exhibits a high degree of “plasticity,” as many elementary analytic functions can be expressed by them.

First, as a prerequisite, let us define the gamma function. Then we proceed to second order Fuchsian differential equations; followed by rewriting a Fuchsian differential equation into a hypergeometric equation. Then we study the hypergeometric function as a solution to the hypergeometric equation. Finally, we mention some particular hypergeometric functions, such as the Legendre orthogonal polynomials, and others.

Again, if not mentioned otherwise, we shall restrict our attention to second order differential equations. Sometimes – such as for the Fuchsian class – a generalization is possible but not very relevant for physics.

### 14.1 Gamma function

The gamma function  $\Gamma(x)$  is an extension of the factorial function  $n!$ , because it generalizes the factorial to real or complex arguments (different

<sup>1</sup> N. N. Lebedev. *Special Functions and Their Applications*. Prentice-Hall Inc., Englewood Cliffs, N.J., 1965. R. A. Silverman, translator and editor; reprinted by Dover, New York, 1972; Herbert S. Wilf. *Mathematics for the physical sciences*. Dover, New York, 1962. URL [http://www.math.upenn.edu/~wilf/website/Mathematics\\_for\\_the\\_Physical\\_Sciences.html](http://www.math.upenn.edu/~wilf/website/Mathematics_for_the_Physical_Sciences.html); W. W. Bell. *Special Functions for Scientists and Engineers*. D. Van Nostrand Company Ltd, London, 1968; Nico M. Temme. *Special functions: an introduction to the classical functions of mathematical physics*. John Wiley & Sons, Inc., New York, 1996. ISBN 0-471-11313-1; Nico M. Temme. Numerical aspects of special functions. *Acta Numerica*, 16:379–478, 2007. ISSN 0962-4929. DOI: 10.1017/S0962492904000077. URL <http://dx.doi.org/10.1017/S0962492904000077>; George E. Andrews, Richard Askey, and Ranjan Roy. *Special Functions*, volume 71 of *Encyclopedia of Mathematics and its Applications*. Cambridge University Press, Cambridge, 1999. ISBN 0-521-62321-9; Vadim Kuznetsov. Special functions and their symmetries. Part I: Algebraic and analytic methods. Postgraduate Course in Applied Analysis, May 2003. URL <http://www1.maths.leeds.ac.uk/~kisilv/courses/sp-funct.pdf>; and Vladimir Kisil. Special functions and their symmetries. Part II: Algebraic and symmetry methods. Postgraduate Course in Applied Analysis, May 2003. URL <http://www1.maths.leeds.ac.uk/~kisilv/courses/sp-repr.pdf>

<sup>2</sup> Milton Abramowitz and Irene A. Stegun, editors. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Number 55 in National Bureau of Standards Applied Mathematics Series. U.S. Government Printing Office, Washington, D.C., 1964. Corrections appeared in later printings up to the 10th Printing, December, 1972. Reproductions by other publishers, in whole or in part, have been available since 1965; Yuri Alexandrovich Brychkov and Anatolii Platonovich Prudnikov. *Handbook of special functions: derivatives, integrals, series and other formulas*. CRC/Chapman

from the negative integers and from zero); that is,

$$\Gamma(n+1) = n! \text{ for } n \in \mathbb{N}. \quad (14.1)$$

Let us first define the *shifted factorial* or, by another naming, the *Pochhammer symbol*

$$(a)_n \stackrel{\text{def}}{=} a(a+1)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}, \quad (14.2)$$

where  $n > 0$  and  $a$  can be any real or complex number.

With this definition,

$$\begin{aligned} z!(z+1)_n &= 1 \cdot 2 \cdots z \cdot (z+1)((z+1)+1) \cdots ((z+1)+n-1) \\ &= 1 \cdot 2 \cdots z \cdot (z+1)(z+2) \cdots (z+n) \\ &= (z+n)!, \\ \text{or } z! &= \frac{(z+n)!}{(z+1)_n}. \end{aligned} \quad (14.3)$$

Since

$$\begin{aligned} (z+n)! &= (n+z)! \\ &= 1 \cdot 2 \cdots n \cdot (n+1)(n+2) \cdots (n+z) \\ &= n! \cdot (n+1)(n+2) \cdots (n+z) \\ &= n!(n+1)_z, \end{aligned} \quad (14.4)$$

we can rewrite Eq. (14.3) into

$$z! = \frac{n!(n+1)_z}{(z+1)_n} = \frac{n!n^z}{(z+1)_n} \frac{(n+1)_z}{n^z}. \quad (14.5)$$

Since the latter factor, for large  $n$ , converges as [ $O(x)$ ] means “of the order of  $x$ ”]

$$\begin{aligned} \frac{(n+1)_z}{n^z} &= \frac{(n+1)((n+1)+1) \cdots ((n+1)+z-1)}{n^z} \\ &= \frac{n^z + O(n^{z-1})}{n^z} \\ &= \frac{n^z}{n^z} + \frac{O(n^{z-1})}{n^z} \\ &= 1 + O(n^{-1}) \xrightarrow{n \rightarrow \infty} 1, \end{aligned} \quad (14.6)$$

in this limit, Eq. (14.5) can be written as

$$z! = \lim_{n \rightarrow \infty} z! = \lim_{n \rightarrow \infty} \frac{n!n^z}{(z+1)_n}. \quad (14.7)$$

Hence, for all  $z \in \mathbb{C}$  which are not equal to a negative integer – that is,  $z \notin \{-1, -2, \dots\}$  – we can, in analogy to the “classical factorial,” define a “factorial function shifted by one” as

$$\Gamma(z+1) \stackrel{\text{def}}{=} \lim_{n \rightarrow \infty} \frac{n!n^z}{(z+1)_n}, \quad (14.8)$$

and thus, because for very large  $n$  and constant  $z$  (i.e.,  $z \ll n$ ),  $(z+n) \approx n$ ,

$$\begin{aligned}
 \Gamma(z) &= \lim_{n \rightarrow \infty} \frac{n! n^{z-1}}{(z)_n} \\
 &= \lim_{n \rightarrow \infty} \frac{n! n^{z-1}}{z(z+1) \cdots (z+n-1)} \\
 &= \lim_{n \rightarrow \infty} \frac{n! n^{z-1}}{z(z+1) \cdots (z+n-1)} \underbrace{\left( \frac{z+n}{z+n} \right)}_1 \\
 &= \lim_{n \rightarrow \infty} \frac{n! n^{z-1} (z+n)}{z(z+1) \cdots (z+n)} \\
 &= \frac{1}{z} \lim_{n \rightarrow \infty} \frac{n! n^z}{(z+1)_n}.
 \end{aligned} \tag{14.9}$$

$\Gamma(z+1)$  has thus been redefined in terms of  $z!$  in Eq. (14.3), which, by comparing Eqs. (14.8) and (14.9), also implies that

$$\Gamma(z+1) = z\Gamma(z). \tag{14.10}$$

Note that, since

$$(1)_n = 1(1+1)(1+2) \cdots (1+n-1) = n!, \tag{14.11}$$

Eq. (14.8) yields

$$\Gamma(1) = \lim_{n \rightarrow \infty} \frac{n! n^0}{(1)_n} = \lim_{n \rightarrow \infty} \frac{n!}{n!} = 1. \tag{14.12}$$

By induction, Eqs. (14.12) and (14.10) yield  $\Gamma(n+1) = n!$  for  $n \in \mathbb{N}$ .

We state without proof that, for complex numbers  $z$  with positive real parts  $\Re z > 0$ ,  $\Gamma(z)$  can be defined by an integral representation as

$$\Gamma(z) \stackrel{\text{def}}{=} \int_0^\infty t^{z-1} e^{-t} dt. \tag{14.13}$$

Note that Eq. (14.10) can be derived from this integral representation of  $\Gamma(z)$  by partial integration; that is,

$$\begin{aligned}
 \Gamma(z+1) &= \int_0^\infty t^z e^{-t} dt \\
 &= \underbrace{-t^z e^{-t}}_0 \Big|_0^\infty - \left[ - \int_0^\infty \left( \frac{d}{dt} t^z \right) e^{-t} dt \right] \\
 &= \int_0^\infty z t^{z-1} e^{-t} dt \\
 &= z \int_0^\infty t^{z-1} e^{-t} dt = z\Gamma(z).
 \end{aligned} \tag{14.14}$$

We also mention without proof following the formulæ:

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \tag{14.15}$$

or, more generally,

$$\Gamma\left(\frac{n}{2}\right) = \sqrt{\pi} \frac{(n-2)!!}{2^{(n-1)/2}}, \text{ for } n > 0; \text{ and} \quad (14.16)$$

$$\text{Euler's reflection formula } \Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin(\pi x)}. \quad (14.17)$$

Here, the *double factorial* is defined by

$$n!! = \begin{cases} 1 \text{ for } n = -1, 0, \text{ and} \\ 2 \cdot 4 \cdots (n-2) \cdot n \\ = (2k)!! = \prod_{i=1}^k (2i) \\ = 2^{n/2} \left(1 \cdot 2 \cdots \frac{(n-2)}{2} \cdot \frac{n}{2}\right) \\ = k!2^k \text{ for positive even } n = 2k, k \geq 1, \text{ and} \\ 1 \cdot 3 \cdots (n-2) \cdot n \\ = (2k-1)!! = \prod_{i=1}^k (2i-1) \\ = \frac{1 \cdot 2 \cdots (2k-2) \cdot (2k-1) \cdot (2k)}{(2k)!!} \\ = \frac{(2k)!}{k!2^k} \text{ for odd positive } n = 2k-1, k \geq 1. \end{cases} \quad (14.18)$$

Stirling's formula [again,  $O(x)$  means “of the order of  $x$ ”]

$$\begin{aligned} \log n! &= n \log n - n + O(\log(n)), \text{ or} \\ n! &\xrightarrow{n \rightarrow \infty} \sqrt{2\pi n} \left(\frac{n}{e}\right)^n, \text{ or, more generally,} \\ \Gamma(x) &= \sqrt{\frac{2\pi}{x}} \left(\frac{x}{e}\right)^x \left(1 + O\left(\frac{1}{x}\right)\right) \end{aligned} \quad (14.19)$$

is stated without proof.

## 14.2 Beta function

The *beta function*, also called the *Euler integral of the first kind*, is a special function defined by

$$B(x, y) = \int_0^1 t^{x-1} (1-t)^{y-1} dt = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \text{ for } \Re x, \Re y > 0 \quad (14.20)$$

No proof of the identity of the two representations in terms of an integral, and of  $\Gamma$ -functions is given.

## 14.3 Fuchsian differential equations

Many differential equations of theoretical physics are Fuchsian equations.

We shall therefore study this class in some generality.

### 14.3.1 Regular, regular singular, and irregular singular point

Consider the homogenous differential equation [Eq. (12.1) on page 193 is inhomogeneous]

$$\mathcal{L}_x y(x) = a_2(x) \frac{d^2}{dx^2} y(x) + a_1(x) \frac{d}{dx} y(x) + a_0(x) y(x) = 0. \quad (14.21)$$

If  $a_0(x)$ ,  $a_1(x)$  and  $a_2(x)$  are analytic at some point  $x_0$  and in its neighborhood, and if  $a_2(x_0) \neq 0$  at  $x_0$ , then  $x_0$  is called an *ordinary point*, or *regular point*. We state without proof that in this case the solutions around  $x_0$  can be expanded as power series. In this case we can divide equation (14.21) by  $a_2(x)$  and rewrite it

$$\frac{1}{a_2(x)} \mathcal{L}_x y(x) = \frac{d^2}{dx^2} y(x) + p_1(x) \frac{d}{dx} y(x) + p_2(x) y(x) = 0, \quad (14.22)$$

with  $p_1(x) = a_1(x)/a_2(x)$  and  $p_2(x) = a_0(x)/a_2(x)$ .

If, however,  $a_2(x_0) = 0$  and  $a_1(x_0)$  or  $a_0(x_0)$  are nonzero, then the  $x_0$  is called *singular point* of (14.21). The simplest case is if  $a_0(x)$  has a *simple zero* at  $x_0$ ; then both  $p_1(x)$  and  $p_2(x)$  in (14.22) have at most simple poles.

Furthermore, for reasons disclosed later – mainly motivated by the possibility to write the solutions as power series – a point  $x_0$  is called a *regular singular point* of Eq. (14.21) if

$$\lim_{x \rightarrow x_0} (x - x_0) \frac{a_1(x)}{a_2(x)}, \text{ as well as } \lim_{x \rightarrow x_0} (x - x_0)^2 \frac{a_0(x)}{a_2(x)} \quad (14.23)$$

both exist. If any one of these limits does not exist, the singular point is an *irregular singular point*.

A linear ordinary differential equation is called *Fuchsian*, or *Fuchsian differential equation* generalizable to arbitrary order  $n$  of differentiation

$$\left[ \frac{d^n}{dx^n} + p_1(x) \frac{d^{n-1}}{dx^{n-1}} + \cdots + p_{n-1}(x) \frac{d}{dx} + p_n(x) \right] y(x) = 0, \quad (14.24)$$

if every singular point, including infinity, is regular, meaning that  $p_k(x)$  has at most poles of order  $k$ .

A very important case is a Fuchsian of the second order (up to second derivatives occur). In this case, we suppose that the coefficients in (14.22) satisfy the following conditions:

- $p_1(x)$  has at most *single poles*, and
- $p_2(x)$  has at most *double poles*.

The simplest realization of this case is for  $a_2(x) = a(x - x_0)^2$ ,  $a_1(x) = b(x - x_0)$ ,  $a_0(x) = c$  for some constant  $a, b, c \in \mathbb{C}$ .



### 14.3.2 Behavior at infinity

In order to cope with infinity  $z = \infty$  let us transform the Fuchsian equation  $w'' + p_1(z)w' + p_2(z)w = 0$  into the new variable  $t = \frac{1}{z}$ .

$$\begin{aligned}
 t &= \frac{1}{z}, \quad z = \frac{1}{t}, \quad u(t) \stackrel{\text{def}}{=} w\left(\frac{1}{t}\right) = w(z) \\
 \frac{dz}{dt} &= -\frac{1}{t^2}, \text{ and thus } \frac{d}{dz} = -t^2 \frac{d}{dt} \\
 \frac{d^2}{dz^2} &= -t^2 \frac{d}{dt} \left( -t^2 \frac{d}{dt} \right) = -t^2 \left( -2t \frac{d}{dt} - t^2 \frac{d^2}{dt^2} \right) = 2t^3 \frac{d}{dt} + t^4 \frac{d^2}{dt^2} \quad (14.25) \\
 w'(z) &= \frac{d}{dz} w(z) = -t^2 \frac{d}{dt} u(t) = -t^2 u'(t) \\
 w''(z) &= \frac{d^2}{dz^2} w(z) = \left( 2t^3 \frac{d}{dt} + t^4 \frac{d^2}{dt^2} \right) u(t) = 2t^3 u'(t) + t^4 u''(t)
 \end{aligned}$$

Insertion into the Fuchsian equation  $w'' + p_1(z)w' + p_2(z)w = 0$  yields

$$2t^3 u' + t^4 u'' + p_1\left(\frac{1}{t}\right)(-t^2 u') + p_2\left(\frac{1}{t}\right)u = 0, \quad (14.26)$$

and hence,

$$u'' + \left[ \frac{2}{t} - \frac{p_1\left(\frac{1}{t}\right)}{t^2} \right] u' + \frac{p_2\left(\frac{1}{t}\right)}{t^4} u = 0. \quad (14.27)$$

From

$$\tilde{p}_1(t) \stackrel{\text{def}}{=} \left[ \frac{2}{t} - \frac{p_1\left(\frac{1}{t}\right)}{t^2} \right] \quad (14.28)$$

and

$$\tilde{p}_2(t) \stackrel{\text{def}}{=} \frac{p_2\left(\frac{1}{t}\right)}{t^4} \quad (14.29)$$

follows the form of the rewritten differential equation

$$u'' + \tilde{p}_1(t)u' + \tilde{p}_2(t)u = 0. \quad (14.30)$$

This equation is Fuchsian if 0 is an ordinary point, or at least a regular singular point.

Note that, for infinity to be a regular singular point,  $\tilde{p}_1(t)$  must have at most a pole of the order of  $t^{-1}$ , and  $\tilde{p}_2(t)$  must have at most a pole of the order of  $t^{-2}$  at  $t = 0$ . Therefore,  $(1/t)p_1(1/t) = zp_1(z)$  as well as  $(1/t^2)p_2(1/t) = z^2p_2(z)$  must both be analytic functions as  $t \rightarrow 0$ , or  $z \rightarrow \infty$ .

### 14.3.3 Functional form of the coefficients in Fuchsian differential equations

Let us hint on the functional form of the coefficients  $p_1(x)$  and  $p_2(x)$ , resulting from the assumption of regular singular poles.

First, let us start with poles at finite complex numbers. Suppose there are  $k$  finite poles (the behavior of  $p_1(x)$  and  $p_2(x)$  at infinity will be treated later). Hence, in Eq. (14.22), the coefficients must be of the form

$$\begin{aligned} p_1(x) &= \frac{P_1(x)}{\prod_{j=1}^k (x - x_j)}, \\ \text{and } p_2(x) &= \frac{P_2(x)}{\prod_{j=1}^k (x - x_j)^2}, \end{aligned} \quad (14.31)$$

where the  $x_1, \dots, x_k$  are  $k$  the points of the (regular singular) poles, and  $P_1(x)$  and  $P_2(x)$  *entire functions*; that is, they are analytic (or, by another wording, holomorphic) over the whole complex plane formed by  $\{x \mid x \in \mathbb{C}\}$ .

Second, consider possible poles at infinity. Note that, as has been shown earlier, because of the requirement that infinity is a regular singular point,  $p_1(x)x$  as well as  $p_2(x)x^2$ , as  $x \rightarrow \infty$  approaches infinity, must both be analytic. Therefore,  $p_1(x)$  cannot grow faster than  $|x|^{-1}$ , and  $p_2(x)$  cannot grow faster than  $|x|^{-2}$ .

Therefore, as  $x \rightarrow \infty$  approaches infinity,  $P_1(x) = p_1(x) \prod_{j=1}^k (x - x_j)$  does not grow faster than  $|x|^{k-1}$ , and  $P_2(x) = p_2(x) \prod_{j=1}^k (x - x_j)^2$  does not grow faster than  $|x|^{2k-2}$ .

Recall that both  $P_1(x)$  and  $P_2(x)$  are *entire functions*. Therefore, because of the *generalized Liouville theorem*<sup>3</sup> (mentioned on page 136), both  $P_1(x)$  and  $P_2(x)$  must be rational functions – that is, polynomials of the form  $\frac{P(x)}{Q(x)}$  – of degree of at most  $k-1$  and  $2k-2$ , respectively.

Moreover, by using *partial fraction decomposition*<sup>4</sup> of the rational functions in terms of their pole factors  $(x - x_j)$ , we obtain the general form of the coefficients

$$\begin{aligned} p_1(x) &= \sum_{j=1}^k \frac{A_j}{x - x_j}, \\ \text{and } p_2(x) &= \sum_{j=1}^k \left[ \frac{B_j}{(x - x_j)^2} + \frac{C_j}{x - x_j} \right], \end{aligned} \quad (14.32)$$

with constant  $A_j, B_j, C_j \in \mathbb{C}$ . The resulting Fuchsian differential equation is called *Riemann differential equation*.

Although we have considered an arbitrary finite number of poles, for reasons that are unclear to this author, in physics we are mainly concerned with two poles (i.e.,  $k = 2$ ) at finite points, and one at infinity.

The *hypergeometric differential equation* is a *Fuchsian differential equation* which has at most *three regular singularities*, including infinity, at 0, 1, and  $\infty$ <sup>5</sup>.

#### 14.3.4 Frobenius method by power series

Now let us get more concrete about the solution of Fuchsian equations by *power series*.

<sup>3</sup> Robert E. Greene and Stephen G. Krantz. *Function theory of one complex variable*, volume 40 of *Graduate Studies in Mathematics*. American mathematical Society, Providence, Rhode Island, third edition, 2006

<sup>4</sup> Gerhard Kristensson. Equations of Fuchsian type. In *Second Order Differential Equations*, pages 29–42. Springer, New York, 2010. ISBN 978-1-4419-7019-0. DOI: 10.1007/978-1-4419-7020-6. URL <http://dx.doi.org/10.1007/978-1-4419-7020-6>

<sup>5</sup> Vadim Kuznetsov. Special functions and their symmetries. Part I: Algebraic and analytic methods. Postgraduate Course in Applied Analysis, May 2003. URL <http://www1.maths.leeds.ac.uk/~kisilv/courses/sp-funct.pdf>

In order to obtain a feeling for power series solutions of differential equations, consider the “first order” Fuchsian equation <sup>6</sup>

$$y' - \lambda y = 0. \quad (14.33)$$

Make the *Ansatz*, also known as known as *Frobenius method* <sup>7</sup>, that the solution can be expanded into a power series of the form

$$y(x) = \sum_{j=0}^{\infty} a_j x^j. \quad (14.34)$$

Then, Eq. (14.33) can be written as

$$\begin{aligned} \left( \frac{d}{dx} \sum_{j=0}^{\infty} a_j x^j \right) - \lambda \sum_{j=0}^{\infty} a_j x^j &= 0, \\ \sum_{j=0}^{\infty} j a_j x^{j-1} - \lambda \sum_{j=0}^{\infty} a_j x^j &= 0, \\ \sum_{j=1}^{\infty} j a_j x^{j-1} - \lambda \sum_{j=0}^{\infty} a_j x^j &= 0, \\ \sum_{m=j-1=0}^{\infty} (m+1) a_{m+1} x^m - \lambda \sum_{j=0}^{\infty} a_j x^j &= 0, \\ \sum_{j=0}^{\infty} (j+1) a_{j+1} x^j - \lambda \sum_{j=0}^{\infty} a_j x^j &= 0, \end{aligned} \quad (14.35)$$

and hence, by comparing the coefficients of  $x^j$ , for  $n \geq 0$ ,

$$\begin{aligned} (j+1) a_{j+1} &= \lambda a_j, \text{ or} \\ a_{j+1} &= \frac{\lambda a_j}{j+1} = a_0 \frac{\lambda^{j+1}}{(j+1)!}, \text{ and} \\ a_j &= a_0 \frac{\lambda^j}{j!}. \end{aligned} \quad (14.36)$$

Therefore,

$$y(x) = \sum_{j=0}^{\infty} a_0 \frac{\lambda^j}{j!} x^j = a_0 \sum_{j=0}^{\infty} \frac{(\lambda x)^j}{j!} = a_0 e^{\lambda x}. \quad (14.37)$$

In the Fuchsian case let us consider the following *Frobenius Ansatz* to expand the solution as a *generalized power series* around a regular singular point  $x_0$ , which can be motivated by Eq. (14.31), and by the *Laurent series expansion* (8.28)–(8.30) on page 129:

$$\begin{aligned} p_1(x) &= \frac{A_1(x)}{x - x_0} = \sum_{j=0}^{\infty} \alpha_j (x - x_0)^{j-1} \text{ for } 0 < |x - x_0| < r_1, \\ p_2(x) &= \frac{A_2(x)}{(x - x_0)^2} = \sum_{j=0}^{\infty} \beta_j (x - x_0)^{j-2} \text{ for } 0 < |x - x_0| < r_2, \\ y(x) &= (x - x_0)^\sigma \sum_{l=0}^{\infty} (x - x_0)^l w_l = \sum_{l=0}^{\infty} (x - x_0)^{l+\sigma} w_l, \text{ with } w_0 \neq 0, \end{aligned} \quad (14.38)$$

<sup>6</sup> Ron Larson and Bruce H. Edwards. *Calculus*. Brooks/Cole Cengage Learning, Belmont, CA, 9th edition, 2010. ISBN 978-0-547-16702-2

<sup>7</sup> George B. Arfken and Hans J. Weber. *Mathematical Methods for Physicists*. Elsevier, Oxford, 6th edition, 2005. ISBN 0-12-059876-0; 0-12-088584-0

where  $A_1(x) = [(x - x_0)a_1(x)]/a_2(x)$  and  $A_2(x) = [(x - x_0)^2 a_0(x)]/a_2(x)$ . Eq. (14.22) then becomes

$$\begin{aligned}
 & \frac{d^2}{dx^2} y(x) + p_1(x) \frac{d}{dx} y(x) + p_2(x) y(x) = 0, \\
 & \left[ \frac{d^2}{dx^2} + \sum_{j=0}^{\infty} \alpha_j (x - x_0)^{j-1} \frac{d}{dx} + \sum_{j=0}^{\infty} \beta_j (x - x_0)^{j-2} \right] \sum_{l=0}^{\infty} w_l (x - x_0)^{l+\sigma} = 0, \\
 & \sum_{l=0}^{\infty} (l + \sigma)(l + \sigma - 1) w_l (x - x_0)^{l+\sigma-2} \\
 & + \left[ \sum_{l=0}^{\infty} (l + \sigma) w_l (x - x_0)^{l+\sigma-1} \right] \sum_{j=0}^{\infty} \alpha_j (x - x_0)^{j-1} \\
 & + \left[ \sum_{l=0}^{\infty} w_l (x - x_0)^{l+\sigma} \right] \sum_{j=0}^{\infty} \beta_j (x - x_0)^{j-2} = 0, \\
 & (x - x_0)^{\sigma-2} \sum_{l=0}^{\infty} (x - x_0)^l [(l + \sigma)(l + \sigma - 1) w_l \\
 & + (l + \sigma) w_l \sum_{j=0}^{\infty} \alpha_j (x - x_0)^j + w_l \sum_{j=0}^{\infty} \beta_j (x - x_0)^j] = 0, \\
 & (x - x_0)^{\sigma-2} \left[ \sum_{l=0}^{\infty} (l + \sigma)(l + \sigma - 1) w_l (x - x_0)^l \right. \\
 & \left. + \sum_{l=0}^{\infty} (l + \sigma) w_l \sum_{j=0}^{\infty} \alpha_j (x - x_0)^{l+j} + \sum_{l=0}^{\infty} w_l \sum_{j=0}^{\infty} \beta_j (x - x_0)^{l+j} \right] = 0.
 \end{aligned}$$

Next, in order to reach a common power of  $(x - x_0)$ , we perform an index identification in the second and third summands (where the order of the sums change):  $l = m$  in the first summand, as well as an index shift  $l + j = m$ , and thus  $j = m - l$ . Since  $l \geq 0$  and  $j \geq 0$ , also  $m = l + j$  cannot be

negative. Furthermore,  $0 \leq j = m - l$ , so that  $l \leq m$ .

$$\begin{aligned}
& (x - x_0)^{\sigma-2} \left[ \sum_{l=0}^{\infty} (l + \sigma)(l + \sigma - 1) w_l (x - x_0)^l \right. \\
& \quad + \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} (l + \sigma) w_l \alpha_j (x - x_0)^{l+j} \\
& \quad \left. + \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} w_l \beta_j (x - x_0)^{l+j} \right] = 0, \\
& (x - x_0)^{\sigma-2} \left[ \sum_{m=0}^{\infty} (m + \sigma)(m + \sigma - 1) w_m (x - x_0)^m \right. \\
& \quad + \sum_{m=0}^{\infty} \sum_{l=0}^m (l + \sigma) w_l \alpha_{m-l} (x - x_0)^{l+m-l} \\
& \quad \left. + \sum_{m=0}^{\infty} \sum_{l=0}^m w_l \beta_{m-l} (x - x_0)^{l+m-l} \right] = 0, \tag{14.39} \\
& (x - x_0)^{\sigma-2} \left\{ \sum_{m=0}^{\infty} (x - x_0)^m [(m + \sigma)(m + \sigma - 1) w_m \right. \\
& \quad \left. + \sum_{l=0}^m (l + \sigma) w_l \alpha_{m-l} + \sum_{l=0}^m w_l \beta_{m-l}] \right\} = 0, \\
& (x - x_0)^{\sigma-2} \left\{ \sum_{m=0}^{\infty} (x - x_0)^m [(m + \sigma)(m + \sigma - 1) w_m \right. \\
& \quad \left. + \sum_{l=0}^m w_l ((l + \sigma) \alpha_{m-l} + \beta_{m-l})] \right\} = 0.
\end{aligned}$$

If we can divide this equation through  $(x - x_0)^{\sigma-2}$  and exploit the linear independence of the polynomials  $(x - x_0)^m$ , we obtain an infinite number of equations for the infinite number of coefficients  $w_m$  by requiring that all the terms “inbetween” the  $[\dots]$ -brackets in Eq. (14.39) vanish *individually*. In particular, for  $m = 0$  and  $w_0 \neq 0$ ,

$$\begin{aligned}
& (0 + \sigma)(0 + \sigma - 1) w_0 + w_0 ((0 + \sigma) \alpha_0 + \beta_0) = 0 \\
& f_0(\sigma) \stackrel{\text{def}}{=} \sigma(\sigma - 1) + \sigma \alpha_0 + \beta_0 = 0. \tag{14.40}
\end{aligned}$$

The *radius of convergence* of the solution will, in accordance with the Laurent series expansion, extend to the next singularity.

Note that in Eq. (14.40) we have defined  $f_0(\sigma)$  which we will use now. Furthermore, for successive  $m$ , and with the definition of

$$f_k(\sigma) \stackrel{\text{def}}{=} \alpha_k \sigma + \beta_k, \tag{14.41}$$

we obtain the sequence of linear equations

$$\begin{aligned}
& w_0 f_0(\sigma) = 0 \\
& w_1 f_0(\sigma + 1) + w_0 f_1(\sigma) = 0, \\
& w_2 f_0(\sigma + 2) + w_1 f_1(\sigma + 1) + w_0 f_2(\sigma) = 0, \\
& \vdots \\
& w_n f_0(\sigma + n) + w_{n-1} f_1(\sigma + n - 1) + \dots + w_0 f_n(\sigma) = 0.
\end{aligned} \tag{14.42}$$

which can be used for an inductive determination of the coefficients  $w_k$ .

Eq. (14.40) is a quadratic equation  $\sigma^2 + \sigma(\alpha_0 - 1) + \beta_0 = 0$  for the *characteristic exponents*

$$\sigma_{1,2} = \frac{1}{2} \left[ 1 - \alpha_0 \pm \sqrt{(1 - \alpha_0)^2 - 4\beta_0} \right] \quad (14.43)$$

We state without proof that, if the difference of the characteristic exponents

$$\sigma_1 - \sigma_2 = \sqrt{(1 - \alpha_0)^2 - 4\beta_0} \quad (14.44)$$

is *nonzero* and *not* an integer, then the two solutions found from  $\sigma_{1,2}$  through the generalized series Ansatz (14.38) are linear independent.

Intuitively speaking, the Frobenius method “is in obvious trouble” to find the general solution of the Fuchsian equation if the two characteristic exponents coincide (e.g.,  $\sigma_1 = \sigma_2$ ), but it “is also in trouble” to find the general solution if  $\sigma_1 - \sigma_2 = m \in \mathbb{N}$ ; that is, if, for some positive integer  $m$ ,  $\sigma_1 = \sigma_2 + m > \sigma_2$ . Because in this case, “eventually” at  $n = m$  in Eq. (14.42), we obtain as iterative solution for the coefficient  $w_m$  the term

$$\begin{aligned} w_m &= - \frac{w_{m-1}f_1(\sigma_2 + m - 1) + \cdots + w_0f_m(\sigma_2)}{f_0(\sigma_2 + m)} \\ &= - \frac{w_{m-1}f_1(\sigma_1 - 1) + \cdots + w_0f_m(\sigma_2)}{\underbrace{f_0(\sigma_1)}_{=0}}, \end{aligned} \quad (14.45)$$

as the greater critical exponent  $\sigma_1$  is a solution of Eq. (14.40) and thus vanishes, leaving us with a vanishing denominator.

### 14.3.5 d’Alambert reduction of order

If  $\sigma_1 = \sigma_2 + n$  with  $n \in \mathbb{Z}$ , then we find only a *single* solution of the Fuchsian equation. In order to obtain another linear independent solution we have to employ a method based on the Wronskian<sup>8</sup>, or the d’Alambert reduction<sup>9</sup>, which is a general method to obtain another, linear independent solution  $y_2(x)$  from an existing particular solution  $y_1(x)$  by the *Ansatz* (no proof is presented here)

$$y_2(x) = y_1(x) \int_x v(s) ds. \quad (14.46)$$

<sup>8</sup> George B. Arfken and Hans J. Weber. *Mathematical Methods for Physicists*. Elsevier, Oxford, 6th edition, 2005. ISBN 0-12-059876-0; 0-12-088584-0

<sup>9</sup> Gerald Teschl. *Ordinary Differential Equations and Dynamical Systems. Graduate Studies in Mathematics, volume 140*. American Mathematical Society, Providence, Rhode Island, 2012. ISBN 0-8218-8328-3 / ISBN-13: 978-0-8218-8328-0. URL <http://www.mat.univie.ac.at/~gerald/ftp/book-ode/ode.pdf>

Inserting  $y_2(x)$  from (14.46) into the Fuchsian equation (14.22), and using the fact that by assumption  $y_1(x)$  is a solution of it, yields

$$\begin{aligned}
& \frac{d^2}{dx^2} y_2(x) + p_1(x) \frac{d}{dx} y_2(x) + p_2(x) y_2(x) = 0, \\
& \frac{d^2}{dx^2} y_1(x) \int_x v(s) ds + p_1(x) \frac{d}{dx} y_1(x) \int_x v(s) ds + p_2(x) y_1(x) \int_x v(s) ds = 0, \\
& \frac{d}{dx} \left\{ \left[ \frac{d}{dx} y_1(x) \right] \int_x v(s) ds + y_1(x) v(x) \right\} \\
& + p_1(x) \left[ \frac{d}{dx} y_1(x) \right] \int_x v(s) ds + p_1(x) v(x) + p_2(x) y_1(x) \int_x v(s) ds = 0, \\
& \left[ \frac{d^2}{dx^2} y_1(x) \right] \int_x v(s) ds + \left[ \frac{d}{dx} y_1(x) \right] v(x) + \left[ \frac{d}{dx} y_1(x) \right] v(x) + y_1(x) \left[ \frac{d}{dx} v(x) \right] \\
& + p_1(x) \left[ \frac{d}{dx} y_1(x) \right] \int_x v(s) ds + p_1(x) y_1(x) v(x) + p_2(x) y_1(x) \int_x v(s) ds = 0, \\
& \left[ \frac{d^2}{dx^2} y_1(x) \right] \int_x v(s) ds + p_1(x) \left[ \frac{d}{dx} y_1(x) \right] \int_x v(s) ds + p_2(x) y_1(x) \int_x v(s) ds \\
& + p_1(x) y_1(x) v(x) + \left[ \frac{d}{dx} y_1(x) \right] v(x) + \left[ \frac{d}{dx} y_1(x) \right] v(x) + y_1(x) \left[ \frac{d}{dx} v(x) \right] = 0, \\
& \left[ \frac{d^2}{dx^2} y_1(x) \right] \int_x v(s) ds + p_1(x) \left[ \frac{d}{dx} y_1(x) \right] \int_x v(s) ds + p_2(x) y_1(x) \int_x v(s) ds \\
& + y_1(x) \left[ \frac{d}{dx} v(x) \right] + 2 \left[ \frac{d}{dx} y_1(x) \right] v(x) + p_1(x) y_1(x) v(x) = 0, \\
& \underbrace{\left\{ \left[ \frac{d^2}{dx^2} y_1(x) \right] + p_1(x) \left[ \frac{d}{dx} y_1(x) \right] + p_2(x) y_1(x) \right\} \int_x v(s) ds}_{=0} \\
& + y_1(x) \left[ \frac{d}{dx} v(x) \right] + \left\{ 2 \left[ \frac{d}{dx} y_1(x) \right] + p_1(x) y_1(x) \right\} v(x) = 0, \\
& y_1(x) \left[ \frac{d}{dx} v(x) \right] + \left\{ 2 \left[ \frac{d}{dx} y_1(x) \right] + p_1(x) y_1(x) \right\} v(x) = 0,
\end{aligned}$$

and finally,

$$v'(x) + v(x) \left\{ 2 \frac{y_1'(x)}{y_1(x)} + p_1(x) \right\} = 0. \quad (14.47)$$

### 14.3.6 Computation of the characteristic exponent

Let  $w'' + p_1(z)w' + p_2(z)w = 0$  be a Fuchsian equation. From the Laurent series expansion of  $p_1(z)$  and  $p_2(z)$  with Cauchy's integral formula we can derive the following equations, which are helpful in determining the characteristic exponent  $\sigma$ :

$$\begin{aligned}
\alpha_0 &= \lim_{z \rightarrow z_0} (z - z_0) p_1(z), \\
\beta_0 &= \lim_{z \rightarrow z_0} (z - z_0)^2 p_2(z),
\end{aligned} \quad (14.48)$$

where  $z_0$  is a regular singular point.

Let us consider  $\alpha_0$  and the Laurent series for

$$p_1(z) = \sum_{k=-1}^{\infty} \tilde{a}_k (z - z_0)^k \text{ with } \tilde{a}_k = \frac{1}{2\pi i} \oint p_1(s) (s - z_0)^{-(k+1)} ds.$$

The summands vanish for  $k < -1$ , because  $p_1(z)$  has at most a pole of order one at  $z_0$ . Let us change the index :  $n = k + 1$  ( $\implies k = n - 1$ ) and  $\alpha_n \stackrel{\text{def}}{=} \tilde{a}_{n-1}$ ; then

$$p_1(z) = \sum_{n=0}^{\infty} \alpha_n (z - z_0)^{n-1},$$

where

$$\alpha_n = \tilde{a}_{n-1} = \frac{1}{2\pi i} \oint p_1(s) (s - z_0)^{-n} ds;$$

in particular,

$$\alpha_0 = \frac{1}{2\pi i} \oint p_1(s) ds.$$

Because the equation is Fuchsian,  $p_1(z)$  has only a pole of order one at  $z_0$ ; and  $p_1(z)$  is of the form

$$p_1(z) = \frac{a_1(z)}{(z - z_0)a_2(z)} = \frac{(z - z_0)p_1(z)}{(z - z_0)}$$

and

$$\alpha_0 = \frac{1}{2\pi i} \oint \frac{p_1(s)(s - z_0)}{(s - z_0)} ds,$$

where  $(s - z_0)p_1(s)$  is analytic around  $z_0$ ; hence we can apply Cauchy's integral formula:

$$\alpha_0 = \lim_{s \rightarrow z_0} p_1(s)(s - z_0)$$

An easy way to see this is with the *Ansatz*:  $p_1(z) = \sum_{n=0}^{\infty} \alpha_n (z - z_0)^{n-1}$ ; multiplication with  $(z - z_0)$  yields

$$(z - z_0)p_1(z) = \sum_{n=0}^{\infty} \alpha_n (z - z_0)^n.$$

In the limit  $z \rightarrow z_0$ ,

$$\lim_{z \rightarrow z_0} (z - z_0)p_1(z) = \alpha_n$$

Let us consider  $\beta_0$  and the Laurent series for

$$p_2(z) = \sum_{k=-2}^{\infty} \tilde{b}_k (z - z_0)^k \text{ with } \tilde{b}_k = \frac{1}{2\pi i} \oint p_2(s) (s - z_0)^{-(k+1)} ds.$$

The summands vanish for  $k < -2$ , because  $p_2(z)$  has at most a pole of second order at  $z_0$ . Let us change the index :  $n = k + 2$  ( $\implies k = n - 2$ ) and  $\beta_n \stackrel{\text{def}}{=} \tilde{b}_{n-2}$ . Hence,

$$p_2(z) = \sum_{n=0}^{\infty} \beta_n (z - z_0)^{n-2},$$

where

$$\beta_n = \frac{1}{2\pi i} \oint p_2(s) (s - z_0)^{-(n-1)} ds,$$



in particular,

$$\beta_0 = \frac{1}{2\pi i} \oint p_2(s)(s - z_0) ds.$$

Because the equation is Fuchsian,  $p_2(z)$  has only a pole of the order of two at  $z_0$ ; and  $p_2(z)$  is of the form

$$p_2(z) = \frac{a_2(z)}{(z - z_0)^2 a_2(z)} = \frac{(z - z_0)^2 p_2(z)}{(z - z_0)^2}$$

where  $a_2(z) = p_2(z)(z - z_0)^2$  is analytic around  $z_0$

$$\beta_0 = \frac{1}{2\pi i} \oint \frac{p_2(s)(s - z_0)^2}{(s - z_0)} ds;$$

hence we can apply Cauchy's integral formula

$$\beta_0 = \lim_{s \rightarrow z_0} p_2(s)(s - z_0)^2.$$

An easy way to see this is with the *Ansatz*:  $p_2(z) = \sum_{n=0}^{\infty} \beta_n (z - z_0)^{n-2}$ . multiplication with  $(z - z_0)^2$ , in the limit  $z \rightarrow z_0$ , yields

$$\lim_{z \rightarrow z_0} (z - z_0)^2 p_2(z) = \beta_n$$

#### 14.3.7 Examples

Let us consider some examples involving Fuchsian equations of the second order.

1. Find out whether the following differential equations are Fuchsian, and enumerate the regular singular points:

$$\begin{aligned} z w'' + (1 - z) w' &= 0, \\ z^2 w'' + z w' - v^2 w &= 0, \\ z^2(1 + z)^2 w'' + 2z(z + 1)(z + 2) w' - 4w &= 0, \\ 2z(z + 2) w'' + w' - zw &= 0. \end{aligned} \tag{14.49}$$

$$\text{ad 1: } z w'' + (1 - z) w' = 0 \implies w'' + \frac{(1 - z)}{z} w' = 0$$

$z = 0$ :

$$\alpha_0 = \lim_{z \rightarrow 0} z \frac{(1 - z)}{z} = 1, \quad \beta_0 = \lim_{z \rightarrow 0} z^2 \cdot 0 = 0.$$

The equation for the characteristic exponent is

$$\sigma(\sigma - 1) + \sigma \alpha_0 + \beta_0 = 0 \implies \sigma^2 - \sigma + \sigma = 0 \implies \sigma_{1,2} = 0.$$

$z = \infty$ :  $z = \frac{1}{t}$

$$\tilde{p}_1(t) = \frac{2}{t} - \frac{\frac{(1 - \frac{1}{t})}{\frac{1}{t}}}{t^2} = \frac{2}{t} - \frac{(1 - \frac{1}{t})}{t} = \frac{1}{t} + \frac{1}{t^2} = \frac{t + 1}{t^2}$$

$\Rightarrow$  not Fuchsian.

$$\text{ad 2: } z^2 w'' + zw' - v^2 w = 0 \Rightarrow w'' + \frac{1}{z} w' - \frac{v^2}{z^2} w = 0.$$

$z = 0$ :

$$\alpha_0 = \lim_{z \rightarrow 0} z \frac{1}{z} = 1, \quad \beta_0 = \lim_{z \rightarrow 0} z^2 \left( -\frac{v^2}{z^2} \right) = -v^2.$$

$$\Rightarrow \sigma^2 - \sigma + \sigma - v^2 = 0 \Rightarrow \sigma_{1,2} = \pm v$$

$z = \infty$ :  $z = \frac{1}{t}$

$$\begin{aligned} \tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2} t = \frac{1}{t} \\ \tilde{p}_2(t) &= \frac{1}{t^4} (-t^2 v^2) = -\frac{v^2}{t^2} \\ \Rightarrow u'' + \frac{1}{t} u' - \frac{v^2}{t^2} u &= 0 \Rightarrow \sigma_{1,2} = \pm v \end{aligned}$$

$\Rightarrow$  Fuchsian equation.

ad 3:

$$z^2(1+z)^2 w'' + 2z(z+1)(z+2)w' - 4w = 0 \Rightarrow w'' + \frac{2(z+2)}{z(z+1)} w' - \frac{4}{z^2(1+z)^2} w = 0$$

$z = 0$ :

$$\alpha_0 = \lim_{z \rightarrow 0} z \frac{2(z+2)}{z(z+1)} = 4, \quad \beta_0 = \lim_{z \rightarrow 0} z^2 \left( -\frac{4}{z^2(1+z)^2} \right) = -4.$$

$$\Rightarrow \sigma(\sigma-1) + 4\sigma - 4 = \sigma^2 + 3\sigma - 4 = 0 \Rightarrow \sigma_{1,2} = \frac{-3 \pm \sqrt{9+16}}{2} = \begin{cases} -4 \\ +1 \end{cases}$$

$z = -1$ :

$$\alpha_0 = \lim_{z \rightarrow -1} (z+1) \frac{2(z+2)}{z(z+1)} = -2, \quad \beta_0 = \lim_{z \rightarrow -1} (z+1)^2 \left( -\frac{4}{z^2(1+z)^2} \right) = -4.$$

$$\Rightarrow \sigma(\sigma-1) - 2\sigma - 4 = \sigma^2 - 3\sigma - 4 = 0 \Rightarrow \sigma_{1,2} = \frac{3 \pm \sqrt{9+16}}{2} = \begin{cases} +4 \\ -1 \end{cases}$$

$z = \infty$ :

$$\begin{aligned} \tilde{p}_1(t) &= \frac{2}{t} - \frac{1}{t^2} \frac{2\left(\frac{1}{t}+2\right)}{\frac{1}{t}\left(\frac{1}{t}+1\right)} = \frac{2}{t} - \frac{2\left(\frac{1}{t}+2\right)}{1+t} = \frac{2}{t} \left( 1 - \frac{1+2t}{1+t} \right) \\ \tilde{p}_2(t) &= \frac{1}{t^4} \left( -\frac{4}{\frac{1}{t^2}\left(1+\frac{1}{t}\right)^2} \right) = -\frac{4}{t^2} \frac{t^2}{(t+1)^2} = -\frac{4}{(t+1)^2} \\ \Rightarrow u'' + \frac{2}{t} \left( 1 - \frac{1+2t}{1+t} \right) u' - \frac{4}{(t+1)^2} u &= 0 \\ \alpha_0 = \lim_{t \rightarrow 0} t \frac{2}{t} \left( 1 - \frac{1+2t}{1+t} \right) &= 0, \quad \beta_0 = \lim_{t \rightarrow 0} t^2 \left( -\frac{4}{(t+1)^2} \right) = 0. \end{aligned}$$

$$\Rightarrow \sigma(\sigma - 1) = 0 \Rightarrow \sigma_{1,2} = \begin{cases} 0 \\ 1 \end{cases}$$

$\Rightarrow$  Fuchsian equation.

ad 4:

$$2z(z+2)w'' + w' - zw = 0 \Rightarrow w'' + \frac{1}{2z(z+2)}w' - \frac{1}{2(z+2)}w = 0$$

$z = 0$ :

$$\alpha_0 = \lim_{z \rightarrow 0} z \frac{1}{2z(z+2)} = \frac{1}{4}, \quad \beta_0 = \lim_{z \rightarrow 0} z^2 \frac{-1}{2(z+2)} = 0.$$

$$\Rightarrow \sigma^2 - \sigma + \frac{1}{4}\sigma = 0 \Rightarrow \sigma^2 - \frac{3}{4}\sigma = 0 \Rightarrow \sigma_1 = 0, \sigma_2 = \frac{3}{4}.$$

$z = -2$ :

$$\alpha_0 = \lim_{z \rightarrow -2} (z+2) \frac{1}{2z(z+2)} = -\frac{1}{4}, \quad \beta_0 = \lim_{z \rightarrow -2} (z+2)^2 \frac{-1}{2(z+2)} = 0.$$

$$\Rightarrow \sigma_1 = 0, \quad \sigma_2 = \frac{5}{4}.$$

$z = \infty$ :

$$\tilde{p}_1(t) = \frac{2}{t} - \frac{1}{t^2} \left( \frac{1}{2\frac{1}{t}(\frac{1}{t}+2)} \right) = \frac{2}{t} - \frac{1}{2(1+2t)}$$

$$\tilde{p}_2(t) = \frac{1}{t^4} \frac{(-1)}{2(\frac{1}{t}+2)} = -\frac{1}{2t^3(1+2t)}$$

$\Rightarrow$  not a Fuchsian.

2. Determine the solutions of

$$z^2 w'' + (3z+1)w' + w = 0$$

around the regular singular points.

The singularities are at  $z = 0$  and  $z = \infty$ .

Singularities at  $z = 0$ :

$$p_1(z) = \frac{3z+1}{z^2} = \frac{a_1(z)}{z} \text{ with } a_1(z) = 3 + \frac{1}{z}$$

$p_1(z)$  has a pole of higher order than one; hence this is no Fuchsian equation; and  $z = 0$  is an irregular singular point.

Singularities at  $z = \infty$ :

- Transformation  $z = \frac{1}{t}$ ,  $w(z) \rightarrow u(t)$ :

$$u''(t) + \left[ \frac{2}{t} - \frac{1}{t^2} p_1\left(\frac{1}{t}\right) \right] \cdot u'(t) + \frac{1}{t^4} p_2\left(\frac{1}{t}\right) \cdot u(t) = 0.$$

The new coefficient functions are

$$\tilde{p}_1(t) = \frac{2}{t} - \frac{1}{t^2} p_1\left(\frac{1}{t}\right) = \frac{2}{t} - \frac{1}{t^2} (3t + t^2) = \frac{2}{t} - \frac{3}{t} - 1 = -\frac{1}{t} - 1$$

$$\tilde{p}_2(t) = \frac{1}{t^4} p_2\left(\frac{1}{t}\right) = \frac{t^2}{t^4} = \frac{1}{t^2}$$

- check whether this is a regular singular point:

$$\begin{aligned}\tilde{p}_1(t) &= -\frac{1+t}{t} = \frac{\tilde{a}_1(t)}{t} & \text{with } \tilde{a}_1(t) &= -(1+t) & \text{regular} \\ \tilde{p}_2(t) &= \frac{1}{t^2} = \frac{\tilde{a}_2(t)}{t^2} & \text{with } \tilde{a}_2(t) &= 1 & \text{regular}\end{aligned}$$

$\tilde{a}_1$  and  $\tilde{a}_2$  are regular at  $t = 0$ , hence this is a regular singular point.

- *Ansatz* around  $t = 0$ : the transformed equation is

$$\begin{aligned}u''(t) + \tilde{p}_1(t)u'(t) + \tilde{p}_2(t)u(t) &= 0 \\ u''(t) - \left(\frac{1}{t} + 1\right)u'(t) + \frac{1}{t^2}u(t) &= 0 \\ t^2u''(t) - (t + t^2)u'(t) + u(t) &= 0\end{aligned}$$

The generalized power series is

$$\begin{aligned}u(t) &= \sum_{n=0}^{\infty} w_n t^{n+\sigma} \\ u'(t) &= \sum_{n=0}^{\infty} w_n (n+\sigma) t^{n+\sigma-1} \\ u''(t) &= \sum_{n=0}^{\infty} w_n (n+\sigma)(n+\sigma-1) t^{n+\sigma-2}\end{aligned}$$

If we insert this into the transformed differential equation we obtain

$$\begin{aligned}& t^2 \sum_{n=0}^{\infty} w_n (n+\sigma)(n+\sigma-1) t^{n+\sigma-2} - \\ & - (t + t^2) \sum_{n=0}^{\infty} w_n (n+\sigma) t^{n+\sigma-1} + \sum_{n=0}^{\infty} w_n t^{n+\sigma} = 0 \\ & \sum_{n=0}^{\infty} w_n (n+\sigma)(n+\sigma-1) t^{n+\sigma} - \sum_{n=0}^{\infty} w_n (n+\sigma) t^{n+\sigma} - \\ & - \sum_{n=0}^{\infty} w_n (n+\sigma) t^{n+\sigma+1} + \sum_{n=0}^{\infty} w_n t^{n+\sigma} = 0\end{aligned}$$

Change of index:  $m = n + 1$ ,  $n = m - 1$  in the third sum yields

$$\sum_{n=0}^{\infty} w_n \left[ (n+\sigma)(n+\sigma-2) + 1 \right] t^{n+\sigma} - \sum_{m=1}^{\infty} w_{m-1} (m-1+\sigma) t^{m+\sigma} = 0.$$

In the second sum, substitute  $m$  for  $n$

$$\sum_{n=0}^{\infty} w_n \left[ (n+\sigma)(n+\sigma-2) + 1 \right] t^{n+\sigma} - \sum_{n=1}^{\infty} w_{n-1} (n+\sigma-1) t^{n+\sigma} = 0.$$

We write out explicitly the  $n = 0$  term of the first sum

$$\begin{aligned}w_0 \left[ \sigma(\sigma-2) + 1 \right] t^{\sigma} + \sum_{n=1}^{\infty} w_n \left[ (n+\sigma)(n+\sigma-2) + 1 \right] t^{n+\sigma} - \\ - \sum_{n=1}^{\infty} w_{n-1} (n+\sigma-1) t^{n+\sigma} = 0.\end{aligned}$$

Now we can combine the two sums

$$w_0 \left[ \sigma(\sigma-2)+1 \right] t^\sigma + \sum_{n=1}^{\infty} \left\{ w_n \left[ (n+\sigma)(n+\sigma-2)+1 \right] - w_{n-1} (n+\sigma-1) \right\} t^{n+\sigma} = 0.$$

The left hand side can only vanish for all  $t$  if the coefficients vanish; hence

$$w_0 \left[ \sigma(\sigma-2)+1 \right] = 0, \quad (14.50)$$

$$w_n \left[ (n+\sigma)(n+\sigma-2)+1 \right] - w_{n-1} (n+\sigma-1) = 0. \quad (14.51)$$

ad (14.50) for  $w_0$ :

$$\begin{aligned} \sigma(\sigma-2)+1 &= 0 \\ \sigma^2-2\sigma+1 &= 0 \\ (\sigma-1)^2 &= 0 \implies \sigma_{\infty}^{(1,2)} = 1 \end{aligned}$$

The characteristic exponent is  $\sigma_{\infty}^{(1)} = \sigma_{\infty}^{(2)} = 1$ .

ad (14.51) for  $w_n$ : For the coefficients  $w_n$  we obtain the recursion formula

$$\begin{aligned} w_n \left[ (n+\sigma)(n+\sigma-2)+1 \right] &= w_{n-1} (n+\sigma-1) \\ \implies w_n &= \frac{n+\sigma-1}{(n+\sigma)(n+\sigma-2)+1} w_{n-1}. \end{aligned}$$

Let us insert  $\sigma = 1$ :

$$w_n = \frac{n}{(n+1)(n-1)+1} w_{n-1} = \frac{n}{n^2-1+1} w_{n-1} = \frac{n}{n^2} w_{n-1} = \frac{1}{n} w_{n-1}.$$

We can fix  $w_0 = 1$ , hence:

$$\begin{aligned} w_0 &= 1 = \frac{1}{1} = \frac{1}{0!} \\ w_1 &= \frac{1}{1} = \frac{1}{1!} \\ w_2 &= \frac{1}{1 \cdot 2} = \frac{1}{2!} \\ w_3 &= \frac{1}{1 \cdot 2 \cdot 3} = \frac{1}{3!} \\ &\vdots \\ w_n &= \frac{1}{1 \cdot 2 \cdot 3 \cdot \dots \cdot n} = \frac{1}{n!} \end{aligned}$$

And finally,

$$u_1(t) = t^\sigma \sum_{n=0}^{\infty} w_n t^n = t \sum_{n=0}^{\infty} \frac{t^n}{n!} = t e^t.$$

- Notice that both characteristic exponents are equal; hence we have to employ the d'Alembert reduction

$$u_2(t) = u_1(t) \int_0^t v(s) ds$$

with

$$v'(t) + v(t) \left[ 2 \frac{u_1'(t)}{u_1(t)} + \tilde{p}_1(t) \right] = 0.$$

Insertion of  $u_1$  and  $\tilde{p}_1$ ,

$$\begin{aligned} u_1(t) &= te^t \\ u_1'(t) &= e^t(1+t) \\ \tilde{p}_1(t) &= -\left(\frac{1}{t} + 1\right), \end{aligned}$$

yields

$$\begin{aligned} v'(t) + v(t) \left( 2 \frac{e^t(1+t)}{te^t} - \frac{1}{t} - 1 \right) &= 0 \\ v'(t) + v(t) \left( 2 \frac{(1+t)}{t} - \frac{1}{t} - 1 \right) &= 0 \\ v'(t) + v(t) \left( \frac{2}{t} + 2 - \frac{1}{t} - 1 \right) &= 0 \\ v'(t) + v(t) \left( \frac{1}{t} + 1 \right) &= 0 \\ \frac{dv}{dt} &= -v \left( 1 + \frac{1}{t} \right) \\ \frac{dv}{v} &= -\left( 1 + \frac{1}{t} \right) dt \end{aligned}$$

Upon integration of both sides we obtain

$$\begin{aligned} \int \frac{dv}{v} &= -\int \left( 1 + \frac{1}{t} \right) dt \\ \log v &= -(t + \log t) = -t - \log t \\ v &= \exp(-t - \log t) = e^{-t} e^{-\log t} = \frac{e^{-t}}{t}, \end{aligned}$$

and hence an explicit form of  $v(t)$ :

$$v(t) = \frac{1}{t} e^{-t}.$$

If we insert this into the equation for  $u_2$  we obtain

$$u_2(t) = te^t \int_0^t \frac{1}{s} e^{-s} ds.$$

- Therefore, with  $t = \frac{1}{z}$ ,  $u(t) = w(z)$ , the two linear independent solutions around the regular singular point at  $z = \infty$  are

$$\begin{aligned} w_1(z) &= \frac{1}{z} \exp\left(\frac{1}{z}\right), \text{ and} \\ w_2(z) &= \frac{1}{z} \exp\left(\frac{1}{z}\right) \int_0^{\frac{1}{z}} \frac{1}{t} e^{-t} dt. \end{aligned} \quad (14.52)$$

## 14.4 Hypergeometric function

### 14.4.1 Definition

A *hypergeometric series* is a series

$$\sum_{j=0}^{\infty} c_j, \quad (14.53)$$

where the quotients  $\frac{c_{j+1}}{c_j}$  are *rational functions* (that is, the quotient of two polynomials) of  $j$ , so that they can be factorized by

$$\begin{aligned} \frac{c_{j+1}}{c_j} &= \frac{(j+a_1)(j+a_2)\cdots(j+a_p)}{(j+b_1)(j+b_2)\cdots(j+b_q)} \left(\frac{x}{j+1}\right), \\ \text{or } c_{j+1} &= c_j \frac{(j+a_1)(j+a_2)\cdots(j+a_p)}{(j+b_1)(j+b_2)\cdots(j+b_q)} \left(\frac{x}{j+1}\right) \\ &= c_{j-1} \frac{(j-1+a_1)(j-1+a_2)\cdots(j-1+a_p)}{(j-1+b_1)(j-1+b_2)\cdots(j-1+b_q)} \times \\ &\quad \times \frac{(j+a_1)(j+a_2)\cdots(j+a_p)}{(j+b_1)(j+b_2)\cdots(j+b_q)} \left(\frac{x}{j}\right) \left(\frac{x}{j+1}\right) \\ &= c_0 \frac{a_1 a_2 \cdots a_p}{b_1 b_2 \cdots b_q} \cdots \frac{(j-1+a_1)(j-1+a_2)\cdots(j-1+a_p)}{(j-1+b_1)(j-1+b_2)\cdots(j-1+b_q)} \times \\ &\quad \times \frac{(j+a_1)(j+a_2)\cdots(j+a_p)}{(j+b_1)(j+b_2)\cdots(j+b_q)} \left(\frac{x}{1}\right) \cdots \left(\frac{x}{j}\right) \left(\frac{x}{j+1}\right) \\ &= c_0 \frac{(a_1)_{j+1} (a_2)_{j+1} \cdots (a_p)_{j+1}}{(b_1)_{j+1} (b_2)_{j+1} \cdots (b_q)_{j+1}} \left(\frac{x^{j+1}}{(j+1)!}\right). \end{aligned} \quad (14.54)$$

The factor  $j+1$  in the denominator has been chosen to define the particular factor  $j!$  in a definition given later and below; if it does not arise “naturally” we may just obtain it by compensating it with a factor  $j+1$  in the numerator. With this ratio, the hypergeometric series (14.53) can be written in terms of *shifted factorials*, or, by another naming, the *Pochhammer symbol*, as

$$\begin{aligned} \sum_{j=0}^{\infty} c_j &= c_0 \sum_{j=0}^{\infty} \frac{(a_1)_j (a_2)_j \cdots (a_p)_j}{(b_1)_j (b_2)_j \cdots (b_q)_j} \frac{x^j}{j!} \\ &= c_0 {}_pF_q \left( \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_p \end{matrix} ; x \right), \text{ or} \\ &= c_0 {}_pF_q (a_1, \dots, a_p; b_1, \dots, b_p; x). \end{aligned} \quad (14.55)$$

Apart from this definition *via* hypergeometric series, the Gauss *hypergeometric function*, or, used synonymously, the *Gauss series*

$$\begin{aligned} {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix}; x\right) &= {}_2F_1(a, b; c; x) = \sum_{j=0}^{\infty} \frac{(a)_j (b)_j}{(c)_j} \frac{x^j}{j!} \\ &= 1 + \frac{ab}{c}x + \frac{1}{2!} \frac{a(a+1)b(b+1)}{c(c+1)}x^2 + \dots \end{aligned} \quad (14.56)$$

can be defined as a solution of a *Fuchsian differential equation* which has at most *three regular singularities* at 0, 1, and  $\infty$ .

Indeed, any Fuchsian equation with finite regular singularities at  $x_1$  and  $x_2$  can be rewritten into the *Riemann differential equation* (14.32), which in turn can be rewritten into the *Gaussian differential equation* or *hypergeometric differential equation* with regular singularities at 0, 1, and  $\infty$ <sup>10</sup>. This can be demonstrated by rewriting any such equation of the form

$$\begin{aligned} w''(x) + \left(\frac{A_1}{x-x_1} + \frac{A_2}{x-x_2}\right)w'(x) \\ + \left(\frac{B_1}{(x-x_1)^2} + \frac{B_2}{(x-x_2)^2} + \frac{C_1}{x-x_1} + \frac{C_2}{x-x_2}\right)w(x) = 0 \end{aligned} \quad (14.57)$$

through transforming Eq. (14.57) into the *hypergeometric equation*

$$\left[\frac{d^2}{dx^2} + \frac{(a+b+1)x-c}{x(x-1)}\frac{d}{dx} + \frac{ab}{x(x-1)}\right] {}_2F_1(a, b; c; x) = 0, \quad (14.58)$$

where the solution is proportional to the Gauss hypergeometric function

$$w(x) \longrightarrow (x-x_1)^{\sigma_1^{(1)}}(x-x_2)^{\sigma_2^{(2)}} {}_2F_1(a, b; c; x), \quad (14.59)$$

and the variable transform as

$$\begin{aligned} x &\longrightarrow x = \frac{x-x_1}{x_2-x_1}, \text{ with} \\ a &= \sigma_1^{(1)} + \sigma_2^{(1)} + \sigma_{\infty}^{(1)}, \\ b &= \sigma_1^{(1)} + \sigma_2^{(1)} + \sigma_{\infty}^{(2)}, \\ c &= 1 + \sigma_1^{(1)} - \sigma_1^{(2)}. \end{aligned} \quad (14.60)$$

where  $\sigma_j^{(i)}$  stands for the  $i$ th characteristic exponent of the  $j$ th singularity.

Whereas the full transformation from Eq. (14.57) to the hypergeometric equation (14.58) will not be given, we shall show that the Gauss hypergeometric function  ${}_2F_1$  satisfies the hypergeometric equation (14.58).

First, define the differential operator

$$\vartheta = x \frac{d}{dx}, \quad (14.61)$$

<sup>10</sup> Einar Hille. *Lectures on ordinary differential equations*. Addison-Wesley, Reading, Mass., 1969; Garrett Birkhoff and Gian-Carlo Rota. *Ordinary Differential Equations*. John Wiley & Sons, New York, Chichester, Brisbane, Toronto, fourth edition, 1959, 1960, 1962, 1969, 1978, and 1989; and Gerhard Kristensson. *Equations of Fuchsian type*. In *Second Order Differential Equations*, pages 29–42. Springer, New York, 2010. ISBN 978-1-4419-7019-0. DOI: 10.1007/978-1-4419-7020-6. URL <http://dx.doi.org/10.1007/978-1-4419-7020-6>

The Bessel equation has a regular singular point at 0, and an irregular singular point at infinity.



and observe that

$$\begin{aligned}
 \vartheta(\vartheta + c - 1)x^n &= x \frac{d}{dx} \left( x \frac{d}{dx} + c - 1 \right) x^n \\
 &= x \frac{d}{dx} (x n x^{n-1} + c x^n - x^n) \\
 &= x \frac{d}{dx} (n x^n + c x^n - x^n) \\
 &= x \frac{d}{dx} (n + c - 1) x^n \\
 &= n(n + c - 1) x^n.
 \end{aligned} \tag{14.62}$$

Thus, if we apply  $\vartheta(\vartheta + c - 1)$  to  ${}_2F_1$ , then

$$\begin{aligned}
 \vartheta(\vartheta + c - 1) {}_2F_1(a, b; c; x) &= \vartheta(\vartheta + c - 1) \sum_{j=0}^{\infty} \frac{(a)_j (b)_j}{(c)_j} \frac{x^j}{j!} \\
 &= \sum_{j=0}^{\infty} \frac{(a)_j (b)_j}{(c)_j} \frac{j(j + c - 1)x^j}{j!} = \sum_{j=1}^{\infty} \frac{(a)_j (b)_j}{(c)_j} \frac{j(j + c - 1)x^j}{j!} \\
 &= \sum_{j=1}^{\infty} \frac{(a)_j (b)_j}{(c)_j} \frac{(j + c - 1)x^j}{(j - 1)!} \\
 &\quad [\text{index shift: } j \rightarrow n + 1, n = j - 1, n \geq 0] \\
 &= \sum_{n=0}^{\infty} \frac{(a)_{n+1} (b)_{n+1}}{(c)_{n+1}} \frac{(n + 1 + c - 1)x^{n+1}}{n!} \\
 &= x \sum_{n=0}^{\infty} \frac{(a)_n (a + n) (b)_n (b + n)}{(c)_n (c + n)} \frac{(n + c)x^n}{n!} \\
 &= x \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{(a + n)(b + n)x^n}{n!} \\
 &= x(\vartheta + a)(\vartheta + b) \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{x^n}{n!} = x(\vartheta + a)(\vartheta + b) {}_2F_1(a, b; c; x),
 \end{aligned} \tag{14.63}$$

where we have used

$$\begin{aligned}
 (a + n)x^n &= (a + \vartheta)x^n, \text{ and} \\
 (a)_{n+1} &= a(a + 1) \cdots (a + n - 1)(a + n) = (a)_n(a + n).
 \end{aligned} \tag{14.64}$$

Writing out  $\vartheta$  in Eq. (14.63) explicitly yields

$$\begin{aligned}
 & \{\vartheta(\vartheta + c - 1) - x(\vartheta + a)(\vartheta + b)\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ x \frac{d}{dx} \left( x \frac{d}{dx} + c - 1 \right) - x \left( x \frac{d}{dx} + a \right) \left( x \frac{d}{dx} + b \right) \right\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ \frac{d}{dx} \left( x \frac{d}{dx} + c - 1 \right) - \left( x \frac{d}{dx} + a \right) \left( x \frac{d}{dx} + b \right) \right\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ \frac{d}{dx} + x \frac{d^2}{dx^2} + (c - 1) \frac{d}{dx} - \left( x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} + bx \frac{d}{dx} \right. \right. \\
 & \quad \left. \left. + ax \frac{d}{dx} + ab \right) \right\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ (x - x^2) \frac{d^2}{dx^2} + (1 + c - 1 - x - x(a + b)) \frac{d}{dx} + ab \right\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ -x(x - 1) \frac{d^2}{dx^2} - (c - x(1 + a + b)) \frac{d}{dx} - ab \right\} {}_2F_1(a, b; c; x) = 0, \\
 & \left\{ \frac{d^2}{dx^2} + \frac{x(1 + a + b) - c}{x(x - 1)} \frac{d}{dx} + \frac{ab}{x(x - 1)} \right\} {}_2F_1(a, b; c; x) = 0.
 \end{aligned} \tag{14.65}$$

#### 14.4.2 Properties

There exist many properties of the hypergeometric series. In the following we shall mention a few.

$$\frac{d}{dz} {}_2F_1(a, b; c; z) = \frac{ab}{c} {}_2F_1(a + 1, b + 1; c + 1; z). \tag{14.66}$$

$$\begin{aligned}
 \frac{d}{dz} {}_2F_1(a, b; c; z) &= \frac{d}{dz} \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!} = \\
 &= \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} n \frac{z^{n-1}}{n!} \\
 &= \sum_{n=1}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^{n-1}}{(n-1)!}
 \end{aligned}$$

An index shift  $n \rightarrow m + 1$ ,  $m = n - 1$ , and a subsequent renaming  $m \rightarrow n$ , yields

$$\frac{d}{dz} {}_2F_1(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_{n+1} (b)_{n+1}}{(c)_{n+1}} \frac{z^n}{n!}.$$

As

$$\begin{aligned}
 (x)_{n+1} &= x(x+1)(x+2) \cdots (x+n-1)(x+n) \\
 (x+1)_n &= (x+1)(x+2) \cdots (x+n-1)(x+n) \\
 (x)_{n+1} &= x(x+1)_n
 \end{aligned}$$

holds, we obtain

$$\frac{d}{dz} {}_2F_1(a, b; c; z) = \sum_{n=0}^{\infty} \frac{ab}{c} \frac{(a+1)_n (b+1)_n}{(c+1)_n} \frac{z^n}{n!} = \frac{ab}{c} {}_2F_1(a+1, b+1; c+1; z).$$

We state *Euler's integral representation* for  $\Re c > 0$  and  $\Re b > 0$  without proof:

$${}_2F_1(a, b; c; x) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1} (1-t)^{c-b-1} (1-xt)^{-a} dt. \quad (14.67)$$

For  $\Re(c-a-b) > 0$ , we also state Gauss' theorem

$${}_2F_1(a, b; c; 1) = \sum_{j=0}^{\infty} \frac{(a)_j (b)_j}{j! (c)_j} = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}. \quad (14.68)$$

For a proof, we can set  $x = 1$  in Euler's integral representation, and the Beta function defined in Eq. (14.20).

#### 14.4.3 Plasticity

Some of the most important elementary functions can be expressed as hypergeometric series; most importantly the Gaussian one  ${}_2F_1$ , which is sometimes denoted by just  $F$ . Let us enumerate a few.

$$e^x = {}_0F_0(-; -; x) \quad (14.69)$$

$$\cos x = {}_0F_1(-; \frac{1}{2}; -\frac{x^2}{4}) \quad (14.70)$$

$$\sin x = x {}_0F_1(-; \frac{3}{2}; -\frac{x^2}{4}) \quad (14.71)$$

$$(1-x)^{-a} = {}_1F_0(a; -; x) \quad (14.72)$$

$$\sin^{-1} x = x {}_2F_1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; x^2) \quad (14.73)$$

$$\tan^{-1} x = x {}_2F_1(\frac{1}{2}, 1; \frac{3}{2}; -x^2) \quad (14.74)$$

$$\log(1+x) = x {}_2F_1(1, 1; 2; -x) \quad (14.75)$$

$$H_{2n}(x) = \frac{(-1)^n (2n)!}{n!} {}_1F_1(-n; \frac{1}{2}; x^2) \quad (14.76)$$

$$H_{2n+1}(x) = 2x \frac{(-1)^n (2n+1)!}{n!} {}_1F_1(-n; \frac{3}{2}; x^2) \quad (14.77)$$

$$L_n^\alpha(x) = \binom{n+\alpha}{n} {}_1F_1(-n; \alpha+1; x) \quad (14.78)$$

$$P_n(x) = P_n^{(0,0)}(x) = {}_2F_1(-n, n+1; 1; \frac{1-x}{2}), \quad (14.79)$$

$$C_n^\gamma(x) = \frac{(2\gamma)_n}{(\gamma + \frac{1}{2})_n} P_n^{(\gamma-\frac{1}{2}, \gamma-\frac{1}{2})}(x), \quad (14.80)$$

$$T_n(x) = \frac{n!}{(\frac{1}{2})_n} P_n^{(-\frac{1}{2}, -\frac{1}{2})}(x), \quad (14.81)$$

$$J_\alpha(x) = \frac{(\frac{x}{2})^\alpha}{\Gamma(\alpha+1)} {}_0F_1(-; \alpha+1; -\frac{1}{4}x^2), \quad (14.82)$$

where  $H$  stands for *Hermite polynomials*,  $L$  for *Laguerre polynomials*,

$$P_n^{(\alpha, \beta)}(x) = \frac{(\alpha+1)_n}{n!} {}_2F_1(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}) \quad (14.83)$$

for *Jacobi polynomials*, *C* for *Gegenbauer polynomials*, *T* for *Chebyshev polynomials*, *P* for *Legendre polynomials*, and *J* for the *Bessel functions of the first kind*, respectively.

1. Let us prove that

$$\log(1-z) = -z {}_2F_1(1, 1, 2; z).$$

Consider

$${}_2F_1(1, 1, 2; z) = \sum_{m=0}^{\infty} \frac{[(1)_m]^2}{(2)_m} \frac{z^m}{m!} = \sum_{m=0}^{\infty} \frac{[1 \cdot 2 \cdots m]^2}{2 \cdot (2+1) \cdots (2+m-1)} \frac{z^m}{m!}$$

With

$$(1)_m = 1 \cdot 2 \cdots m = m!, \quad (2)_m = 2 \cdot (2+1) \cdots (2+m-1) = (m+1)!$$

follows

$${}_2F_1(1, 1, 2; z) = \sum_{m=0}^{\infty} \frac{[m!]^2}{(m+1)!} \frac{z^m}{m!} = \sum_{m=0}^{\infty} \frac{z^m}{m+1}.$$

Index shift  $k = m + 1$

$${}_2F_1(1, 1, 2; z) = \sum_{k=1}^{\infty} \frac{z^{k-1}}{k}$$

and hence

$$-z {}_2F_1(1, 1, 2; z) = -\sum_{k=1}^{\infty} \frac{z^k}{k}.$$

Compare with the series

$$\log(1+x) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{x^k}{k} \quad \text{for } -1 < x \leq 1$$

If one substitutes  $-x$  for  $x$ , then

$$\log(1-x) = -\sum_{k=1}^{\infty} \frac{x^k}{k}.$$

The identity follows from the analytic continuation of  $x$  to the complex  $z$  plane.

2. Let us prove that, because of  $(a+z)^n = \sum_{k=0}^n \binom{n}{k} z^k a^{n-k}$ ,

$$(1-z)^n = {}_2F_1(-n, 1, 1; z).$$

$${}_2F_1(-n, 1, 1; z) = \sum_{i=0}^{\infty} \frac{(-n)_i (1)_i}{(1)_i} \frac{z^i}{i!} = \sum_{i=0}^{\infty} (-n)_i \frac{z^i}{i!}.$$

Consider  $(-n)_i$

$$(-n)_i = (-n)(-n+1) \cdots (-n+i-1).$$

For even  $n \geq 0$  the series stops after a finite number of terms, because the factor  $-n+i-1=0$  for  $i=n+1$  vanishes; hence the sum of  $i$  extends only from 0 to  $n$ . Hence, if we collect the factors  $(-1)$  which yield  $(-1)^i$  we obtain

$$(-n)_i = (-1)^i n(n-1) \cdots [n-(i-1)] = (-1)^i \frac{n!}{(n-i)!}.$$

Hence, insertion into the Gauss hypergeometric function yields

$${}_2F_1(-n, 1, 1; z) = \sum_{i=0}^n (-1)^i z^i \frac{n!}{i!(n-i)!} = \sum_{i=0}^n \binom{n}{i} (-z)^i.$$

This is the binomial series

$$(1+x)^n = \sum_{k=0}^n \binom{n}{k} x^k$$

with  $x = -z$ ; and hence,

$${}_2F_1(-n, 1, 1; z) = (1-z)^n.$$

3. Let us prove that, because of  $\arcsin x = \sum_{k=0}^{\infty} \frac{(2k)! x^{2k+1}}{2^{2k}(k!)^2(2k+1)}$ ,

$${}_2F_1\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \sin^2 z\right) = \frac{z}{\sin z}.$$

Consider

$${}_2F_1\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \sin^2 z\right) = \sum_{m=0}^{\infty} \frac{\left[\left(\frac{1}{2}\right)_m\right]^2}{\left(\frac{3}{2}\right)_m} \frac{(\sin z)^{2m}}{m!}.$$

We take

$$\begin{aligned} (2n)!! &= 2 \cdot 4 \cdot \cdots \cdot (2n) = n! 2^n \\ (2n-1)!! &= 1 \cdot 3 \cdot \cdots \cdot (2n-1) = \frac{(2n)!}{2^n n!} \end{aligned}$$

Hence

$$\begin{aligned} \left(\frac{1}{2}\right)_m &= \frac{1}{2} \cdot \left(\frac{1}{2} + 1\right) \cdots \left(\frac{1}{2} + m - 1\right) = \frac{1 \cdot 3 \cdot 5 \cdots (2m-1)}{2^m} = \frac{(2m-1)!!}{2^m} \\ \left(\frac{3}{2}\right)_m &= \frac{3}{2} \cdot \left(\frac{3}{2} + 1\right) \cdots \left(\frac{3}{2} + m - 1\right) = \frac{3 \cdot 5 \cdot 7 \cdots (2m+1)}{2^m} = \frac{(2m+1)!!}{2^m} \end{aligned}$$

Therefore,

$$\frac{\left(\frac{1}{2}\right)_m}{\left(\frac{3}{2}\right)_m} = \frac{1}{2m+1}.$$

On the other hand,

$$\begin{aligned} (2m)! &= 1 \cdot 2 \cdot 3 \cdots (2m-1)(2m) = (2m-1)!!(2m)!! = \\ &= 1 \cdot 3 \cdot 5 \cdots (2m-1) \cdot 2 \cdot 4 \cdot 6 \cdots (2m) = \\ &= \left(\frac{1}{2}\right)_m 2^m \cdot 2^m m! = 2^{2m} m! \left(\frac{1}{2}\right)_m \Rightarrow \left(\frac{1}{2}\right)_m = \frac{(2m)!}{2^{2m} m!} \end{aligned}$$

Upon insertion one obtains

$$F\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \sin^2 z\right) = \sum_{m=0}^{\infty} \frac{(2m)!(\sin z)^{2m}}{2^{2m}(m!)^2(2m+1)}.$$

Comparing with the series for arcsin one finally obtains

$$\sin z F\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \sin^2 z\right) = \arcsin(\sin z) = z.$$

#### 14.4.4 Four forms

We state without proof the four forms of the Gauss hypergeometric function <sup>11</sup>.

$${}_2F_1(a, b; c; x) = (1-x)^{c-a-b} {}_2F_1(c-a, c-b; c; x) \quad (14.84)$$

$$= (1-x)^{-a} {}_2F_1\left(a, c-b; c; \frac{x}{x-1}\right) \quad (14.85)$$

$$= (1-x)^{-b} {}_2F_1\left(b, c-a; c; \frac{x}{x-1}\right). \quad (14.86)$$

### 14.5 Orthogonal polynomials

Many systems or sequences of functions may serve as a *basis of linearly independent functions* which are capable to “cover” – that is, to approximate – certain functional classes <sup>12</sup>. We have already encountered at least two such prospective bases [cf. Eq. (9.12)]:

$$\{1, x, x^2, \dots, x^k, \dots\} \text{ with } f(x) = \sum_{k=0}^{\infty} c_k x^k, \quad (14.87)$$

and

$$\left\{e^{ikx} \mid k \in \mathbb{Z}\right\} \quad \text{for } f(x+2\pi) = f(x) \\ \text{with } f(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx}, \quad (14.88)$$

$$\text{where } c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} dx.$$

In order to claim existence of such functional basis systems, let us first define what *orthogonality* means in the functional context. Just as for linear vector spaces, we can define an *inner product* or *scalar product* [cf. also Eq. (9.4)] of two real-valued functions  $f(x)$  and  $g(x)$  by the integral <sup>13</sup>

$$\langle f \mid g \rangle = \int_a^b f(x) g(x) \rho(x) dx \quad (14.89)$$

for some suitable *weight function*  $\rho(x) \geq 0$ . Very often, the weight function is set to unity; that is,  $\rho(x) = \rho = 1$ . We notice without proof that  $\langle f \mid$

<sup>11</sup> T. M. MacRobert. *Spherical Harmonics. An Elementary Treatise on Harmonic Functions with Applications*, volume 98 of *International Series of Monographs in Pure and Applied Mathematics*. Pergamon Press, Oxford, 3rd edition, 1967

<sup>12</sup> Russell Herman. *A Second Course in Ordinary Differential Equations: Dynamical Systems and Boundary Value Problems*. University of North Carolina Wilmington, Wilmington, NC, 2008. URL [http://people.uncw.edu/hermanr/mat463/ODEBook/Book/ODE\\_LargeFont.pdf](http://people.uncw.edu/hermanr/mat463/ODEBook/Book/ODE_LargeFont.pdf). Creative Commons Attribution-NoncommercialShare Alike 3.0 United States License; and Francisco Marcellán and Walter Van Assche. *Orthogonal Polynomials and Special Functions*, volume 1883 of *Lecture Notes in Mathematics*. Springer, Berlin, 2006. ISBN 3-540-31062-2

<sup>13</sup> Herbert S. Wilf. *Mathematics for the physical sciences*. Dover, New York, 1962. URL [http://www.math.upenn.edu/~wilf/website/Mathematics\\_for\\_the\\_Physical\\_Sciences.html](http://www.math.upenn.edu/~wilf/website/Mathematics_for_the_Physical_Sciences.html)

$g\rangle$  satisfies all requirements of a scalar product. A system of functions  $\{\psi_0, \psi_1, \psi_2, \dots, \psi_k, \dots\}$  is orthogonal if, for  $j \neq k$ ,

$$\langle \psi_j | \psi_k \rangle = \int_a^b \psi_j(x) \psi_k(x) \rho(x) dx = 0. \quad (14.90)$$

Suppose, in some generality, that  $\{f_0, f_1, f_2, \dots, f_k, \dots\}$  is a sequence of nonorthogonal functions. Then we can apply a *Gram-Schmidt orthogonalization process* to these functions and thereby obtain orthogonal functions  $\{\phi_0, \phi_1, \phi_2, \dots, \phi_k, \dots\}$  by

$$\begin{aligned} \phi_0(x) &= f_0(x), \\ \phi_k(x) &= f_k(x) - \sum_{j=0}^{k-1} \frac{\langle f_k | \phi_j \rangle}{\langle \phi_j | \phi_j \rangle} \phi_j(x). \end{aligned} \quad (14.91)$$

Note that the proof of the Gram-Schmidt process in the functional context is analogous to the one in the vector context.

### 14.6 Legendre polynomials

The system of polynomial functions  $\{1, x, x^2, \dots, x^k, \dots\}$  is such a non orthogonal sequence in this sense, as, for instance, with  $\rho = 1$  and  $b = -a = 1$ ,

$$\langle 1 | x^2 \rangle = \int_{a=-1}^{b=1} x^2 dx = \frac{x^3}{3} \Big|_{x=-1}^{x=1} = \frac{2}{3}. \quad (14.92)$$

Hence, by the Gram-Schmidt process we obtain

$$\begin{aligned} \phi_0(x) &= 1, \\ \phi_1(x) &= x - \frac{\langle x | 1 \rangle}{\langle 1 | 1 \rangle} 1 \\ &= x - 0 = x, \\ \phi_2(x) &= x^2 - \frac{\langle x^2 | 1 \rangle}{\langle 1 | 1 \rangle} 1 - \frac{\langle x^2 | x \rangle}{\langle x | x \rangle} x \\ &= x^2 - \frac{2/3}{2} 1 - 0x = x^2 - \frac{1}{3}, \\ &\vdots \end{aligned} \quad (14.93)$$

If, on top of orthogonality, we are “forcing” a type of “normalization” by defining

$$\begin{aligned} P_l(x) &\stackrel{\text{def}}{=} \frac{\phi_l(x)}{\phi_l(1)}, \\ &\text{with } P_l(1) = 1, \end{aligned} \quad (14.94)$$

then the resulting orthogonal polynomials are the *Legendre polynomials*  $P_l$ ; in particular,

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= \left(x^2 - \frac{1}{3}\right) / \frac{2}{3} = \frac{1}{2}(3x^2 - 1), \\ &\vdots \end{aligned} \quad (14.95)$$

with  $P_l(1) = 1$ ,  $l \in \mathbb{N}_0$ .

Why should we be interested in orthonormal systems of functions? Because, as pointed out earlier in the context of hypergeometric functions, they could be alternatively defined as the eigenfunctions and solutions of certain differential equation, such as, for instance, the Schrödinger equation, which may be subjected to a separation of variables. For Legendre polynomials the associated differential equation is the *Legendre equation*

$$\begin{aligned} &\left\{ (1-x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + l(l+1) \right\} P_l(x) = 0, \\ &\text{or } \left\{ \frac{d}{dx} \left( (1-x^2) \frac{d}{dx} \right) + l(l+1) \right\} P_l(x) = 0 \end{aligned} \quad (14.96)$$

for  $l \in \mathbb{N}_0$ , whose Sturm-Liouville form has been mentioned earlier in Table 12.1 on page 200. For a proof, we refer to the literature.

#### 14.6.1 Rodrigues formula

A third alternative definition of Legendre polynomials is by the Rodrigues formula

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l, \text{ for } l \in \mathbb{N}_0. \quad (14.97)$$

Again, no proof of equivalence will be given.

For even  $l$ ,  $P_l(x) = P_l(-x)$  is an even function of  $x$ , whereas for odd  $l$ ,  $P_l(x) = -P_l(-x)$  is an odd function of  $x$ ; that is,

$$P_l(-x) = (-1)^l P_l(x). \quad (14.98)$$

Moreover,

$$P_l(-1) = (-1)^l \quad (14.99)$$

and

$$P_{2k+1}(0) = 0. \quad (14.100)$$

This can be shown by the substitution  $t = -x$ ,  $dt = -dx$ , and insertion into the Rodrigues formula:

$$\begin{aligned} P_l(-x) &= \frac{1}{2^l l!} \frac{d^l}{du^l} (u^2 - 1)^l \Big|_{u=-x} = [u \rightarrow -u] = \\ &= \frac{1}{(-1)^l} \frac{1}{2^l l!} \frac{d^l}{du^l} (u^2 - 1)^l \Big|_{u=x} = (-1)^l P_l(x). \end{aligned}$$



Because of the “normalization”  $P_l(1) = 1$  we obtain

$$P_l(-1) = (-1)^l P_l(1) = (-1)^l.$$

And as  $P_l(-0) = P_l(0) = (-1)^l P_l(0)$ , we obtain  $P_l(0) = 0$  for odd  $l$ .

### 14.6.2 Generating function

For  $|x| < 1$  and  $|t| < 1$  the Legendre polynomials  $P_l(x)$  are the coefficients in the Taylor series expansion of the following generating function

$$g(x, t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{l=0}^{\infty} P_l(x) t^l \quad (14.101)$$

around  $t = 0$ . No proof is given here.

### 14.6.3 The three term and other recursion formulae

Among other things, generating functions are useful for the derivation of certain recursion relations involving Legendre polynomials.

For instance, for  $l = 1, 2, \dots$ , the three term recursion formula

$$(2l+1)xP_l(x) = (l+1)P_{l+1}(x) + lP_{l-1}(x), \quad (14.102)$$

or, by substituting  $l-1$  for  $l$ , for  $l = 2, 3, \dots$ ,

$$(2l-1)xP_{l-1}(x) = lP_l(x) + (l-1)P_{l-2}(x), \quad (14.103)$$

can be proven as follows.

$$\begin{aligned} g(x, t) &= \frac{1}{\sqrt{1-2tx+t^2}} = \sum_{n=0}^{\infty} t^n P_n(x) \\ \frac{\partial}{\partial t} g(x, t) &= -\frac{1}{2}(1-2tx+t^2)^{-\frac{3}{2}}(-2x+2t) = \frac{1}{\sqrt{1-2tx+t^2}} \frac{x-t}{1-2tx+t^2} \\ \frac{\partial}{\partial t} g(x, t) &= \frac{x-t}{1-2tx+t^2} \sum_{n=0}^{\infty} t^n P_n(x) = \sum_{n=0}^{\infty} n t^{n-1} P_n(x) \\ (x-t) \sum_{n=0}^{\infty} t^n P_n(x) - (1-2tx+t^2) \sum_{n=0}^{\infty} n t^{n-1} P_n(x) &= 0 \\ \sum_{n=0}^{\infty} x t^n P_n(x) - \sum_{n=0}^{\infty} t^{n+1} P_n(x) - \sum_{n=1}^{\infty} n t^{n-1} P_n(x) + \\ &\quad + \sum_{n=0}^{\infty} 2x n t^n P_n(x) - \sum_{n=0}^{\infty} n t^{n+1} P_n(x) = 0 \\ \sum_{n=0}^{\infty} (2n+1) x t^n P_n(x) - \sum_{n=0}^{\infty} (n+1) t^{n+1} P_n(x) - \sum_{n=1}^{\infty} n t^{n-1} P_n(x) &= 0 \\ \sum_{n=0}^{\infty} (2n+1) x t^n P_n(x) - \sum_{n=1}^{\infty} n t^n P_{n-1}(x) - \sum_{n=0}^{\infty} (n+1) t^n P_{n+1}(x) &= 0, \end{aligned}$$

$$xP_0(x) - P_1(x) + \sum_{n=1}^{\infty} t^n \left[ (2n+1)xP_n(x) - nP_{n-1}(x) - (n+1)P_{n+1}(x) \right] = 0,$$

hence

$$xP_0(x) - P_1(x) = 0, \quad (2n+1)xP_n(x) - nP_{n-1}(x) - (n+1)P_{n+1}(x) = 0,$$

hence

$$P_1(x) = xP_0(x), \quad (n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

Let us prove

$$P_{l-1}(x) = P'_l(x) - 2xP'_{l-1}(x) + P'_{l-2}(x). \quad (14.104)$$

$$\begin{aligned} g(x, t) &= \frac{1}{\sqrt{1-2tx+t^2}} = \sum_{n=0}^{\infty} t^n P_n(x) \\ \frac{\partial}{\partial x} g(x, t) &= -\frac{1}{2}(1-2tx+t^2)^{-\frac{3}{2}}(-2t) = \frac{1}{\sqrt{1-2tx+t^2}} \frac{t}{1-2tx+t^2} \\ \frac{\partial}{\partial x} g(x, t) &= \frac{t}{1-2tx+t^2} \sum_{n=0}^{\infty} t^n P_n(x) = \sum_{n=0}^{\infty} t^n P'_n(x) \\ \sum_{n=0}^{\infty} t^{n+1} P_n(x) &= \sum_{n=0}^{\infty} t^n P'_n(x) - \sum_{n=0}^{\infty} 2xt^{n+1} P'_n(x) + \sum_{n=0}^{\infty} t^{n+2} P'_n(x) \\ \sum_{n=1}^{\infty} t^n P_{n-1}(x) &= \sum_{n=0}^{\infty} t^n P'_n(x) - \sum_{n=1}^{\infty} 2xt^n P'_{n-1}(x) + \sum_{n=2}^{\infty} t^n P'_{n-2}(x) \\ tP_0 + \sum_{n=2}^{\infty} t^n P_{n-1}(x) &= P'_0(x) + tP'_1(x) + \sum_{n=2}^{\infty} t^n P'_n(x) - \\ &\quad - 2xtP'_0 - \sum_{n=2}^{\infty} 2xt^n P'_{n-1}(x) + \sum_{n=2}^{\infty} t^n P'_{n-2}(x) \\ P'_0(x) + t \left[ P'_1(x) - P_0(x) - 2xP'_0(x) \right] &+ \\ &+ \sum_{n=2}^{\infty} t^n [P'_n(x) - 2xP'_{n-1}(x) + P'_{n-2}(x) - P_{n-1}(x)] = 0 \\ P'_0(x) &= 0, \text{ hence } P_0(x) = \text{const.} \\ P'_1(x) - P_0(x) - 2xP'_0(x) &= 0. \end{aligned}$$

Because of  $P'_0(x) = 0$  we obtain  $P'_1(x) - P_0(x) = 0$ , hence  $P'_1(x) = P_0(x)$ , and

$$P'_n(x) - 2xP'_{n-1}(x) + P'_{n-2}(x) - P_{n-1}(x) = 0.$$

Finally we substitute  $n+1$  for  $n$ :

$$P'_{n+1}(x) - 2xP'_n(x) + P'_{n-1}(x) - P_n(x) = 0,$$

hence

$$P_n(x) = P'_{n+1}(x) - 2xP'_n(x) + P'_{n-1}(x).$$

Let us prove

$$P'_{l+1}(x) - P'_{l-1}(x) = (2l+1)P_l(x). \quad (14.105)$$

$$\begin{aligned} (n+1)P_{n+1}(x) &= (2n+1)xP_n(x) - nP_{n-1}(x) \quad \left| \frac{d}{dx} \right. \\ (n+1)P'_{n+1}(x) &= (2n+1)P_n(x) + (2n+1)xP'_n(x) - nP'_{n-1}(x) \quad \left| \cdot 2 \right. \\ \text{(i): } (2n+2)P'_{n+1}(x) &= 2(2n+1)P_n(x) + 2(2n+1)xP'_n(x) - 2nP'_{n-1}(x) \\ P'_{n+1}(x) - 2xP'_n(x) + P'_{n-1}(x) &= P_n(x) \quad \left| \cdot (2n+1) \right. \\ \text{(ii): } (2n+1)P'_{n+1}(x) - 2(2n+1)xP'_n(x) + (2n+1)P'_{n-1}(x) &= (2n+1)P_n(x) \end{aligned}$$

We subtract (ii) from (i):

$$\begin{aligned} P'_{n+1}(x) + 2(2n+1)xP'_n(x) - (2n+1)P'_{n-1}(x) &= \\ &= (2n+1)P_n(x) + 2(2n+1)xP'_n(x) - 2nP'_{n-1}(x); \end{aligned}$$

hence

$$P'_{n+1}(x) - P'_{n-1}(x) = (2n+1)P_n(x).$$

#### 14.6.4 Expansion in Legendre polynomials

We state without proof that square integrable functions  $f(x)$  can be written as series of Legendre polynomials as

$$\begin{aligned} f(x) &= \sum_{l=0}^{\infty} a_l P_l(x), \\ \text{with expansion coefficients } a_l &= \frac{2l+1}{2} \int_{-1}^{+1} f(x) P_l(x) dx. \end{aligned} \quad (14.106)$$

Let us expand the Heaviside function defined in Eq. (10.109)

$$H(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{for } x < 0 \end{cases} \quad (14.107)$$

in terms of Legendre polynomials.

We shall use the recursion formula  $(2l+1)P_l = P'_{l+1} - P'_{l-1}$  and rewrite

$$\begin{aligned} a_l &= \frac{1}{2} \int_0^1 (P'_{l+1}(x) - P'_{l-1}(x)) dx = \frac{1}{2} (P_{l+1}(x) - P_{l-1}(x)) \Big|_{x=0}^1 = \\ &= \frac{1}{2} \underbrace{[P_{l+1}(1) - P_{l-1}(1)]}_{=0 \text{ because of "normalization"}} - \frac{1}{2} [P_{l+1}(0) - P_{l-1}(0)]. \end{aligned}$$

Note that  $P_n(0) = 0$  for *odd*  $n$ ; hence  $a_l = 0$  for *even*  $l \neq 0$ . We shall treat the case  $l = 0$  with  $P_0(x) = 1$  separately. Upon substituting  $2l + 1$  for  $l$  one obtains

$$a_{2l+1} = -\frac{1}{2} \left[ P_{2l+2}(0) - P_{2l}(0) \right].$$

We shall next use the formula

$$P_l(0) = (-1)^{\frac{l}{2}} \frac{l!}{2^l \left( \left( \frac{l}{2} \right)! \right)^2},$$

and for *even*  $l \geq 0$  one obtains

$$\begin{aligned} a_{2l+1} &= -\frac{1}{2} \left[ \frac{(-1)^{l+1} (2l+2)!}{2^{2l+2} ((l+1)!)^2} - \frac{(-1)^l (2l)!}{2^{2l} (l!)^2} \right] = \\ &= (-1)^l \frac{(2l)!}{2^{2l+1} (l!)^2} \left[ \frac{(2l+1)(2l+2)}{2^2 (l+1)^2} + 1 \right] = \\ &= (-1)^l \frac{(2l)!}{2^{2l+1} (l!)^2} \left[ \frac{2(2l+1)(l+1)}{2^2 (l+1)^2} + 1 \right] = \\ &= (-1)^l \frac{(2l)!}{2^{2l+1} (l!)^2} \left[ \frac{2l+1+2l+2}{2(l+1)} \right] = \\ &= (-1)^l \frac{(2l)!}{2^{2l+1} (l!)^2} \left[ \frac{4l+3}{2(l+1)} \right] = \\ &= (-1)^l \frac{(2l)!(4l+3)}{2^{2l+2} l!(l+1)!} \\ a_0 &= \frac{1}{2} \int_{-1}^{+1} H(x) \underbrace{P_0(x)}_{=1} dx = \frac{1}{2} \int_0^1 dx = \frac{1}{2}; \end{aligned}$$

and finally

$$H(x) = \frac{1}{2} + \sum_{l=0}^{\infty} (-1)^l \frac{(2l)!(4l+3)}{2^{2l+2} l!(l+1)!} P_{2l+1}(x).$$

## 14.7 Associated Legendre polynomial

Associated Legendre polynomials  $P_l^m(x)$  are the solutions of the *general Legendre equation*

$$\begin{aligned} \left\{ (1-x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx} + \left[ l(l+1) - \frac{m^2}{1-x^2} \right] \right\} P_l^m(x) &= 0, \\ \text{or } \left[ \frac{d}{dx} \left( (1-x^2) \frac{d}{dx} \right) + l(l+1) - \frac{m^2}{1-x^2} \right] P_l^m(x) &= 0 \end{aligned} \quad (14.108)$$

Eq. (14.108) reduces to the Legendre equation (14.96) on page 233 for  $m = 0$ ; hence

$$P_l^0(x) = P_l(x). \quad (14.109)$$

More generally, by differentiating  $m$  times the Legendre equation (14.96) it can be shown that

$$P_l^m(x) = (-1)^m (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x). \quad (14.110)$$

By inserting  $P_l(x)$  from the *Rodrigues formula* for Legendre polynomials (14.97) we obtain

$$\begin{aligned} P_l^m(x) &= (-1)^m (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2-1)^l \\ &= \frac{(-1)^m (1-x^2)^{\frac{m}{2}}}{2^l l!} \frac{d^{m+l}}{dx^{m+l}} (x^2-1)^l. \end{aligned} \quad (14.111)$$

In terms of the Gauss hypergeometric function the associated Legendre polynomials can be generalised to arbitrary complex indices  $\mu$ ,  $\lambda$  and argument  $x$  by

$$P_\lambda^\mu(x) = \frac{1}{\Gamma(1-\mu)} \left( \frac{1+x}{1-x} \right)^{\frac{\mu}{2}} {}_2F_1 \left( -\lambda, \lambda+1; 1-\mu; \frac{1-x}{2} \right). \quad (14.112)$$

No proof is given here.

## 14.8 Spherical harmonics

Let us define the *spherical harmonics*  $Y_l^m(\theta, \varphi)$  by

$$Y_l^m(\theta, \varphi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\varphi} \text{ for } -l \leq m \leq l. \quad (14.113)$$

Spherical harmonics are solutions of the differential equation

$$\{\Delta + l(l+1)\} Y_l^m(\theta, \varphi) = 0. \quad (14.114)$$

This equation is what typically remains after separation and “removal” of the radial part of the Laplace equation  $\Delta\psi(r, \theta, \varphi) = 0$  in three dimensions when the problem is invariant (symmetric) under rotations.

## 14.9 Solution of the Schrödinger equation for a hydrogen atom

Suppose Schrödinger, in his 1926 *annus mirabilis* – a year which seems to have been initiated by a trip to Arosa with ‘an old girlfriend from Vienna’ (apparently it was neither his wife Anny who remained in Zurich, nor Lotte, nor Irene nor Felicie<sup>14</sup>), – came down from the mountains or from whatever realm he was in – and handed you over some partial differential equation for the hydrogen atom – an equation (note that the quantum mechanical “momentum operator”  $\mathcal{P}$  is identified with  $-i\hbar\nabla$ )

$$\begin{aligned} \frac{1}{2\mu} \mathcal{P}^2 \psi &= \frac{1}{2\mu} \left( \mathcal{P}_x^2 + \mathcal{P}_y^2 + \mathcal{P}_z^2 \right) \psi = (E - V) \psi, \\ \text{or, with } V &= -\frac{e^2}{4\pi\epsilon_0 r}, \\ -\left[ \frac{\hbar^2}{2\mu} \Delta + \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(\mathbf{x}) &= E\psi, \\ \text{or } \left[ \Delta + \frac{2\mu}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) \right] \psi(\mathbf{x}) &= 0, \end{aligned} \quad (14.115)$$

Twice continuously differentiable, complex-valued solutions  $u$  of the Laplace equation  $\Delta u = 0$  are called *harmonic functions*

Sheldon Axler, Paul Bourdon, and Wade Ramey. *Harmonic Function Theory*, volume 137 of *Graduate texts in mathematics*, second edition, 1994. ISBN 0-387-97875-5

<sup>14</sup> Walter Moore. *Schrödinger life and thought*. Cambridge University Press, Cambridge, UK, 1989

which would later bear his name – and asked you if you could be so kind to please solve it for him. Actually, by Schrödinger's own account <sup>15</sup> he handed over this eigenwert equation to Hermann Klaus Hugo Weyl; in this instance he was not dissimilar from Einstein, who seemed to have employed a (human) computator on a very regular basis. Schrödinger might also have hinted that  $\mu$ ,  $e$ , and  $\epsilon_0$  stand for some (reduced) mass, charge, and the permittivity of the vacuum, respectively,  $-\hbar$  is a constant of (the dimension of) action, and  $E$  is some eigenvalue which must be determined from the solution of (14.115).

So, what could you do? First, observe that the problem is spherical symmetric, as the potential just depends on the radius  $r = \sqrt{\mathbf{x} \cdot \mathbf{x}}$ , and also the Laplace operator  $\Delta = \nabla \cdot \nabla$  allows spherical symmetry. Thus we could write the Schrödinger equation (14.115) in terms of spherical coordinates  $(r, \theta, \varphi)$  with  $x = r \sin \theta \cos \varphi$ ,  $y = r \sin \theta \sin \varphi$ ,  $z = r \cos \theta$ , whereby  $\theta$  is the polar angle in the  $x$ - $z$ -plane measured from the  $z$ -axis, with  $0 \leq \theta \leq \pi$ , and  $\varphi$  is the azimuthal angle in the  $x$ - $y$ -plane, measured from the  $x$ -axis with  $0 \leq \varphi < 2\pi$  (cf page 267). In terms of spherical coordinates the Laplace operator essentially “decays into” (i.e. consists additively of) a radial part and an angular part

$$\begin{aligned} \Delta &= \left( \frac{\partial}{\partial x} \right)^2 + \left( \frac{\partial}{\partial y} \right)^2 + \left( \frac{\partial}{\partial z} \right)^2 \\ &= \frac{1}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right. \\ &\quad \left. + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]. \end{aligned} \quad (14.116)$$

#### 14.9.1 Separation of variables Ansatz

This can be exploited for a *separation of variable Ansatz*, which, according to Schrödinger, should be well known (in German *sattsam bekannt*) by now (cf chapter 13). We thus write the solution  $\psi$  as a product of functions of separate variables

$$\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi) = R(r)Y_l^m(\theta, \varphi) \quad (14.117)$$

That the angular part  $\Theta(\theta)\Phi(\varphi)$  of this product will turn out to be the spherical harmonics  $Y_l^m(\theta, \varphi)$  introduced earlier on page 238 is nontrivial – indeed, at this point it is an *ad hoc* assumption. We will come back to its derivation in fuller detail later.

#### 14.9.2 Separation of the radial part from the angular one

For the time being, let us first concentrate on the radial part  $R(r)$ . Let us first totally separate the variables of the Schrödinger equation (14.115) in

<sup>15</sup> Erwin Schrödinger. Quantisierung als Eigenwertproblem. *Annalen der Physik*, 384(4):361–376, 1926. ISSN 1521-3889. DOI: 10.1002/andp.19263840404. URL <http://dx.doi.org/10.1002/andp.19263840404>

radial coordinates

$$\left\{ \frac{1}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] + \frac{2\mu}{-\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) \right\} \psi(r, \theta, \varphi) = 0, \quad (14.118)$$

and multiplying it with  $r^2$

$$\left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{2\mu r^2}{-\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right\} \psi(r, \theta, \varphi) = 0, \quad (14.119)$$

so that, after division by  $\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi)$  and writing separate variables on separate sides of the equation,

$$\begin{aligned} & \frac{1}{R(r)} \left\{ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{2\mu r^2}{-\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) \right\} R(r) \\ &= -\frac{1}{\Theta(\theta)\Phi(\varphi)} \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right\} \Theta(\theta)\Phi(\varphi) \end{aligned} \quad (14.120)$$

Because the left hand side of this equation is independent of the angular variables  $\theta$  and  $\varphi$ , and its right hand side is independent of the radius  $r$ , both sides have to be constant; say  $\lambda$ . Thus we obtain two differential equations for the radial and the angular part, respectively

$$\left\{ \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{2\mu r^2}{-\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) \right\} R(r) = \lambda R(r), \quad (14.121)$$

and

$$\left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right\} \Theta(\theta)\Phi(\varphi) = -\lambda \Theta(\theta)\Phi(\varphi). \quad (14.122)$$

### 14.9.3 Separation of the polar angle $\theta$ from the azimuthal angle $\varphi$

As already hinted in Eq. (14.117) The angular portion can still be separated into a polar and an azimuthal part because, when multiplied by  $\sin^2 \theta / [\Theta(\theta)\Phi(\varphi)]$ , Eq. (14.122) can be rewritten as

$$\left\{ \frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} + \lambda \sin^2 \theta \right\} + \frac{1}{\Phi(\varphi)} \frac{\partial^2 \Phi(\varphi)}{\partial \varphi^2} = 0, \quad (14.123)$$

and hence

$$\frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} + \lambda \sin^2 \theta = -\frac{1}{\Phi(\varphi)} \frac{\partial^2 \Phi(\varphi)}{\partial \varphi^2} = m^2, \quad (14.124)$$

where  $m$  is some constant.

#### 14.9.4 Solution of the equation for the azimuthal angle factor $\Phi(\varphi)$

The resulting differential equation for  $\Phi(\varphi)$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2} = -m^2\Phi(\varphi), \quad (14.125)$$

has the general solution

$$\Phi(\varphi) = Ae^{im\varphi} + Be^{-im\varphi}. \quad (14.126)$$

As  $\Phi$  must obey the periodic boundary conditions  $\Phi(\varphi) = \Phi(\varphi + 2\pi)$ ,  $m$  must be an integer. The two constants  $A, B$  must be equal if we require the system of functions  $\{e^{im\varphi} | m \in \mathbb{Z}\}$  to be orthonormalized. Indeed, if we define

$$\Phi_m(\varphi) = Ae^{im\varphi} \quad (14.127)$$

and require that it is normalized, it follows that

$$\begin{aligned} & \int_0^{2\pi} \overline{\Phi}_m(\varphi) \Phi_m(\varphi) d\varphi \\ &= \int_0^{2\pi} \overline{A} e^{-im\varphi} A e^{im\varphi} d\varphi \\ &= \int_0^{2\pi} |A|^2 d\varphi \\ &= 2\pi |A|^2 \\ &= 1, \end{aligned} \quad (14.128)$$

it is consistent to set

$$A = \frac{1}{\sqrt{2\pi}}; \quad (14.129)$$

and hence,

$$\Phi_m(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \quad (14.130)$$

Note that, for different  $m \neq n$ ,

$$\begin{aligned} & \int_0^{2\pi} \overline{\Phi}_n(\varphi) \Phi_m(\varphi) d\varphi \\ &= \int_0^{2\pi} \frac{e^{-in\varphi}}{\sqrt{2\pi}} \frac{e^{im\varphi}}{\sqrt{2\pi}} d\varphi \\ &= \int_0^{2\pi} \frac{e^{i(m-n)\varphi}}{2\pi} d\varphi \\ &= -\frac{ie^{i(m-n)\varphi}}{2(m-n)\pi} \Big|_{\varphi=0}^{\varphi=2\pi} \\ &= 0, \end{aligned} \quad (14.131)$$

because  $m - n \in \mathbb{Z}$ .



14.9.5 Solution of the equation for the polar angle factor  $\Theta(\theta)$ 

The left hand side of Eq. (14.124) contains only the polar coordinate. Upon division by  $\sin^2 \theta$  we obtain

$$\begin{aligned} \frac{1}{\Theta(\theta) \sin \theta} \frac{d}{d\theta} \sin \theta \frac{d\Theta(\theta)}{d\theta} + \lambda &= \frac{m^2}{\sin^2 \theta}, \text{ or} \\ \frac{1}{\Theta(\theta) \sin \theta} \frac{d}{d\theta} \sin \theta \frac{d\Theta(\theta)}{d\theta} - \frac{m^2}{\sin^2 \theta} &= -\lambda, \end{aligned} \quad (14.132)$$

Now, first, let us consider the case  $m = 0$ . With the variable substitution  $x = \cos \theta$ , and thus  $\frac{dx}{d\theta} = -\sin \theta$  and  $dx = -\sin \theta d\theta$ , we obtain from (14.132)

$$\begin{aligned} \frac{d}{dx} \sin^2 \theta \frac{d\Theta(x)}{dx} &= -\lambda \Theta(x), \\ \frac{d}{dx} (1 - x^2) \frac{d\Theta(x)}{dx} + \lambda \Theta(x) &= 0, \\ (x^2 - 1) \frac{d^2 \Theta(x)}{dx^2} + 2x \frac{d\Theta(x)}{dx} &= \lambda \Theta(x), \end{aligned} \quad (14.133)$$

which is of the same form as the *Legendre equation* (14.96) mentioned on page 233.

Consider the series *Ansatz*

$$\Theta(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots \quad (14.134)$$

for solving (14.133). Insertion into (14.133) and comparing the coefficients

This is actually a “shortcut” solution of the Fuchian Equation mentioned earlier.

of  $x$  for equal degrees yields the recursion relation

$$\begin{aligned}
& (x^2 - 1) \frac{d^2}{dx^2} [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots] \\
& + 2x \frac{d}{dx} [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots] \\
& = \lambda [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots], \\
& (x^2 - 1) [2a_2 + \cdots + k(k-1)a_k x^{k-2} + \cdots] \\
& + [2xa_1 + 2x2a_2 x + \cdots + 2xka_k x^{k-1} + \cdots] \\
& = \lambda [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots], \\
& (x^2 - 1) [2a_2 + \cdots + k(k-1)a_k x^{k-2} + \cdots] \\
& + [2a_1 x + 4a_2 x^2 + \cdots + 2ka_k x^k + \cdots] \\
& = \lambda [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots], \quad (14.135) \\
& [2a_2 x^2 + \cdots + k(k-1)a_k x^k + \cdots] \\
& - [2a_2 + \cdots + k(k-1)a_k x^{k-2} + \cdots] \\
& + [2a_1 x + 4a_2 x^2 + \cdots + 2ka_k x^k + \cdots] \\
& = \lambda [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots], \\
& [2a_2 x^2 + \cdots + k(k-1)a_k x^k + \cdots] \\
& - [2a_2 + \cdots + k(k-1)a_k x^{k-2} \\
& + (k+1)ka_{k+1}x^{k-1} + (k+2)(k+1)a_{k+2}x^k + \cdots] \\
& + [2a_1 x + 4a_2 x^2 + \cdots + 2ka_k x^k + \cdots] \\
& = \lambda [a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots],
\end{aligned}$$

and thus, by taking all polynomials of the order of  $k$  and proportional to  $x^k$ , so that, for  $x^k \neq 0$  (and thus excluding the trivial solution),

$$\begin{aligned}
& k(k-1)a_k x^k - (k+2)(k+1)a_{k+2}x^k + 2ka_k x^k - \lambda a_k x^k = 0, \\
& k(k+1)a_k - (k+2)(k+1)a_{k+2} - \lambda a_k = 0, \quad (14.136) \\
& a_{k+2} = a_k \frac{k(k+1) - \lambda}{(k+2)(k+1)}.
\end{aligned}$$

In order to converge also for  $x = \pm 1$ , and hence for  $\theta = 0$  and  $\theta = \pi$ , the sum in (14.134) has to have only a *finite number of terms*. Because if the sum would be infinite, the terms  $a_k$ , for large  $k$ , would be dominated by  $a_{k-2}O(k^2/k^2) = a_{k-2}O(1)$ , and thus would converge to  $a_k \xrightarrow{k \rightarrow \infty} a_\infty$  with constant  $a_\infty \neq 0$ , and thus  $\Theta$  would diverge as  $\Theta(1) \approx ka_\infty \xrightarrow{k \rightarrow \infty} \infty$ . That means that, in Eq. (14.136) for some  $k = l \in \mathbb{N}$ , the coefficient  $a_{l+2} = 0$  has to vanish; thus

$$\lambda = l(l+1). \quad (14.137)$$

This results in *Legendre polynomials*  $\Theta(x) \equiv P_l(x)$ .

Let us now shortly mention the case  $m \neq 0$ . With the same variable substitution  $x = \cos \theta$ , and thus  $\frac{dx}{d\theta} = -\sin \theta$  and  $dx = -\sin \theta d\theta$  as before,

the equation for the polar angle dependent factor (14.132) becomes

$$\left\{ \frac{d}{dx} (1-x^2) \frac{d}{dx} + l(l+1) - \frac{m^2}{1-x^2} \right\} \Theta(x) = 0, \quad (14.138)$$

This is exactly the form of the general Legendre equation (14.108), whose solution is a multiple of the associated Legendre polynomial  $P_l^m(x)$ , with  $|m| \leq l$ .

Note (without proof) that, for equal  $m$ , the  $P_l^m(x)$  satisfy the orthogonality condition

$$\int_{-1}^1 P_l^m(x) P_{l'}^m(x) dx = \frac{2(l+m)!}{(2l+1)(l-m)!} \delta_{ll'}. \quad (14.139)$$

Therefore we obtain a normalized polar solution by dividing  $P_l^m(x)$  by  $\{[2(l+m)!] / [(2l+1)(l-m)!]\}^{1/2}$ .

In putting both normalized polar and azimuthal angle factors together we arrive at the spherical harmonics (14.113); that is,

$$\Theta(\theta)\Phi(\varphi) = \sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}} P_l^m(\cos\theta) \frac{e^{im\varphi}}{\sqrt{2\pi}} = Y_l^m(\theta, \varphi) \quad (14.140)$$

for  $-l \leq m \leq l$ ,  $l \in \mathbb{N}_0$ . Note that the discreteness of these solutions follows from physical requirements about their finite existence.

#### 14.9.6 Solution of the equation for radial factor $R(r)$

The solution of the equation (14.121)

$$\left\{ \frac{d}{dr} r^2 \frac{d}{dr} + \frac{2\mu r^2}{-\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) \right\} R(r) = l(l+1)R(r), \text{ or} \quad (14.141)$$

$$-\frac{1}{R(r)} \frac{d}{dr} r^2 \frac{d}{dr} R(r) + l(l+1) - 2 \frac{\mu e^2}{4\pi\epsilon_0 - \hbar^2} r = \frac{2\mu}{-\hbar^2} r^2 E$$

for the radial factor  $R(r)$  turned out to be the most difficult part for Schrödinger<sup>16</sup>.

Note that, since the additive term  $l(l+1)$  in (14.141) is non-dimensional, so must be the other terms. We can make this more explicit by the substitution of variables.

First, consider  $y = \frac{r}{a_0}$  obtained by dividing  $r$  by the *Bohr radius*

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \approx 5 \cdot 10^{-11} \text{ m}, \quad (14.142)$$

thereby assuming that the reduced mass is equal to the electron mass  $\mu \approx m_e$ . More explicitly,  $r = ya_0 = y(4\pi\epsilon_0 \hbar^2)/(m_e e^2)$ , or  $y = r/a_0 = r(m_e e^2)/(4\pi\epsilon_0 \hbar^2)$ . Furthermore, let us define  $\varepsilon = E \frac{2\mu a_0^2}{-\hbar^2}$ .

These substitutions yield

$$-\frac{1}{R(y)} \frac{d}{dy} y^2 \frac{d}{dy} R(y) + l(l+1) - 2y = y^2 \varepsilon, \text{ or} \quad (14.143)$$

$$-y^2 \frac{d^2}{dy^2} R(y) - 2y \frac{d}{dy} R(y) + [l(l+1) - 2y - \varepsilon y^2] R(y) = 0.$$

<sup>16</sup> Walter Moore. *Schrödinger life and thought*. Cambridge University Press, Cambridge, UK, 1989

Now we introduce a new function  $\hat{R}$  via

$$R(\xi) = \xi^l e^{-\frac{1}{2}\xi} \hat{R}(\xi), \quad (14.144)$$

with  $\xi = \frac{2y}{n}$  and by replacing the energy variable with  $\varepsilon = -\frac{1}{n^2}$ . (It will later be argued that  $\varepsilon$  must be discrete; with  $n \in \mathbb{N} - 0$ .) This yields

$$\xi \frac{d^2}{d\xi^2} \hat{R}(\xi) + [2(l+1) - \xi] \frac{d}{d\xi} \hat{R}(\xi) + (n-l-1) \hat{R}(\xi) = 0. \quad (14.145)$$

The discretization of  $n$  can again be motivated by requiring physical properties from the solution; in particular, convergence. Consider again a series solution *Ansatz*

$$\hat{R}(\xi) = c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots, \quad (14.146)$$

which, when inserted into (14.143), yields

$$\begin{aligned} & \xi \frac{d^2}{d\xi^2} [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & + [2(l+1) - \xi] \frac{d}{d\xi} [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & + (n-l-1) [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & = 0, \\ & \xi [2c_2 + \cdots + k(k-1)c_k \xi^{k-2} + \cdots] \\ & + [2(l+1) - \xi] [c_1 + 2c_2 \xi + \cdots + k c_k \xi^{k-1} + \cdots] \\ & + (n-l-1) [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & = 0, \\ & [2c_2 \xi + \cdots + k(k-1)c_k \xi^{k-1} + \cdots] \quad (14.147) \\ & + 2(l+1) [c_1 + 2c_2 \xi + \cdots + k c_k \xi^{k-1} + \cdots] \\ & - [c_1 \xi + 2c_2 \xi^2 + \cdots + k c_k \xi^k + \cdots] \\ & + (n-l-1) [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & = 0, \\ & [2c_2 \xi + \cdots + k(k-1)c_k \xi^{k-1} + k(k+1)c_{k+1} \xi^k + \cdots] \\ & + 2(l+1) [c_1 + 2c_2 \xi + \cdots + k c_k \xi^{k-1} + (k+1)c_{k+1} \xi^k + \cdots] \\ & - [c_1 \xi + 2c_2 \xi^2 + \cdots + k c_k \xi^k + \cdots] \\ & + (n-l-1) [c_0 + c_1 \xi + c_2 \xi^2 + \cdots + c_k \xi^k + \cdots] \\ & = 0, \end{aligned}$$

so that, by comparing the coefficients of  $\xi^k$ , we obtain

$$\begin{aligned} k(k+1)c_{k+1}\xi^k + 2(l+1)(k+1)c_{k+1}\xi^k &= k c_k \xi^k - (n-l-1)c_k \xi^k, \\ c_{k+1}[k(k+1) + 2(l+1)(k+1)] &= c_k[k - (n-l-1)], \\ c_{k+1}(k+1)(k+2l+2) &= c_k(k-n+l+1), \quad (14.148) \\ c_{k+1} &= c_k \frac{k-n+l+1}{(k+1)(k+2l+2)}. \end{aligned}$$

Because of convergence of  $\hat{R}$  and thus of  $R$  – note that, for large  $\xi$  and  $k$ , the  $k$ 'th term in Eq. (14.146) determining  $\hat{R}(\xi)$  would behave as  $\xi^k/k!$  and thus  $\hat{R}(\xi)$  would roughly behave as  $e^\xi$  – the series solution (14.146) should terminate at some  $k = n - l - 1$ , or  $n = k + l + 1$ . Since  $k$ ,  $l$ , and 1 are all integers,  $n$  must be an integer as well. And since  $k \geq 0$ ,  $n$  must be at least  $l + 1$ , or

$$l \leq n - 1. \quad (14.149)$$

Thus, we end up with an *associated Laguerre equation* of the form

$$\left\{ \xi \frac{d^2}{d\xi^2} + [2(l+1) - \xi] \frac{d}{d\xi} + (n - l - 1) \right\} \hat{R}(\xi) = 0, \text{ with } n \geq l + 1, \text{ and } n, l \in \mathbb{Z}. \quad (14.150)$$

Its solutions are the *associated Laguerre polynomials*  $L_{n+l}^{2l+1}$  which are the  $(2l+1)$ -th derivatives of the Laguerre's polynomials  $L_{n+l}$ ; that is,

$$\begin{aligned} L_n(x) &= e^x \frac{d^n}{dx^n} (x^n e^{-x}), \\ L_n^m(x) &= \frac{d^m}{dx^m} L_n(x). \end{aligned} \quad (14.151)$$

This yields a normalized wave function

$$\begin{aligned} R_n(r) &= \mathcal{N} \left( \frac{2r}{na_0} \right)^l e^{-\frac{r}{a_0 n}} L_{n+l}^{2l+1} \left( \frac{2r}{na_0} \right), \text{ with} \\ \mathcal{N} &= -\frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{[(n+l)!a_0]^3}}, \end{aligned} \quad (14.152)$$

where  $\mathcal{N}$  stands for the normalization factor.

#### 14.9.7 Composition of the general solution of the Schrödinger Equation

Now we shall coagulate and combine the factorized solutions (14.117) into a complete solution of the Schrödinger equation for  $n+1$ ,  $l$ ,  $|m| \in \mathbb{N}_0$ ,  $0 \leq l \leq n-1$ , and  $|m| \leq l$ ,

Always remember the alchemic principle of *solve et coagula!*

$$\begin{aligned} \psi_{n,l,m}(r, \theta, \varphi) &= R_n(r) Y_l^m(\theta, \varphi) \\ &= -\frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{[(n+l)!a_0]^3}} \left( \frac{2r}{na_0} \right)^l e^{-\frac{r}{a_0 n}} L_{n+l}^{2l+1} \left( \frac{2r}{na_0} \right) \sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}} P_l^m(\cos \theta) \frac{e^{im\varphi}}{\sqrt{2\pi}}. \end{aligned} \quad (14.153)$$



## Divergent series

In this final chapter we will consider *divergent series*, which, as has already been mentioned earlier, seem to have been “invented by the devil”<sup>1</sup>. Unfortunately such series occur very often in physical situations; for instance in celestial mechanics or in quantum field theory<sup>2</sup>, and one may wonder with Abel why, “for the most part, it is true that the results are correct, which is very strange”<sup>3</sup>. On the other hand, there appears to be another view on diverging series, a view that has been expressed by Berry as follows<sup>4</sup>: “... an asymptotic series ... is a compact encoding of a function, and its divergence should be regarded not as a deficiency but as a source of information about the function.”

### 15.1 Convergence and divergence

Let us first define *convergence* in the context of series. A series

$$\sum_{j=0}^{\infty} a_j = a_0 + a_1 + a_2 + \cdots \quad (15.1)$$

is said to converge to the *sum*  $s$ , if the *partial sum*

$$s_n = \sum_{j=0}^n a_j = a_0 + a_1 + a_2 + \cdots + a_n \quad (15.2)$$

tends to a finite limit  $s$  when  $n \rightarrow \infty$ ; otherwise it is said to be divergent.

One of the most prominent series is the Leibniz series<sup>5</sup>

$$s = \sum_{j=0}^{\infty} (-1)^j = 1 - 1 + 1 - 1 + 1 - \cdots, \quad (15.3)$$

whose summands may be – inconsistently – “rearranged,” yielding

$$\begin{aligned} \text{either } 1 - 1 + 1 - 1 + 1 - 1 + \cdots &= (1 - 1) + (1 - 1) + (1 - 1) - \cdots = 0 \\ \text{or } 1 - 1 + 1 - 1 + 1 - 1 + \cdots &= 1 + (-1 + 1) + (-1 + 1) + \cdots = 1. \end{aligned}$$

Note that, by *Riemann's rearrangement theorem*, even convergent series which do not absolutely converge (i.e.,  $\sum_{j=0}^n a_j$  converges but  $\sum_{j=0}^n |a_j|$

<sup>1</sup> Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949

<sup>2</sup> John P. Boyd. The devil's invention: Asymptotic, superasymptotic and hyperasymptotic series. *Acta Applicandae Mathematica*, 56:1–98, 1999. ISSN 0167-8019. DOI: 10.1023/A:1006145903624. URL <http://dx.doi.org/10.1023/A:1006145903624>; Freeman J. Dyson. Divergence of perturbation theory in quantum electrodynamics. *Phys. Rev.*, 85(4):631–632, Feb 1952. DOI: 10.1103/PhysRev.85.631. URL <http://dx.doi.org/10.1103/PhysRev.85.631>; Sergio A. Pernice and Gerardo Oleaga. Divergence of perturbation theory: Steps towards a convergent series. *Physical Review D*, 57:1144–1158, Jan 1998. DOI: 10.1103/PhysRevD.57.1144. URL <http://dx.doi.org/10.1103/PhysRevD.57.1144>; and Ulrich D. Jentschura. Resummation of nonalternating divergent perturbative expansions. *Physical Review D*, 62:076001, Aug 2000. DOI: 10.1103/PhysRevD.62.076001. URL <http://dx.doi.org/10.1103/PhysRevD.62.076001>

<sup>3</sup> Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL <http://www.dms.umontreal.ca/~rousseau/divergent.pdf>

<sup>4</sup> Michael Berry. Asymptotics, superasymptotics, hyperasymptotics... In Harvey Segur, Saleh Tanveer, and Herbert Levine, editors, *Asymptotics beyond All Orders*, volume 284 of *NATO ASI Series*, pages 1–14. Springer, 1992. ISBN 978-1-4757-0437-2. DOI: 10.1007/978-1-4757-0435-8. URL <http://dx.doi.org/10.1007/978-1-4757-0435-8>

<sup>5</sup> Gottfried Wilhelm Leibniz. Letters LXX, LXXI. In Carl Immanuel Gerhardt, editor, *Briefwechsel zwischen Leibniz und Christian Wolf. Handschriften der Königlichen Bibliothek zu Hannover*, H. W. Schmidt, Halle, 1860. URL <http://books.google.de/books?id=TUKJAAAQAAJ>; Charles N. Moore. *Summable Series and Convergence Factors*. American Mathematical Society, New York, NY, 1938; Godfrey Harold Hardy. *Divergent Series*. Oxford University Press, 1949; and Graham Everest, Alf van der Poorten, Igor Shparlinski, and Thomas Ward. *Recurrence sequences. Volume*

diverges) can converge to any arbitrary (even infinite) value by permuting (rearranging) the (ratio of) positive and negative terms (the series of which must both be divergent).

The Leibniz series is a particular case  $q = -1$  of a *geometric series*

$$s = \sum_{j=0}^{\infty} q^j = 1 + q + q^2 + q^3 + \cdots = 1 + qs \quad (15.4)$$

which, since  $s = 1 + qs$ , for  $|q| < 1$ , converges to

$$s = \sum_{j=0}^{\infty} q^j = \frac{1}{1-q}. \quad (15.5)$$

One way to sum the Leibniz series is by “continuing” Eq. (15.5) for arbitrary  $q \neq 1$ , thereby defining the *Abel sum*

$$\sum_{j=0}^{\infty} (-1)^j \stackrel{\text{A}}{=} \frac{1}{1-(-1)} = \frac{1}{2}. \quad (15.6)$$

Another divergent series, which can be obtained by formally expanding the square of the Abel sum of the Leibniz series  $s^2 \stackrel{\text{A}}{=} (1+x)^{-2}$  around 0 and inserting  $x = 1$ <sup>6</sup> is

$$s^2 = \left( \sum_{j=0}^{\infty} (-1)^j \right) \left( \sum_{k=0}^{\infty} (-1)^k \right) = \sum_{j=0}^{\infty} (-1)^{j+1} j = 0 + 1 - 2 + 3 - 4 + 5 - \cdots. \quad (15.7)$$

In the same sense as the Leibniz series, this yields the Abel sum  $s^2 \stackrel{\text{A}}{=} 1/4$ .

Note that the sequence of its partial sums  $s_n^2 = \sum_{j=0}^n (-1)^{j+1} j$  yield every integer once; that is,  $s_0^2 = 0$ ,  $s_1^2 = 0 + 1 = 1$ ,  $s_2^2 = 0 + 1 - 2 = -1$ ,  $s_3^2 = 0 + 1 - 2 + 3 = 2$ ,  $s_4^2 = 0 + 1 - 2 + 3 - 4 = -2$ , ...,  $s_n^2 = -\frac{n}{2}$  for even  $n$ , and  $s_n^2 = -\frac{n+1}{2}$  for odd  $n$ . It thus establishes a strict one-to-one mapping  $s^2 : \mathbb{N} \rightarrow \mathbb{Z}$  of the natural numbers onto the integers.

## 15.2 Euler differential equation

In what follows we demonstrate that divergent series may make sense, in the way Abel wondered. That is, we shall show that the first partial sums of divergent series may yield “good” approximations of the exact result; and that, from a certain point onward, more terms contributing to the sum might worsen the approximation rather than make it better – a situation totally different from convergent series, where more terms always result in better approximations.

Let us, with Rousseau, for the sake of demonstration of the former situation, consider the *Euler differential equation*

$$\left( x^2 \frac{d}{dx} + 1 \right) y(x) = x, \text{ or } \left( \frac{d}{dx} + \frac{1}{x^2} \right) y(x) = \frac{1}{x}. \quad (15.8)$$

<sup>6</sup> Morris Kline. Euler and infinite series. *Mathematics Magazine*, 56(5):307–314, 1983. ISSN 0025570X. DOI: 10.2307/2690371. URL <http://dx.doi.org/10.2307/2690371>

We shall solve this equation by two methods: we shall, on the one hand, present a divergent series solution, and on the other hand, an exact solution. Then we shall compare the series approximation to the exact solution by considering the difference.

A series solution of the Euler differential equation can be given by

$$y_s(x) = \sum_{j=0}^{\infty} (-1)^j j! x^{j+1}. \quad (15.9)$$

That (15.9) solves (15.8) can be seen by inserting the former into the latter; that is,

$$\begin{aligned} & \left( x^2 \frac{d}{dx} + 1 \right) \sum_{j=0}^{\infty} (-1)^j j! x^{j+1} = x, \\ & \sum_{j=0}^{\infty} (-1)^j (j+1)! x^{j+2} + \sum_{j=0}^{\infty} (-1)^j j! x^{j+1} = x, \\ & \text{[change of variable in the first sum: } j \rightarrow j-1 \text{]} \\ & \sum_{j=1}^{\infty} (-1)^{j-1} (j+1-1)! x^{j+2-1} + \sum_{j=0}^{\infty} (-1)^j j! x^{j+1} = x, \\ & \sum_{j=1}^{\infty} (-1)^{j-1} j! x^{j+1} + x + \sum_{j=1}^{\infty} (-1)^j j! x^{j+1} = x, \\ & x + \sum_{j=1}^{\infty} (-1)^j [(-1)^{-1} + 1] j! x^{j+1} = x, \\ & x + \sum_{j=1}^{\infty} (-1)^j \underbrace{[-1 + 1]}_{=0} j! x^{j+1} = x, \\ & x = x. \end{aligned} \quad (15.10)$$

On the other hand, an exact solution can be found by *quadrature*; that is, by explicit integration (see, for instance, Chapter one of Ref. <sup>7</sup>). Consider the homogenous first order differential equation

$$\begin{aligned} & \left( \frac{d}{dx} + p(x) \right) y(x) = 0, \\ & \text{or } \frac{dy(x)}{dx} = -p(x)y(x), \\ & \text{or } \frac{dy(x)}{y(x)} = -p(x)dx. \end{aligned} \quad (15.11)$$

Integrating both sides yields

$$\log|y(x)| = - \int p(x)dx + C, \text{ or } |y(x)| = K e^{-\int p(x)dx}, \quad (15.12)$$

where  $C$  is some constant, and  $K = e^C$ . Let  $P(x) = \int p(x)dx$ . Hence, heuristically,  $y(x)e^{P(x)}$  is constant, as can also be seen by explicit differentiation

<sup>7</sup> Garrett Birkhoff and Gian-Carlo Rota. *Ordinary Differential Equations*. John Wiley & Sons, New York, Chichester, Brisbane, Toronto, fourth edition, 1959, 1960, 1962, 1969, 1978, and 1989



of  $y(x)e^{P(x)}$ ; that is,

$$\begin{aligned}
 \frac{d}{dx} y(x) e^{P(x)} &= e^{P(x)} \frac{dy(x)}{dx} + y(x) \frac{d}{dx} e^{P(x)} \\
 &= e^{P(x)} \frac{dy(x)}{dx} + y(x) p(x) e^{P(x)} \\
 &= e^{P(x)} \left( \frac{d}{dx} + p(x) \right) y(x) \\
 &= 0
 \end{aligned} \tag{15.13}$$

if and, since  $e^{P(x)} \neq 0$ , only if  $y(x)$  satisfies the homogenous equation (15.11). Hence,

$$\begin{aligned}
 y(x) &= c e^{-\int p(x) dx} \text{ is the solution of} \\
 \left( \frac{d}{dx} + p(x) \right) y(x) &= 0
 \end{aligned} \tag{15.14}$$

for some constant  $c$ .

Similarly, we can again find a solution to the inhomogeneous first order differential equation

$$\begin{aligned}
 \left( \frac{d}{dx} + p(x) \right) y(x) + q(x) &= 0, \\
 \text{or } \left( \frac{d}{dx} + p(x) \right) y(x) &= -q(x)
 \end{aligned} \tag{15.15}$$

by differentiating the function  $y(x)e^{P(x)} = y(x)e^{\int p(x) dx}$ ; that is,

$$\begin{aligned}
 \frac{d}{dx} y(x) e^{\int p(x) dx} &= e^{\int p(x) dx} \frac{d}{dx} y(x) + p(x) e^{\int p(x) dx} y(x) \\
 &= e^{\int p(x) dx} \underbrace{\left( \frac{d}{dx} + p(x) \right) y(x)}_{=q(x)} \\
 &= -e^{\int p(x) dx} q(x).
 \end{aligned} \tag{15.16}$$

Hence, for some constant  $y_0$  and some  $a, b$ , we must have, by integration,

$$\begin{aligned}
 \int_b^x \frac{d}{dt} y(t) e^{\int_a^t p(s) ds} dt &= y(x) e^{\int_a^x p(t) dt} \\
 &= y_0 - \int_b^x e^{\int_a^t p(s) ds} q(t) dt,
 \end{aligned} \tag{15.17}$$

$$\text{and hence } y(x) = y_0 e^{-\int_a^x p(t) dt} - e^{-\int_a^x p(t) dt} \int_b^x e^{\int_a^t p(s) ds} q(t) dt.$$

If  $a = b$ , then  $y(b) = y_0$ .

Coming back to the Euler differential equation and identifying  $p(x) = 1/x^2$  and  $q(x) = -1/x$  we obtain, up to a constant, with  $b = 0$  and arbitrary

constant  $a \neq 0$ ,

$$\begin{aligned}
 y(x) &= -e^{-\int_a^x \frac{dt}{t^2}} \int_0^x e^{\int_a^t \frac{ds}{s^2}} \left(-\frac{1}{t}\right) dt \\
 &= e^{-(-\frac{1}{t})|_a^x} \int_0^x e^{-\frac{1}{s}|_a^t} \left(\frac{1}{t}\right) dt \\
 &= e^{\frac{1}{x} - \frac{1}{a}} \int_0^x e^{-\frac{1}{t} + \frac{1}{a}} \left(\frac{1}{t}\right) dt \\
 &= e^{\frac{1}{x}} \underbrace{e^{-\frac{1}{a} + \frac{1}{a}}}_{=e^0=1} \int_0^x e^{-\frac{1}{t}} \left(\frac{1}{t}\right) dt \\
 &= e^{\frac{1}{x}} e^{-\frac{1}{a}} \int_0^x e^{-\frac{1}{t}} e^{\frac{1}{a}} \left(\frac{1}{t}\right) dt \\
 &= e^{\frac{1}{x}} \int_0^x \frac{e^{-\frac{1}{t}}}{t} dt \\
 &= \int_0^x \frac{e^{\frac{1}{x} - \frac{1}{t}}}{t} dt.
 \end{aligned} \tag{15.18}$$

With a change of the integration variable

$$\begin{aligned}
 \frac{\xi}{x} &= \frac{1}{t} - \frac{1}{x}, \text{ and thus } \xi = \frac{x}{t} - 1, \text{ and } t = \frac{x}{1+\xi}, \\
 \frac{dt}{d\xi} &= -\frac{x}{(1+\xi)^2}, \text{ and thus } dt = -\frac{x}{(1+\xi)^2} d\xi, \\
 \text{and thus } \frac{dt}{t} &= \frac{-\frac{x}{(1+\xi)^2}}{\frac{x}{1+\xi}} d\xi = -\frac{d\xi}{1+\xi},
 \end{aligned} \tag{15.19}$$

the integral (15.18) can be rewritten as

$$y(x) = \int_{-\infty}^0 \left(-\frac{e^{-\frac{\xi}{x}}}{1+\xi}\right) d\xi = \int_0^{\infty} \frac{e^{-\frac{\xi}{x}}}{1+\xi} d\xi. \tag{15.20}$$

It is proportional to the *Stieltjes Integral*<sup>8</sup>

$$S(x) = \int_0^{\infty} \frac{e^{-\xi}}{1+x\xi} d\xi. \tag{15.21}$$

Note that whereas the series solution  $y_s(x)$  diverges for all nonzero  $x$ , the solution  $y(x)$  in (15.20) converges and is well defined for all  $x \geq 0$ .

Let us now estimate the absolute difference between  $y_{s_k}(x)$  which represents the partial sum “ $y_s(x)$  truncated after the  $k$ th term” and  $y(x)$ ; that is, let us consider

$$|y(x) - y_{s_k}(x)| = \left| \int_0^{\infty} \frac{e^{-\frac{\xi}{x}}}{1+\xi} d\xi - \sum_{j=0}^k (-1)^j j! x^{j+1} \right|. \tag{15.22}$$

For any  $x \geq 0$  this difference can be estimated<sup>9</sup> by a bound from above

$$|R_k(x)| \stackrel{\text{def}}{=} |y(x) - y_{s_k}(x)| \leq k! x^{k+1}, \tag{15.23}$$

<sup>8</sup> Carl M. Bender Steven A. Orszag. *Advanced Mathematical Methods for Scientists and Engineers*. McGraw-Hill, New York, NY, 1978; and John P. Boyd. The devil's invention: Asymptotic, superasymptotic and hyperasymptotic series. *Acta Applicandae Mathematica*, 56:1–98, 1999. ISSN 0167-8019. DOI: 10.1023/A:1006145903624. URL <http://dx.doi.org/10.1023/A:1006145903624>

<sup>9</sup> Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL <http://www.dms.umontreal.ca/~rousseac/divergent.pdf>

that is, this difference between the exact solution  $y(x)$  and the diverging partial series  $y_{s_k}(x)$  is smaller than the first neglected term; and all subsequent ones.

For a proof, observe that, since a partial *geometric series* is the sum of all the numbers in a geometric progression up to a certain power; that is,

$$\sum_{k=0}^n r^k = 1 + r + r^2 + \cdots + r^k + \cdots + r^n. \quad (15.24)$$

By multiplying both sides with  $1 - r$ , the sum (15.24) can be rewritten as

$$\begin{aligned} (1-r) \sum_{k=0}^n r^k &= (1-r)(1 + r + r^2 + \cdots + r^k + \cdots + r^n) \\ &= 1 + r + r^2 + \cdots + r^k + \cdots + r^n - r(1 + r + r^2 + \cdots + r^k + \cdots + r^n + r^n) \quad (15.25) \\ &= 1 + r + r^2 + \cdots + r^k + \cdots + r^n - (r + r^2 + \cdots + r^k + \cdots + r^n + r^{n+1}) \\ &= 1 - r^{n+1}, \end{aligned}$$

and, since the middle terms all cancel out,

$$\sum_{k=0}^n r^k = \frac{1 - r^{n+1}}{1 - r}, \quad \text{or} \quad \sum_{k=0}^{n-1} r^k = \frac{1 - r^n}{1 - r} = \frac{1}{1 - r} - \frac{r^n}{1 - r}. \quad (15.26)$$

Thus, for  $r = -\zeta$ , it is true that

$$\frac{1}{1 + \zeta} = \sum_{k=0}^{n-1} (-1)^k \zeta^k + (-1)^n \frac{\zeta^n}{1 + \zeta}. \quad (15.27)$$

Thus

$$\begin{aligned} f(x) &= \int_0^\infty \frac{e^{-\frac{\zeta}{x}}}{1 + \zeta} d\zeta \\ &= \int_0^\infty e^{-\frac{\zeta}{x}} \left( \sum_{k=0}^{n-1} (-1)^k \zeta^k + (-1)^n \frac{\zeta^n}{1 + \zeta} \right) d\zeta \quad (15.28) \\ &= \sum_{k=0}^{n-1} \int_0^\infty (-1)^k \zeta^k e^{-\frac{\zeta}{x}} d\zeta + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1 + \zeta} d\zeta. \end{aligned}$$

Since

$$k! = \Gamma(k+1) = \int_0^\infty z^k e^{-z} dz, \quad (15.29)$$

one obtains

$$\begin{aligned} &\int_0^\infty \zeta^k e^{-\frac{\zeta}{x}} d\zeta \\ &[\text{substitution: } z = \frac{\zeta}{x}, d\zeta = x dz] \quad (15.30) \\ &= \int_0^\infty x^{k+1} z^k e^{-z} dz \\ &= x^{k+1} k!, \end{aligned}$$

and hence

$$\begin{aligned}
 f(x) &= \sum_{k=0}^{n-1} \int_0^\infty (-1)^k \zeta^k e^{-\frac{\zeta}{x}} d\zeta + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta \\
 &= \sum_{k=0}^{n-1} (-1)^k x^{k+1} k! + \int_0^\infty (-1)^n \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta \\
 &= f_n(x) + R_n(x),
 \end{aligned} \tag{15.31}$$

where  $f_n(x)$  represents the partial sum of the power series, and  $R_n(x)$  stands for the remainder, the difference between  $f(x)$  and  $f_n(x)$ . The absolute of the remainder can be estimated by

$$\begin{aligned}
 |R_n(x)| &= \int_0^\infty \frac{\zeta^n e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta \\
 &\leq \int_0^\infty \zeta^n e^{-\frac{\zeta}{x}} d\zeta \\
 &= n! x^{n+1}.
 \end{aligned} \tag{15.32}$$

### 15.2.1 Borel's resummation method – “The Master forbids it”

In what follows we shall again follow Christiane Rousseau's treatment<sup>10</sup> and use a resummation method invented by Borel<sup>11</sup> to obtain the exact convergent solution (15.20) of the Euler differential equation (15.8) from the divergent series solution (15.9). First we can rewrite a suitable infinite series by an integral representation, thereby using the integral representation of the factorial (15.29) as follows:

$$\begin{aligned}
 \sum_{j=0}^\infty a_j &= \sum_{j=0}^\infty a_j \frac{j!}{j!} = \sum_{j=0}^\infty \frac{a_j}{j!} j! \\
 &= \sum_{j=0}^\infty \frac{a_j}{j!} \int_0^\infty t^j e^{-t} dt \stackrel{\text{B}}{=} \int_0^\infty \left( \sum_{j=0}^\infty \frac{a_j t^j}{j!} \right) e^{-t} dt.
 \end{aligned} \tag{15.33}$$

A series  $\sum_{j=0}^\infty a_j$  is *Borel summable* if  $\sum_{j=0}^\infty \frac{a_j t^j}{j!}$  has a non-zero radius of convergence, if it can be extended along the positive real axis, and if the integral (15.33) is convergent. This integral is called the *Borel sum* of the series.

In the case of the series solution of the Euler differential equation,  $a_j = (-1)^j j! x^{j+1}$  [cf. Eq. (15.9)]. Thus,

$$\sum_{j=0}^\infty \frac{a_j t^j}{j!} = \sum_{j=0}^\infty \frac{(-1)^j j! x^{j+1} t^j}{j!} = x \sum_{j=0}^\infty (-xt)^j = \frac{x}{1+xt}, \tag{15.34}$$

and therefore, with the substitution  $xt = \zeta$ ,  $dt = \frac{d\zeta}{x}$

$$\sum_{j=0}^\infty (-1)^j j! x^{j+1} \stackrel{\text{B}}{=} \int_0^\infty \sum_{j=0}^\infty \frac{a_j t^j}{j!} e^{-t} dt = \int_0^\infty \frac{x}{1+xt} e^{-t} dt = \int_0^\infty \frac{e^{-\frac{\zeta}{x}}}{1+\zeta} d\zeta, \tag{15.35}$$

<sup>10</sup> Christiane Rousseau. Divergent series: Past, present, future .... preprint, 2004. URL <http://www.dms.umontreal.ca/~rousseac/divergent.pdf>

For more resummation techniques, please see Chapter 16 of

Hagen Kleinert and Verena Schulte-Frohlinde. *Critical Properties of  $\phi^4$  - Theories*. World scientific, Singapore, 2001. ISBN 9810246595

<sup>11</sup> Émile Borel. Mémoire sur les séries divergentes. *Annales scientifiques de l'École Normale Supérieure*, 16:9–131, 1899. URL <http://eudml.org/doc/81143>

“The idea that a function could be determined by a divergent asymptotic series was a foreign one to the nineteenth century mind. Borel, then an unknown young man, discovered that his summation method gave the “right” answer for many classical divergent series. He decided to make a pilgrimage to Stockholm to see Mittag-Leffler, who was the recognized lord of complex analysis. Mittag-Leffler listened politely to what Borel had to say and then, placing his hand upon the complete works by Weierstrass, his teacher, he said in Latin, “The Master forbids it.” A tale of Mark Kac,” quoted (on page 38) by

Michael Reed and Barry Simon. *Methods of Modern Mathematical Physics IV: Analysis of Operators*. Academic Press, New York, 1978

which is the exact solution (15.20) of the Euler differential equation (15.8).

We can also find the Borel sum (which in this case is equal to the Abel sum) of the Leibniz series (15.3) by

$$\begin{aligned}
 s &= \sum_{j=0}^{\infty} (-1)^j \stackrel{\text{B}}{=} \int_0^{\infty} \left( \sum_{j=0}^{\infty} \frac{(-1)^j t^j}{j!} \right) e^{-t} dt \\
 &= \int_0^{\infty} \left( \sum_{j=0}^{\infty} \frac{(-t)^j}{j!} \right) e^{-t} dt = \int_0^{\infty} e^{-2t} dt \\
 &\quad [\text{variable substitution } 2t = \zeta, dt = \frac{1}{2} d\zeta] \\
 &= \frac{1}{2} \int_0^{\infty} e^{-\zeta} d\zeta \\
 &= \frac{1}{2} \left( -e^{-\zeta} \right) \Big|_{\zeta=0}^{\infty} = \frac{1}{2} (-e^{-\infty} + e^{-0}) = \frac{1}{2}.
 \end{aligned} \tag{15.36}$$

A similar calculation for  $s^2$  defined in Eq. (15.7) yields

$$\begin{aligned}
 s^2 &= \sum_{j=0}^{\infty} (-1)^{j+1} j = (-1) \sum_{j=1}^{\infty} (-1)^j j \stackrel{\text{B}}{=} - \int_0^{\infty} \left( \sum_{j=1}^{\infty} \frac{(-1)^j j t^j}{j!} \right) e^{-t} dt \\
 &= - \int_0^{\infty} \left( \sum_{j=1}^{\infty} \frac{(-t)^j}{(j-1)!} \right) e^{-t} dt \\
 &= - \int_0^{\infty} \left( \sum_{j=0}^{\infty} \frac{(-t)^{j+1}}{j!} \right) e^{-t} dt \\
 &= - \int_0^{\infty} (-t) \left( \sum_{j=0}^{\infty} \frac{(-t)^j}{j!} \right) e^{-t} dt \\
 &= - \int_0^{\infty} (-t) e^{-2t} dt \\
 &\quad [\text{variable substitution } 2t = \zeta, dt = \frac{1}{2} d\zeta] \\
 &= \frac{1}{4} \int_0^{\infty} \zeta e^{-\zeta} d\zeta \\
 &= \frac{1}{4} \Gamma(2) = \frac{1}{4} 1! = \frac{1}{4},
 \end{aligned} \tag{15.37}$$

which is again equal to the Abel sum.



## *Appendix*



# A

## Hilbert space quantum mechanics and quantum logic

### A.1 Quantum mechanics

The following is a very brief introduction to quantum mechanics. Introductions to quantum mechanics can be found in Refs. <sup>1</sup>.

All quantum mechanical entities are represented by objects of Hilbert spaces <sup>2</sup>. The following identifications between physical and theoretical objects are made (a *caveat*: this is an incomplete list).

In what follows, unless stated differently, only *finite* dimensional Hilbert spaces are considered. Then, the vectors corresponding to states can be written as usual vectors in complex Hilbert space. Furthermore, bounded self-adjoint operators are equivalent to bounded Hermitean operators. They can be represented by matrices, and the self-adjoint conjugation is just transposition and complex conjugation of the matrix elements. Let  $\mathfrak{B} = \{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_n\}$  be an orthonormal basis in  $n$ -dimensional Hilbert space  $\mathfrak{H}$ . That is, orthonormal base vectors in  $\mathfrak{B}$  satisfy  $\langle \mathbf{b}_i, \mathbf{b}_j \rangle = \delta_{ij}$ , where  $\delta_{ij}$  is the Kronecker delta function.

(I) A quantum *state* is represented by a positive Hermitian operator  $\rho$  of trace class one in the Hilbert space  $\mathfrak{H}$ ; that is

- (i)  $\rho^\dagger = \rho = \sum_{i=1}^n p_i |\mathbf{b}_i\rangle \langle \mathbf{b}_i|$ , with  $p_i \geq 0$  for all  $i = 1, \dots, n$ ,  $\mathbf{b}_i \in \mathfrak{B}$ , and  $\sum_{i=1}^n p_i = 1$ , so that
- (ii)  $\langle \rho \mathbf{x} | \mathbf{x} \rangle = \langle \mathbf{x} | \rho \mathbf{x} \rangle \geq 0$ ,
- (iii)  $\text{Tr}(\rho) = \sum_{i=1}^n \langle \mathbf{b}_i | \rho | \mathbf{b}_i \rangle = 1$ .

A *pure state* is represented by a (unit) vector  $\mathbf{x}$ , also denoted by  $|\mathbf{x}\rangle$ , of the Hilbert space  $\mathfrak{H}$  spanning a one-dimensional subspace (manifold)  $\mathfrak{M}_{\mathbf{x}}$  of the Hilbert space  $\mathfrak{H}$ . Equivalently, it is represented by the one-dimensional subspace (manifold)  $\mathfrak{M}_{\mathbf{x}}$  of the Hilbert space  $\mathfrak{H}$  spanned by the vector  $\mathbf{x}$ . Equivalently, it is represented by the projector  $\mathbf{E}_{\mathbf{x}} = |\mathbf{x}\rangle \langle \mathbf{x}|$  onto the unit vector  $\mathbf{x}$  of the Hilbert space  $\mathfrak{H}$ .

Therefore, if two vectors  $\mathbf{x}, \mathbf{y} \in \mathfrak{H}$  represent pure states, their vector sum  $\mathbf{z} = \mathbf{x} + \mathbf{y} \in \mathfrak{H}$  represents a pure state as well. This state  $\mathbf{z}$  is called the

<sup>1</sup> Richard Phillips Feynman, Robert B. Leighton, and Matthew Sands. *The Feynman Lectures on Physics. Quantum Mechanics*, volume III. Addison-Wesley, Reading, MA, 1965; L. E. Ballentine. *Quantum Mechanics*. Prentice Hall, Englewood Cliffs, NJ, 1989; A. Messiah. *Quantum Mechanics*, volume I. North-Holland, Amsterdam, 1962; Asher Peres. *Quantum Theory: Concepts and Methods*. Kluwer Academic Publishers, Dordrecht, 1993; and John Archibald Wheeler and Wojciech Hubert Zurek. *Quantum Theory and Measurement*. Princeton University Press, Princeton, NJ, 1983

<sup>2</sup> John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932. English translation in Ref. ; and Garrett Birkhoff and John von Neumann. The logic of quantum mechanics. *Annals of Mathematics*, 37(4): 823–843, 1936. DOI: 10.2307/1968621. URL <http://dx.doi.org/10.2307/1968621>

John von Neumann. *Mathematical Foundations of Quantum Mechanics*. Princeton University Press, Princeton, NJ, 1955



*coherent superposition* of state  $\mathbf{x}$  and  $\mathbf{y}$ . Coherent state superpositions between classically mutually exclusive (i.e. orthogonal) states, say  $|\mathbf{0}\rangle$  and  $|\mathbf{1}\rangle$ , will become most important in quantum information theory.

Any pure state  $\mathbf{x}$  can be written as a linear combination of the set of orthonormal base vectors  $\{\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_n\}$ , that is,  $\mathbf{x} = \sum_{i=1}^n \beta_i \mathbf{b}_i$ , where  $n$  is the dimension of  $\mathfrak{H}$  and  $\beta_i = \langle \mathbf{b}_i | \mathbf{x} \rangle \in \mathbb{C}$ .

In the Dirac bra-ket notation, unity is given by  $\mathbf{1} = \sum_{i=1}^n |\mathbf{b}_i\rangle\langle\mathbf{b}_i|$ , or just  $\mathbf{1} = \sum_{i=1}^n |i\rangle\langle i|$ .

- (II) *Observables* are represented by self-adjoint or, synonymously, Hermitian, operators or transformations  $\mathbf{A} = \mathbf{A}^\dagger$  on the Hilbert space  $\mathfrak{H}$  such that  $\langle \mathbf{A}\mathbf{x} | \mathbf{y} \rangle = \langle \mathbf{x} | \mathbf{A}\mathbf{y} \rangle$  for all  $\mathbf{x}, \mathbf{y} \in \mathfrak{H}$ . (Observables and their corresponding operators are identified.)

The trace of an operator  $\mathbf{A}$  is given by  $\text{Tr}\mathbf{A} = \sum_{i=1}^n \langle \mathbf{b}_i | \mathbf{A} | \mathbf{b}_i \rangle$ .

Furthermore, any Hermitian operator has a spectral representation as a spectral sum  $\mathbf{A} = \sum_{i=1}^n \alpha_i \mathbf{E}_i$ , where the  $\mathbf{E}_i$ 's are orthogonal projection operators onto the orthonormal eigenvectors  $\mathbf{a}_i$  of  $\mathbf{A}$  (nondegenerate case).

Observables are said to be *compatible* if they can be defined simultaneously with arbitrary accuracy; i.e., if they are “independent.” A criterion for compatibility is the *commutator*. Two observables  $\mathbf{A}, \mathbf{B}$  are compatible, if their *commutator* vanishes; that is, if  $[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA} = 0$ .

It has recently been demonstrated that (by an analog embodiment using particle beams) every Hermitian operator in a finite dimensional Hilbert space can be experimentally realized<sup>3</sup>.

- (III) The result of any single measurement of the observable  $A$  on a state  $\mathbf{x} \in \mathfrak{H}$  can only be one of the real eigenvalues of the corresponding Hermitian operator  $\mathbf{A}$ . If  $\mathbf{x}$  is in a coherent superposition of eigenstates of  $\mathbf{A}$ , the particular outcome of any such single measurement is believed to be indeterministic<sup>4</sup>; that is, it cannot be predicted with certainty. As a result of the measurement, the system is in the state which corresponds to the eigenvector  $\mathbf{a}_i$  of  $\mathbf{A}$  with the associated real-valued eigenvalue  $\alpha_i$ ; that is,  $\mathbf{A}\mathbf{x} = \alpha_n \mathbf{a}_n$  (no Einstein sum convention here).

This “transition”  $\mathbf{x} \rightarrow \mathbf{a}_n$  has given rise to speculations concerning the “collapse of the wave function (state).” But, subject to technology and in principle, it may be possible to reconstruct coherence; that is, to “reverse the collapse of the wave function (state)” if the process of measurement is reversible. After this reconstruction, no information about the measurement must be left, not even in principle. How did Schrödinger, the creator of wave mechanics, perceive the  $\psi$ -function? In his 1935 paper “Die gegenwärtige Situation in der Quantenmechanik” (“The present situation in quantum mechanics”<sup>5</sup>), on page 53, Schrödinger states, “the  $\psi$ -function as expectation-catalog:

<sup>3</sup> M. Reck, Anton Zeilinger, H. J. Bernstein, and P. Bertani. Experimental realization of any discrete unitary operator. *Physical Review Letters*, 73:58–61, 1994. DOI: 10.1103/PhysRevLett.73.58. URL <http://dx.doi.org/10.1103/PhysRevLett.73.58>

<sup>4</sup> Max Born. Zur Quantenmechanik der Stoßvorgänge. *Zeitschrift für Physik*, 37: 863–867, 1926a. DOI: 10.1007/BF01397477. URL <http://dx.doi.org/10.1007/BF01397477>; Max Born. Quantenmechanik der Stoßvorgänge. *Zeitschrift für Physik*, 38: 803–827, 1926b. DOI: 10.1007/BF01397184. URL <http://dx.doi.org/10.1007/BF01397184>; and Anton Zeilinger. The message of the quantum. *Nature*, 438: 743, 2005. DOI: 10.1038/438743a. URL <http://dx.doi.org/10.1038/438743a>

<sup>5</sup> Erwin Schrödinger. Die gegenwärtige Situation in der Quantenmechanik. *Naturwissenschaften*, 23:807–812, 823–828, 844–849, 1935b. DOI: 10.1007/BF01491891, 10.1007/BF01491914, 10.1007/BF01491987. URL <http://dx.doi.org/10.1007/BF01491891>, <http://dx.doi.org/10.1007/BF01491914>, <http://dx.doi.org/10.1007/BF01491987>

... In it [[the  $\psi$ -function]] is embodied the momentarily-attained sum of theoretically based future expectation, somewhat as laid down in a *catalog*. ... For each measurement one is required to ascribe to the  $\psi$ -function (=the prediction catalog) a characteristic, quite sudden change, which *depends on the measurement result obtained*, and so *cannot be foreseen*; from which alone it is already quite clear that this second kind of change of the  $\psi$ -function has nothing whatever in common with its orderly development *between* two measurements. The abrupt change [[of the  $\psi$ -function (=the prediction catalog)]] by measurement ... is the most interesting point of the entire theory. It is precisely *the* point that demands the break with naive realism. For *this* reason one cannot put the  $\psi$ -function directly in place of the model or of the physical thing. And indeed not because one might never dare impute abrupt unforeseen changes to a physical thing or to a model, but because in the realism point of view observation is a natural process like any other and cannot *per se* bring about an interruption of the orderly flow of natural events."

The late Schrödinger was much more polemic about these issues; compare for instance his remarks in his Dublin Seminars (1949-1955), published in Ref. <sup>6</sup>, pages 19-20: "The idea that [the alternate measurement outcomes] be not alternatives but *all* really happening simultaneously seems lunatic to [the quantum theorist], just *impossible*. He thinks that if the laws of nature took *this* form for, let me say, a quarter of an hour, we should find our surroundings rapidly turning into a quagmire, a sort of a featureless jelly or plasma, all contours becoming blurred, we ourselves probably becoming jelly fish. It is strange that he should believe this. For I understand he grants that unobserved nature does behave this way – namely according to the wave equation. ... according to the quantum theorist, nature is prevented from rapid jellification only by our perceiving or observing it."

- (IV) The probability  $P_{\mathbf{x}}(\mathbf{y})$  to find a system represented by state  $\rho_{\mathbf{x}}$  in some pure state  $\mathbf{y}$  is given by the *Born rule* which is derivable from Gleason's theorem:  $P_{\mathbf{x}}(\mathbf{y}) = \text{Tr}(\rho_{\mathbf{x}} \mathbf{E}_{\mathbf{y}})$ . Recall that the density  $\rho_{\mathbf{x}}$  is a positive Hermitian operator of trace class one.

For pure states with  $\rho_{\mathbf{x}}^2 = \rho_{\mathbf{x}}$ ,  $\rho_{\mathbf{x}}$  is a onedimensional projector  $\rho_{\mathbf{x}} = \mathbf{E}_{\mathbf{x}} = |\mathbf{x}\rangle\langle\mathbf{x}|$  onto the unit vector  $\mathbf{x}$ ; thus expansion of the trace and  $\mathbf{E}_{\mathbf{y}} = |\mathbf{y}\rangle\langle\mathbf{y}|$  yields  $P_{\mathbf{x}}(\mathbf{y}) = \sum_{i=1}^n \langle i | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{y} \rangle \langle \mathbf{y} | i \rangle = \sum_{i=1}^n \langle \mathbf{y} | i \rangle \langle i | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{y} \rangle = \sum_{i=1}^n \langle \mathbf{y} | \mathbf{1} | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{y} \rangle = |\langle \mathbf{y} | \mathbf{x} \rangle|^2$ .

- (V) The *average value* or *expectation value* of an observable  $\mathbf{A}$  in a quantum state  $\mathbf{x}$  is given by  $\langle \mathbf{A} \rangle_{\mathbf{x}} = \text{Tr}(\rho_{\mathbf{x}} \mathbf{A})$ .

The *average value* or *expectation value* of an observable  $\mathbf{A} = \sum_{i=1}^n \alpha_i \mathbf{E}_i$  in a pure state  $\mathbf{x}$  is given by  $\langle \mathbf{A} \rangle_{\mathbf{x}} = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle j | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{a}_i \rangle \langle \mathbf{a}_i | j \rangle = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle \mathbf{a}_i | j \rangle \langle j | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{a}_i \rangle = \sum_{j=1}^n \sum_{i=1}^n \alpha_i \langle \mathbf{a}_i | \mathbf{1} | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{a}_i \rangle =$

German original: "*Die  $\psi$ -Funktion als Katalog der Erwartung*: ... Sie [[die  $\psi$ -Funktion]] ist jetzt das Instrument zur Voraussage der Wahrscheinlichkeit von Maßzahlen. In ihr ist die jeweils erreichte Summe theoretisch begründeter Zukunfts-erwartung verkörpert, gleichsam wie in einem *Katalog* niedergelegt. ... Bei jeder Messung ist man genötigt, der  $\psi$ -Funktion (=dem Voraussagenkatalog) eine eigenartige, etwas plötzliche Veränderung zuzuschreiben, die von der *gefundenen Maßzahl* abhängt und sich *nicht vorhersehen läßt*; woraus allein schon deutlich ist, daß diese zweite Art von Veränderung der  $\psi$ -Funktion mit ihrem regelmäßigen Abrollen *zwischen* zwei Messungen nicht das mindeste zu tun hat. Die abrupte Veränderung durch die Messung ... ist der interessanteste Punkt der ganzen Theorie. Es ist genau *der* Punkt, der den Bruch mit dem naiven Realismus verlangt. Aus *diesem* Grund kann man die  $\psi$ -Funktion *nicht* direkt an die Stelle des Modells oder des Readings setzen. Und zwar nicht etwa weil man einem Reading oder einem Modell nicht abrupte unvorhergesehene Änderungen zumuten dürfte, sondern weil vom realistischen Standpunkt die Beobachtung ein Naturvorgang ist wie jeder andere und nicht *per se* eine Unterbrechung des regelmäßigen Naturlaufs hervorrufen darf.

<sup>6</sup> Erwin Schrödinger. *The Interpretation of Quantum Mechanics. Dublin Seminars (1949-1955) and Other Unpublished Essays*. Ox Bow Press, Woodbridge, Connecticut, 1995

$$\sum_{i=1}^n \alpha_i |\langle \mathbf{x} | \mathbf{a}_i \rangle|^2.$$

(VI) The dynamical law or equation of motion can be written in the form  $x(t) = \mathbf{U}x(t_0)$ , where  $\mathbf{U}^\dagger = \mathbf{U}^{-1}$  (“ $\dagger$ ” stands for transposition and complex conjugation) is a linear *unitary transformation* or *isometry*.

The *Schrödinger equation*  $i\hbar \frac{\partial}{\partial t} \psi(t) = H\psi(t)$  is obtained by identifying  $\mathbf{U}$  with  $\mathbf{U} = e^{-i\mathbf{H}t/\hbar}$ , where  $\mathbf{H}$  is a self-adjoint Hamiltonian (“energy”) operator, by differentiating the equation of motion with respect to the time variable  $t$ .

For stationary  $\psi_n(t) = e^{-(i/\hbar)E_n t} \psi_n$ , the Schrödinger equation can be brought into its time-independent form  $\mathbf{H}\psi_n = E_n \psi_n$ . Here,  $i\hbar \frac{\partial}{\partial t} \psi_n(t) = E_n \psi_n(t)$  has been used;  $E_n$  and  $\psi_n$  stand for the  $n$ ’th eigenvalue and eigenstate of  $\mathbf{H}$ , respectively.

Usually, a physical problem is defined by the Hamiltonian  $\mathbf{H}$ . The problem of finding the physically relevant states reduces to finding a complete set of eigenvalues and eigenstates of  $\mathbf{H}$ . Most elegant solutions utilize the symmetries of the problem; that is, the symmetry of  $\mathbf{H}$ . There exist two “canonical” examples, the  $1/r$ -potential and the harmonic oscillator potential, which can be solved wonderfully by these methods (and they are presented over and over again in standard courses of quantum mechanics), but not many more. (See, for instance,<sup>7</sup> for a detailed treatment of various Hamiltonians  $\mathbf{H}$ .)

<sup>7</sup> A. S. Davydov. *Quantum Mechanics*. Addison-Wesley, Reading, MA, 1965

## A.2 Quantum logic

The dimensionality of the Hilbert space for a given quantum system depends on the number of possible mutually exclusive outcomes. In the spin- $\frac{1}{2}$  case, for example, there are two outcomes “up” and “down,” associated with spin state measurements along arbitrary directions. Thus, the dimensionality of Hilbert space needs to be two.

Then the following identifications can be made. Table A.1 lists the identifications of relations of operations of classical Boolean set-theoretic and quantum Hilbert lattice types.

generic lattice	order relation	“meet”	“join”	“complement”
propositional calculus	implication $\rightarrow$	disjunction “and” $\wedge$	conjunction “or” $\vee$	negation “not” $\neg$
“classical” lattice of subsets of a set	subset $\subset$	intersection $\cap$	union $\cup$	complement
Hilbert lattice	subspace relation $\subset$	intersection of subspaces $\cap$	closure of linear span $\oplus$	orthogonal subspace $\perp$
lattice of commuting {noncommuting} projection operators	$\mathbf{E}_1 \mathbf{E}_2 = \mathbf{E}_1$	$\mathbf{E}_1 \mathbf{E}_2$ $\{\lim_{n \rightarrow \infty} (\mathbf{E}_1 \mathbf{E}_2)^n\}$	$\mathbf{E}_1 + \mathbf{E}_2 - \mathbf{E}_1 \mathbf{E}_2$	orthogonal projection

Table A.1: Comparison of the identifications of lattice relations and operations for the lattices of subsets of a set, for experimental propositional calculi, for Hilbert lattices, and for lattices of commuting projection operators.

- (i) Any closed linear subspace  $\mathfrak{M}_{\mathbf{p}}$  spanned by a vector  $\mathbf{p}$  in a Hilbert space  $\mathfrak{H}$  – or, equivalently, any projection operator  $\mathbf{E}_{\mathbf{p}} = |\mathbf{p}\rangle\langle\mathbf{p}|$  on a Hilbert space  $\mathfrak{H}$  corresponds to an elementary proposition  $\mathbf{p}$ . The elementary “true”-“false” proposition can in English be spelled out explicitly as

“The physical system has a property corresponding to the associated closed linear subspace.”

It is coded into the two eigenvalues 0 and 1 of the projector  $\mathbf{E}_{\mathbf{p}}$  (recall that  $\mathbf{E}_{\mathbf{p}}\mathbf{E}_{\mathbf{p}} = \mathbf{E}_{\mathbf{p}}$ ).

- (ii) The logical “and” operation is identified with the set theoretical intersection of two propositions “ $\cap$ ”; i.e., with the intersection of two subspaces. It is denoted by the symbol “ $\wedge$ ”. So, for two propositions  $\mathbf{p}$  and  $\mathbf{q}$  and their associated closed linear subspaces  $\mathfrak{M}_{\mathbf{p}}$  and  $\mathfrak{M}_{\mathbf{q}}$ ,

$$\mathfrak{M}_{\mathbf{p}\wedge\mathbf{q}} = \{x \mid x \in \mathfrak{M}_{\mathbf{p}}, x \in \mathfrak{M}_{\mathbf{q}}\}.$$

- (iii) The logical “or” operation is identified with the closure of the linear span “ $\oplus$ ” of the subspaces corresponding to the two propositions. It is denoted by the symbol “ $\vee$ ”. So, for two propositions  $\mathbf{p}$  and  $\mathbf{q}$  and their associated closed linear subspaces  $\mathfrak{M}_{\mathbf{p}}$  and  $\mathfrak{M}_{\mathbf{q}}$ ,

$$\mathfrak{M}_{\mathbf{p}\vee\mathbf{q}} = \mathfrak{M}_{\mathbf{p}} \oplus \mathfrak{M}_{\mathbf{q}} = \{\mathbf{x} \mid \mathbf{x} = \alpha\mathbf{y} + \beta\mathbf{z}, \alpha, \beta \in \mathbb{C}, \mathbf{y} \in \mathfrak{M}_{\mathbf{p}}, \mathbf{z} \in \mathfrak{M}_{\mathbf{q}}\}.$$

The symbol  $\oplus$  will be used to indicate the closed linear subspace spanned by two vectors. That is,

$$\mathbf{u} \oplus \mathbf{v} = \{\mathbf{w} \mid \mathbf{w} = \alpha\mathbf{u} + \beta\mathbf{v}, \alpha, \beta \in \mathbb{C}, \mathbf{u}, \mathbf{v} \in \mathfrak{H}\}.$$

Notice that a vector of Hilbert space may be an element of  $\mathfrak{M}_{\mathbf{p}} \oplus \mathfrak{M}_{\mathbf{q}}$  without being an element of either  $\mathfrak{M}_{\mathbf{p}}$  or  $\mathfrak{M}_{\mathbf{q}}$ , since  $\mathfrak{M}_{\mathbf{p}} \oplus \mathfrak{M}_{\mathbf{q}}$  includes all the vectors in  $\mathfrak{M}_{\mathbf{p}} \cup \mathfrak{M}_{\mathbf{q}}$ , as well as all of their linear combinations (superpositions) and their limit vectors.

- (iv) The logical “not”-operation, or “negation” or “complement,” is identified with operation of taking the orthogonal subspace “ $\perp$ ”. It is denoted by the symbol “ $'$ ”. In particular, for a proposition  $\mathbf{p}$  and its associated closed linear subspace  $\mathfrak{M}_{\mathbf{p}}$ , the negation  $\mathbf{p}'$  is associated with

$$\mathfrak{M}_{\mathbf{p}'} = \{\mathbf{x} \mid \langle \mathbf{x} \mid \mathbf{y} \rangle = 0, \mathbf{y} \in \mathfrak{M}_{\mathbf{p}}\},$$

where  $\langle \mathbf{x} \mid \mathbf{y} \rangle$  denotes the scalar product of  $\mathbf{x}$  and  $\mathbf{y}$ .

- (v) The logical “implication” relation is identified with the set theoretical subset relation “ $\subset$ ”. It is denoted by the symbol “ $\rightarrow$ ”. So, for two propositions  $\mathbf{p}$  and  $\mathbf{q}$  and their associated closed linear subspaces  $\mathfrak{M}_{\mathbf{p}}$  and  $\mathfrak{M}_{\mathbf{q}}$ ,

$$\mathbf{p} \rightarrow \mathbf{q} \iff \mathfrak{M}_{\mathbf{p}} \subset \mathfrak{M}_{\mathbf{q}}.$$

- (vi) A trivial statement which is always “true” is denoted by 1. It is represented by the entire Hilbert space  $\mathfrak{H}$ . So,

$$\mathfrak{M}_1 = \mathfrak{H}.$$

- (vii) An absurd statement which is always “false” is denoted by 0. It is represented by the zero vector 0. So,

$$\mathfrak{M}_0 = 0.$$

### A.3 Diagrammatical representation, blocks, complementarity

Propositional structures are often represented by Hasse and Greechie diagrams. A *Hasse diagram* is a convenient representation of the logical implication, as well as of the “and” and “or” operations among propositions. Points “•” represent propositions. Propositions which are implied by other ones are drawn higher than the other ones. Two propositions are connected by a line if one implies the other. Atoms are propositions which “cover” the least element 0; i.e., they lie “just above” 0 in a Hasse diagram of the partial order.

A much more compact representation of the propositional calculus can be given in terms of its *Greechie diagram*<sup>8</sup>. In this representation, the emphasis is on Boolean subalgebras. Points “◦” represent the atoms. If they belong to the same Boolean subalgebra, they are connected by edges or smooth curves. The collection of all atoms and elements belonging to the same Boolean subalgebra is called *block*; i.e., every block represents a Boolean subalgebra within a nonboolean structure. The blocks can be joined or pasted together as follows.

- (i) The tautologies of all blocks are identified.
- (ii) The absurdities of all blocks are identified.
- (iii) Identical elements in different blocks are identified.
- (iii) The logical and algebraic structures of all blocks remain intact.

This construction is often referred to as *pasting* construction. If the blocks are only pasted together at the tautology and the absurdity, one calls the resulting logic a *horizontal sum*.

Every single block represents some “maximal collection of co-measurable observables” which will be identified with some quantum *context*. Hilbert lattices can be thought of as the pasting of a continuity of such blocks or contexts.

Note that whereas all propositions within a given block or context are co-measurable; propositions belonging to different blocks are not. This latter feature is an expression of complementarity. Thus from a strictly

<sup>8</sup> J. R. Greechie. Orthomodular lattices admitting no states. *Journal of Combinatorial Theory*, 10:119–132, 1971.  
DOI: 10.1016/0097-3165(71)90015-X.  
URL [http://dx.doi.org/10.1016/0097-3165\(71\)90015-X](http://dx.doi.org/10.1016/0097-3165(71)90015-X)

operational point of view, it makes no sense to speak of the “real physical existence” of different contexts, as knowledge of a single context makes impossible the measurement of all the other ones.

Einstein-Podolski-Rosen (EPR) type arguments<sup>9</sup> utilizing a configuration sketched in Fig. A.4 claim to be able to infer two different contexts counterfactually. One context is measured on one side of the setup, the other context on the other side of it. By the uniqueness property<sup>10</sup> of certain two-particle states, knowledge of a property of one particle entails the certainty that, if this property were measured on the other particle as well, the outcome of the measurement would be a unique function of the outcome of the measurement performed. This makes possible the measurement of one context, as well as the simultaneous counterfactual inference of another, mutual exclusive, context. Because, one could argue, although one has actually measured on one side a different, incompatible context compared to the context measured on the other side, if on both sides the same context *would be measured*, the outcomes on both sides *would be uniquely correlated*. Hence measurement of one context per side is sufficient, for the outcome could be counterfactually inferred on the other side.

As problematic as counterfactual physical reasoning may appear from an operational point of view even for a two particle state, the simultaneous “counterfactual inference” of three or more blocks or contexts fails because of the missing uniqueness property of quantum states.

#### A.4 Realizations of two-dimensional beam splitters

In what follows, lossless devices will be considered. The matrix

$$\mathbf{T}(\omega, \phi) = \begin{pmatrix} \sin \omega & \cos \omega \\ e^{-i\phi} \cos \omega & -e^{-i\phi} \sin \omega \end{pmatrix} \quad (\text{A.1})$$

introduced in Eq. (A.1) has physical realizations in terms of beam splitters and Mach-Zehnder interferometers equipped with an appropriate number of phase shifters. Two such realizations are depicted in Fig. A.1. The elementary quantum interference device  $\mathbf{T}^{bs}$  in Fig. A.1a) is a unit consisting of two phase shifters  $P_1$  and  $P_2$  in the input ports, followed by a beam splitter  $S$ , which is followed by a phase shifter  $P_3$  in one of the output ports. The device can be quantum mechanically described by<sup>11</sup>

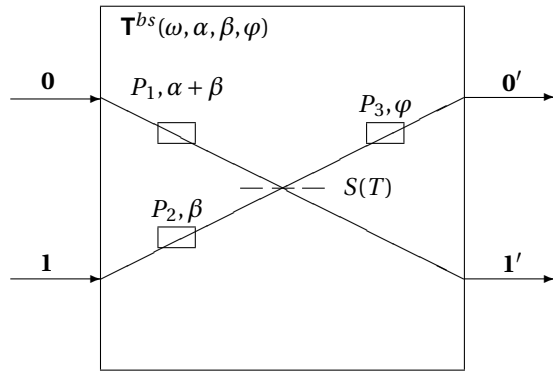
$$\begin{aligned} P_1 : |0\rangle &\rightarrow |0\rangle e^{i(\alpha+\beta)}, \\ P_2 : |1\rangle &\rightarrow |1\rangle e^{i\beta}, \\ S : |0\rangle &\rightarrow \sqrt{T}|1'\rangle + i\sqrt{R}|0'\rangle, \\ S : |1\rangle &\rightarrow \sqrt{T}|0'\rangle + i\sqrt{R}|1'\rangle, \\ P_3 : |0'\rangle &\rightarrow |0'\rangle e^{i\varphi}, \end{aligned} \quad (\text{A.2})$$

where every reflection by a beam splitter  $S$  contributes a phase  $\pi/2$  and thus a factor of  $e^{i\pi/2} = i$  to the state evolution. Transmitted beams remain

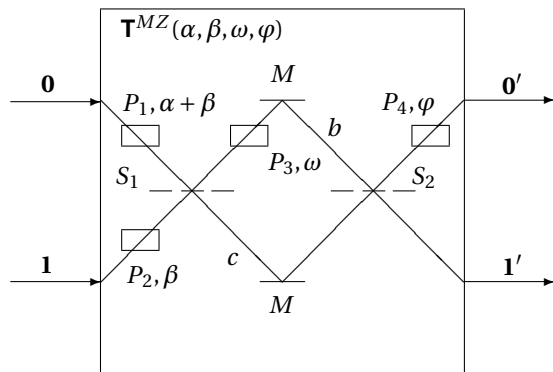
<sup>9</sup> Albert Einstein, Boris Podolsky, and Nathan Rosen. Can quantum-mechanical description of physical reality be considered complete? *Physical Review*, 47(10):777–780, May 1935. DOI: 10.1103/PhysRev.47.777. URL <http://dx.doi.org/10.1103/PhysRev.47.777>

<sup>10</sup> Karl Svozil. Are simultaneous Bell measurements possible? *New Journal of Physics*, 8:39, 1–8, 2006b. DOI: 10.1088/1367-2630/8/3/039. URL <http://dx.doi.org/10.1088/1367-2630/8/3/039>

<sup>11</sup> Daniel M. Greenberger, Mike A. Horne, and Anton Zeilinger. Multiparticle interferometry and the superposition principle. *Physics Today*, 46:22–29, August 1993. DOI: 10.1063/1.881360. URL <http://dx.doi.org/10.1063/1.881360>



a)



b)

Figure A.1: A universal quantum interference device operating on a qubit can be realized by a 4-port interferometer with two input ports  $0, 1$  and two output ports  $0', 1'$ ; a) realization by a single beam splitter  $S(T)$  with variable transmission  $T$  and three phase shifters  $P_1, P_2, P_3$ ; b) realization by two 50:50 beam splitters  $S_1$  and  $S_2$  and four phase shifters  $P_1, P_2, P_3, P_4$ .

unchanged; i.e., there are no phase changes. Global phase shifts from mirror reflections are omitted. With  $\sqrt{T(\omega)} = \cos \omega$  and  $\sqrt{R(\omega)} = \sin \omega$ , the corresponding unitary evolution matrix is given by

$$\mathbf{T}^{bs}(\omega, \alpha, \beta, \varphi) = \begin{pmatrix} i e^{i(\alpha+\beta+\varphi)} \sin \omega & e^{i(\beta+\varphi)} \cos \omega \\ e^{i(\alpha+\beta)} \cos \omega & i e^{i\beta} \sin \omega \end{pmatrix}. \quad (\text{A.3})$$

Alternatively, the action of a lossless beam splitter may be described by the matrix<sup>12</sup>

$$\begin{pmatrix} i \sqrt{R(\omega)} & \sqrt{T(\omega)} \\ \sqrt{T(\omega)} & i \sqrt{R(\omega)} \end{pmatrix} = \begin{pmatrix} i \sin \omega & \cos \omega \\ \cos \omega & i \sin \omega \end{pmatrix}.$$

A phase shifter in two-dimensional Hilbert space is represented by either  $\text{diag}(e^{i\varphi}, 1)$  or  $\text{diag}(1, e^{i\varphi})$ . The action of the entire device consisting of such elements is calculated by multiplying the matrices in reverse order in which the quanta pass these elements<sup>13</sup>; i.e.,

$$\mathbf{T}^{bs}(\omega, \alpha, \beta, \varphi) = \begin{pmatrix} e^{i\varphi} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} i \sin \omega & \cos \omega \\ \cos \omega & i \sin \omega \end{pmatrix} \begin{pmatrix} e^{i(\alpha+\beta)} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\beta} \end{pmatrix}. \quad (\text{A.4})$$

The elementary quantum interference device  $\mathbf{T}^{MZ}$  depicted in Fig. A.1b) is a Mach-Zehnder interferometer with *two* input and output ports and three phase shifters. The process can be quantum mechanically described by

$$\begin{aligned} P_1 : |0\rangle &\rightarrow |0\rangle e^{i(\alpha+\beta)}, \\ P_2 : |1\rangle &\rightarrow |1\rangle e^{i\beta}, \\ S_1 : |1\rangle &\rightarrow (|b\rangle + i|c\rangle)/\sqrt{2}, \\ S_1 : |0\rangle &\rightarrow (|c\rangle + i|b\rangle)/\sqrt{2}, \\ P_3 : |b\rangle &\rightarrow |b\rangle e^{i\omega}, \\ S_2 : |b\rangle &\rightarrow (|1'\rangle + i|0'\rangle)/\sqrt{2}, \\ S_2 : |c\rangle &\rightarrow (|0'\rangle + i|1'\rangle)/\sqrt{2}, \\ P_4 : |0'\rangle &\rightarrow |0'\rangle e^{i\varphi}. \end{aligned} \quad (\text{A.5})$$

The corresponding unitary evolution matrix is given by

$$\mathbf{T}^{MZ}(\alpha, \beta, \omega, \varphi) = i e^{i(\beta+\frac{\omega}{2})} \begin{pmatrix} -e^{i(\alpha+\varphi)} \sin \frac{\omega}{2} & e^{i\varphi} \cos \frac{\omega}{2} \\ e^{i\alpha} \cos \frac{\omega}{2} & \sin \frac{\omega}{2} \end{pmatrix}. \quad (\text{A.6})$$

Alternatively,  $\mathbf{T}^{MZ}$  can be computed by matrix multiplication; i.e.,

$$\begin{aligned} \mathbf{T}^{MZ}(\alpha, \beta, \omega, \varphi) &= i e^{i(\beta+\frac{\omega}{2})} \begin{pmatrix} e^{i\varphi} & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} e^{i\omega} & 0 \\ 0 & 1 \end{pmatrix} \\ &\cdot \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \begin{pmatrix} e^{i(\alpha+\beta)} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\beta} \end{pmatrix}. \end{aligned} \quad (\text{A.7})$$

Both elementary quantum interference devices  $\mathbf{T}^{bs}$  and  $\mathbf{T}^{MZ}$  are universal in the sense that every unitary quantum evolution operator in two-dimensional Hilbert space can be brought into a one-to-one correspondence with  $\mathbf{T}^{bs}$  and  $\mathbf{T}^{MZ}$ . As the emphasis is on the realization of

<sup>12</sup> The standard labelling of the input and output ports are interchanged, therefore sine and cosine are exchanged in the transition matrix.

<sup>13</sup> B. Yurke, S. L. McCall, and J. R. Klauder. SU(2) and SU(1,1) interferometers. *Physical Review A*, 33:4033–4054, 1986. URL <http://dx.doi.org/10.1103/PhysRevA.33.4033>; and Richard A. Campos, Bahaa E. A. Saleh, and Malvin C. Teich. Fourth-order interference of joint single-photon wave packets in lossless optical systems. *Physical Review A*, 42:4127–4137, 1990. DOI: 10.1103/PhysRevA.42.4127. URL <http://dx.doi.org/10.1103/PhysRevA.42.4127>



the elementary beam splitter  $\mathbf{T}$  in Eq. (A.1), which spans a subset of the set of all two-dimensional unitary transformations, the comparison of the parameters in  $\mathbf{T}(\omega, \phi) = \mathbf{T}^{bs}(\omega', \beta', \alpha', \varphi') = \mathbf{T}^{MZ}(\omega'', \beta'', \alpha'', \varphi'')$  yields  $\omega = \omega' = \omega''/2$ ,  $\beta' = \pi/2 - \phi$ ,  $\varphi' = \phi - \pi/2$ ,  $\alpha' = -\pi/2$ ,  $\beta'' = \pi/2 - \omega - \phi$ ,  $\varphi'' = \phi - \pi$ ,  $\alpha'' = \pi$ , and thus

$$\mathbf{T}(\omega, \phi) = \mathbf{T}^{bs}\left(\omega, -\frac{\pi}{2}, \frac{\pi}{2} - \phi, \phi - \frac{\pi}{2}\right) = \mathbf{T}^{MZ}\left(2\omega, \pi, \frac{\pi}{2} - \omega - \phi, \phi - \pi\right). \quad (\text{A.8})$$

Let us examine the realization of a few primitive logical “gates” corresponding to (unitary) unary operations on qubits. The “identity” element  $\mathbb{I}_2$  is defined by  $|\mathbf{0}\rangle \rightarrow |\mathbf{0}\rangle$ ,  $|\mathbf{1}\rangle \rightarrow |\mathbf{1}\rangle$  and can be realized by

$$\mathbb{I}_2 = \mathbf{T}\left(\frac{\pi}{2}, \pi\right) = \mathbf{T}^{bs}\left(\frac{\pi}{2}, -\frac{\pi}{2}, -\frac{\pi}{2}, \frac{\pi}{2}\right) = \mathbf{T}^{MZ}(\pi, \pi, -\pi, 0) = \text{diag}(1, 1) \quad . \quad (\text{A.9})$$

The “not” gate is defined by  $|\mathbf{0}\rangle \rightarrow |\mathbf{1}\rangle$ ,  $|\mathbf{1}\rangle \rightarrow |\mathbf{0}\rangle$  and can be realized by

$$\text{not} = \mathbf{T}(0, 0) = \mathbf{T}^{bs}\left(0, -\frac{\pi}{2}, \frac{\pi}{2}, -\frac{\pi}{2}\right) = \mathbf{T}^{MZ}\left(0, \pi, \frac{\pi}{2}, \pi\right) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad . \quad (\text{A.10})$$

The next gate, a modified “ $\sqrt{\mathbb{I}_2}$ ,” is a truly quantum mechanical, since it converts a classical bit into a coherent superposition; i.e.,  $|\mathbf{0}\rangle$  and  $|\mathbf{1}\rangle$ .  $\sqrt{\mathbb{I}_2}$  is defined by  $|\mathbf{0}\rangle \rightarrow (1/\sqrt{2})(|\mathbf{0}\rangle + |\mathbf{1}\rangle)$ ,  $|\mathbf{1}\rangle \rightarrow (1/\sqrt{2})(|\mathbf{0}\rangle - |\mathbf{1}\rangle)$  and can be realized by

$$\sqrt{\mathbb{I}_2} = \mathbf{T}\left(\frac{\pi}{4}, 0\right) = \mathbf{T}^{bs}\left(\frac{\pi}{4}, -\frac{\pi}{2}, \frac{\pi}{2}, -\frac{\pi}{2}\right) = \mathbf{T}^{MZ}\left(\frac{\pi}{2}, \pi, \frac{\pi}{4}, -\pi\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad . \quad (\text{A.11})$$

Note that  $\sqrt{\mathbb{I}_2} \cdot \sqrt{\mathbb{I}_2} = \mathbb{I}_2$ . However, the reduced parameterization of  $\mathbf{T}(\omega, \phi)$  is insufficient to represent  $\sqrt{\text{not}}$ , such as

$$\sqrt{\text{not}} = \mathbf{T}^{bs}\left(\frac{\pi}{4}, -\pi, \frac{3\pi}{4}, -\pi\right) = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}, \quad (\text{A.12})$$

with  $\sqrt{\text{not}}\sqrt{\text{not}} = \text{not}$ .

## A.5 Two particle correlations

In what follows, spin state measurements along certain directions or angles in spherical coordinates will be considered. Let us, for the sake of clarity, first specify and make precise what we mean by “direction of measurement.” Following, e.g., Ref. <sup>14</sup>, page 1, Fig. 1, and Fig. A.2, when not specified otherwise, we consider a particle travelling along the positive  $z$ -axis; i.e., along  $0Z$ , which is taken to be horizontal. The  $x$ -axis along  $0X$  is also taken to be horizontal. The remaining  $y$ -axis is taken vertically along  $0Y$ . The three axes together form a right-handed system of coordinates.

The Cartesian  $(x, y, z)$ -coordinates can be translated into spherical coordinates  $(r, \theta, \varphi)$  via  $x = r \sin \theta \cos \varphi$ ,  $y = r \sin \theta \sin \varphi$ ,  $z = r \cos \theta$ , whereby  $\theta$  is the polar angle in the  $x$ - $z$ -plane measured from the  $z$ -axis,

<sup>14</sup> G. N. Ramachandran and S. Ramaseshan. Crystal optics. In S. Flügge, editor, *Handbuch der Physik XXV/1*, volume XXV, pages 1–217. Springer, Berlin, 1961

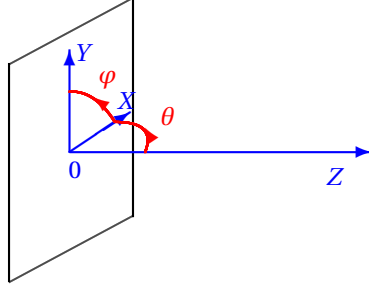


Figure A.2: Coordinate system for measurements of particles travelling along  $OZ$

with  $0 \leq \theta \leq \pi$ , and  $\varphi$  is the azimuthal angle in the  $x$ - $y$ -plane, measured from the  $x$ -axis with  $0 \leq \varphi < 2\pi$ . We shall only consider directions taken from the origin  $0$ , characterized by the angles  $\theta$  and  $\varphi$ , assuming a unit radius  $r = 1$ .

Consider two particles or quanta. On each one of the two quanta, certain measurements (such as the spin state or polarization) of (dichotomic) observables  $O(a)$  and  $O(b)$  along the directions  $a$  and  $b$ , respectively, are performed. The individual outcomes are encoded or labeled by the symbols “−” and “+,” or values “−1” and “+1” are recorded along the directions  $a$  for the first particle, and  $b$  for the second particle, respectively. (Suppose that the measurement direction  $a$  at “Alice’s location” is unknown to an observer “Bob” measuring  $b$  and *vice versa*.) A two-particle correlation function  $E(a, b)$  is defined by averaging over the product of the outcomes  $O(a)_i, O(b)_i \in \{-1, 1\}$  in the  $i$ th experiment for a total of  $N$  experiments; i.e.,

$$E(a, b) = \frac{1}{N} \sum_{i=1}^N O(a)_i O(b)_i. \quad (\text{A.13})$$

Quantum mechanically, we shall follow a standard procedure for obtaining the probabilities upon which the expectation functions are based. We shall start from the angular momentum operators, as for instance defined in Schiff’s “*Quantum Mechanics*”<sup>15</sup>, Chap. VI, Sec.24 in arbitrary directions, given by the spherical angular momentum co-ordinates  $\theta$  and  $\varphi$ , as defined above. Then, the projection operators corresponding to the eigenstates associated with the different eigenvalues are derived from the dyadic (tensor) product of the normalized eigenvectors. In Hilbert space based<sup>16</sup> quantum logic<sup>17</sup>, every projector corresponds to a proposition that the system is in a state corresponding to that observable. The quantum probabilities associated with these eigenstates are derived from the Born rule, assuming singlet states for the physical reasons discussed above. These probabilities contribute to the correlation and expectation functions.

Two-state particles:

Classical case:

<sup>15</sup> Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

<sup>16</sup> John von Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer, Berlin, 1932. English translation in Ref.

John von Neumann. *Mathematical Foundations of Quantum Mechanics*. Princeton University Press, Princeton, NJ, 1955

<sup>17</sup> Garrett Birkhoff and John von Neumann. The logic of quantum mechanics. *Annals of Mathematics*, 37(4):823–843, 1936. DOI: 10.2307/1968621. URL <http://dx.doi.org/10.2307/1968621>

For the two-outcome (e.g., spin one-half case of photon polarization) case, it is quite easy to demonstrate that the *classical* expectation function in the plane perpendicular to the direction connecting the two particles is a *linear* function of the azimuthal measurement angle. Assume uniform distribution of (opposite but otherwise) identical “angular momenta” shared by the two particles and lying on the circumference of the unit circle in the plane spanned by  $OX$  and  $OY$ , as depicted in Figs. A.2 and A.3.

By considering the length  $A_+(a, b)$  and  $A_-(a, b)$  of the positive and negative contributions to expectation function, one obtains for  $0 \leq \theta = |a - b| \leq \pi$ ,

$$\begin{aligned} E_{cl,2,2}(\theta) &= E_{cl,2,2}(a, b) = \frac{1}{2\pi} [A_+(a, b) - A_-(a, b)] \\ &= \frac{1}{2\pi} [2A_+(a, b) - 2\pi] = \frac{2}{\pi} |a - b| - 1 = \frac{2\theta}{\pi} - 1, \end{aligned} \quad (A.14)$$

where the subscripts stand for the number of mutually exclusive measurement outcomes per particle, and for the number of particles, respectively. Note that  $A_+(a, b) + A_-(a, b) = 2\pi$ .

Quantum case:

The two spin one-half particle case is one of the standard quantum mechanical exercises, although it is seldomly computed explicitly. For the sake of completeness and with the prospect to generalize the results to more particles of higher spin, this case will be enumerated explicitly. In what follows, we shall use the following notation: Let  $|+\rangle$  denote the pure state corresponding to  $\mathbf{e}_1 = (0, 1)$ , and  $|-\rangle$  denote the orthogonal pure state corresponding to  $\mathbf{e}_2 = (1, 0)$ . The superscript “ $T$ ,” “ $*$ ” and “ $\dagger$ ” stand for transposition, complex and Hermitian conjugation, respectively.

In finite-dimensional Hilbert space, the matrix representation of projectors  $E_{\mathbf{a}}$  from normalized vectors  $\mathbf{a} = (a_1, a_2, \dots, a_n)^T$  with respect to some basis of  $n$ -dimensional Hilbert space is obtained by taking the dyadic product; i.e., by

$$\mathbf{E}_{\mathbf{a}} = [\mathbf{a}, \mathbf{a}^\dagger] = [\mathbf{a}, (\mathbf{a}^*)^T] = \mathbf{a} \otimes \mathbf{a}^\dagger = \begin{pmatrix} a_1 \mathbf{a}^\dagger \\ a_2 \mathbf{a}^\dagger \\ \vdots \\ a_n \mathbf{a}^\dagger \end{pmatrix} = \begin{pmatrix} a_1 a_1^* & a_1 a_2^* & \dots & a_1 a_n^* \\ a_2 a_1^* & a_2 a_2^* & \dots & a_2 a_n^* \\ \dots & \dots & \dots & \dots \\ a_n a_1^* & a_n a_2^* & \dots & a_n a_n^* \end{pmatrix}. \quad (A.15)$$

The tensor or Kronecker product of two vectors  $\mathbf{a}$  and  $\mathbf{b} = (b_1, b_2, \dots, b_m)^T$  can be represented by

$$\mathbf{a} \otimes \mathbf{b} = (a_1 \mathbf{b}, a_2 \mathbf{b}, \dots, a_n \mathbf{b})^T = (a_1 b_1, a_1 b_2, \dots, a_n b_m)^T \quad (A.16)$$

The tensor or Kronecker product of some operators

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ b_{21} & b_{22} & \dots & b_{2m} \\ \dots & \dots & \dots & \dots \\ b_{m1} & b_{m2} & \dots & b_{mm} \end{pmatrix} \quad (A.17)$$

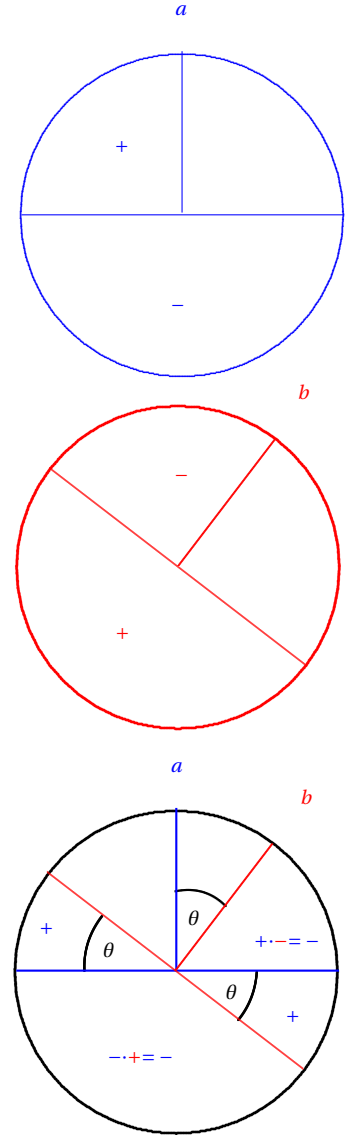


Figure A.3: Planar geometric demonstration of the classical two two-state particles correlation.

is represented by an  $nm \times nm$ -matrix

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \dots & \dots & \dots & \dots \\ a_{n1}B & a_{n2}B & \dots & a_{nn}B \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & \dots & a_{1n}b_{1m} \\ a_{11}b_{21} & a_{11}b_{22} & \dots & a_{2n}b_{2m} \\ \dots & \dots & \dots & \dots \\ a_{nn}b_{m1} & a_{nn}b_{m2} & \dots & a_{nn}b_{mm} \end{pmatrix}. \quad (\text{A.18})$$

Observables:

Let us start with the spin one-half angular momentum observables of a *single* particle along an arbitrary direction in spherical co-ordinates  $\theta$  and  $\varphi$  in units of  $-\hbar$ <sup>18</sup>, i.e.,

$$\mathbf{M}_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{M}_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbf{M}_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{A.19})$$

The angular momentum operator in arbitrary direction  $\theta, \varphi$  is given by its spectral decomposition

$$\begin{aligned} \mathbf{S}_{\frac{1}{2}}(\theta, \varphi) &= x\mathbf{M}_x + y\mathbf{M}_y + z\mathbf{M}_z = \mathbf{M}_x \sin \theta \cos \varphi + \mathbf{M}_y \sin \theta \sin \varphi + \mathbf{M}_z \cos \theta \\ &= \frac{1}{2} \sigma(\theta, \varphi) = \frac{1}{2} \begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix} \\ &= -\frac{1}{2} \begin{pmatrix} \sin^2 \frac{\theta}{2} & -\frac{1}{2} e^{-i\varphi} \sin \theta \\ -\frac{1}{2} e^{i\varphi} \sin \theta & \cos^2 \frac{\theta}{2} \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \cos^2 \frac{\theta}{2} & \frac{1}{2} e^{-i\varphi} \sin \theta \\ \frac{1}{2} e^{i\varphi} \sin \theta & \sin^2 \frac{\theta}{2} \end{pmatrix} \\ &= -\frac{1}{2} \left\{ \frac{1}{2} [\mathbb{I}_2 - \sigma(\theta, \varphi)] \right\} + \frac{1}{2} \left\{ \frac{1}{2} [\mathbb{I}_2 + \sigma(\theta, \varphi)] \right\}. \end{aligned} \quad (\text{A.20})$$

The orthonormal eigenstates (eigenvectors) associated with the eigenvalues  $-\frac{1}{2}$  and  $+\frac{1}{2}$  of  $\mathbf{S}_{\frac{1}{2}}(\theta, \varphi)$  in Eq. (A.20) are

$$\begin{aligned} |-\rangle_{\theta, \varphi} &\equiv \mathbf{x}_{-\frac{1}{2}}(\theta, \varphi) = e^{i\delta_+} \begin{pmatrix} -e^{-\frac{i\varphi}{2}} \sin \frac{\theta}{2}, e^{\frac{i\varphi}{2}} \cos \frac{\theta}{2} \end{pmatrix}, \\ |+\rangle_{\theta, \varphi} &\equiv \mathbf{x}_{+\frac{1}{2}}(\theta, \varphi) = e^{i\delta_-} \begin{pmatrix} e^{-\frac{i\varphi}{2}} \cos \frac{\theta}{2}, e^{\frac{i\varphi}{2}} \sin \frac{\theta}{2} \end{pmatrix}, \end{aligned} \quad (\text{A.21})$$

respectively.  $\delta_+$  and  $\delta_-$  are arbitrary phases. These orthogonal unit vectors correspond to the two orthogonal projectors

$$\mathbf{F}_{\mp}(\theta, \varphi) = \frac{1}{2} [\mathbb{I}_2 \mp \sigma(\theta, \varphi)] \quad (\text{A.22})$$

for the spin down and up states along  $\theta$  and  $\varphi$ , respectively. By setting all the phases and angles to zero, one obtains the original orthonormalized basis  $\{|-\rangle, |+\rangle\}$ .

In what follows, we shall consider two-partite correlation operators based on the spin observables discussed above.

### 1. Two-partite angular momentum observable

If we are only interested in spin state measurements with the associated outcomes of spin states in units of  $-\hbar$ , Eq. (A.24) can be rewritten to include all possible cases at once; i.e.,

$$\mathbf{S}_{\frac{1}{2}\frac{1}{2}}(\hat{\theta}, \hat{\varphi}) = \mathbf{S}_{\frac{1}{2}}(\theta_1, \varphi_1) \otimes \mathbf{S}_{\frac{1}{2}}(\theta_2, \varphi_2). \quad (\text{A.23})$$

<sup>18</sup> Leonard I. Schiff. *Quantum Mechanics*. McGraw-Hill, New York, 1955

## 2. General two-partite observables

The two-particle projectors  $F_{\pm\pm}$  or, by another notation,  $F_{\pm_1\pm_2}$  to indicate the outcome on the first or the second particle, corresponding to a two spin- $\frac{1}{2}$  particle joint measurement aligned (“+”) or antialigned (“−”) along arbitrary directions are

$$\mathbf{F}_{\pm_1\pm_2}(\hat{\theta}, \hat{\varphi}) = \frac{1}{2} [\mathbb{I}_2 \pm_1 \sigma(\theta_1, \varphi_1)] \otimes \frac{1}{2} [\mathbb{I}_2 \pm_2 \sigma(\theta_2, \varphi_2)]; \quad (\text{A.24})$$

where “ $\pm_i$ ,”  $i = 1, 2$  refers to the outcome on the  $i$ 'th particle, and the notation  $\hat{\theta}, \hat{\varphi}$  is used to indicate all angular parameters.

To demonstrate its physical interpretation, let us consider as a concrete example a spin state measurement on two quanta as depicted in Fig. A.4:  $F_{-+}(\hat{\theta}, \hat{\varphi})$  stands for the proposition

*‘The spin state of the first particle measured along  $\theta_1, \varphi_1$  is “−” and the spin state of the second particle measured along  $\theta_2, \varphi_2$  is “+”.’*

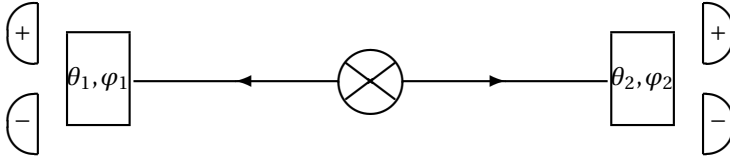


Figure A.4: Simultaneous spin state measurement of the two-partite state represented in Eq. (A.27). Boxes indicate spin state analyzers such as Stern-Gerlach apparatus oriented along the directions  $\theta_1, \varphi_1$  and  $\theta_2, \varphi_2$ ; their two output ports are occupied with detectors associated with the outcomes “+” and “−”, respectively.

More generally, we will consider two different numbers  $\lambda_+$  and  $\lambda_-$ , and the generalized single-particle operator

$$\mathbf{R}_{\frac{1}{2}}(\theta, \varphi) = \lambda_- \left\{ \frac{1}{2} [\mathbb{I}_2 - \sigma(\theta, \varphi)] \right\} + \lambda_+ \left\{ \frac{1}{2} [\mathbb{I}_2 + \sigma(\theta, \varphi)] \right\}, \quad (\text{A.25})$$

as well as the resulting two-particle operator

$$\begin{aligned} \mathbf{R}_{\frac{1}{2}\frac{1}{2}}(\hat{\theta}, \hat{\varphi}) &= \mathbf{R}_{\frac{1}{2}}(\theta_1, \varphi_1) \otimes \mathbf{R}_{\frac{1}{2}}(\theta_2, \varphi_2) \\ &= \lambda_- \lambda_- F_{--} + \lambda_- \lambda_+ F_{-+} + \lambda_+ \lambda_- F_{+-} + \lambda_+ \lambda_+ F_{++}. \end{aligned} \quad (\text{A.26})$$

Singlet state:

Singlet states  $|\Psi_{d,n,i}\rangle$  could be labeled by three numbers  $d$ ,  $n$  and  $i$ , denoting the number  $d$  of outcomes associated with the dimension of Hilbert space per particle, the number  $n$  of participating particles, and the state count  $i$  in an enumeration of all possible singlet states of  $n$  particles of spin  $j = (d-1)/2$ , respectively<sup>19</sup>. For  $n = 2$ , there is only one singlet state, and  $i = 1$  is always one. For historic reasons, this singlet state is also called *Bell state* and denoted by  $|\Psi^-\rangle$ .

Consider the *singlet* “Bell” state of two spin- $\frac{1}{2}$  particles

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle). \quad (\text{A.27})$$

<sup>19</sup> Maria Schimpf and Karl Svozil. A glance at singlet states and four-partite correlations. *Mathematica Slovaca*, 60:701–722, 2010. ISSN 0139-9918. DOI: 10.2478/s12175-010-0041-7. URL <http://dx.doi.org/10.2478/s12175-010-0041-7>

With the identifications  $|+\rangle \equiv \mathbf{e}_1 = (1, 0)$  and  $|-\rangle \equiv \mathbf{e}_2 = (0, 1)$  as before, the Bell state has a vector representation as

$$\begin{aligned} |\Psi^-\rangle &\equiv \frac{1}{\sqrt{2}} (\mathbf{e}_1 \otimes \mathbf{e}_2 - \mathbf{e}_2 \otimes \mathbf{e}_1) \\ &= \frac{1}{\sqrt{2}} [(1, 0) \otimes (0, 1) - (0, 1) \otimes (1, 0)] = \left(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0\right). \end{aligned} \quad (\text{A.28})$$

The density operator  $\rho_{\Psi^-}$  is just the projector of the dyadic product of this vector, corresponding to the one-dimensional linear subspace spanned by  $|\Psi^-\rangle$ ; i.e.,

$$\rho_{\Psi^-} = |\Psi^-\rangle\langle\Psi^-| = \left[|\Psi^-\rangle, |\Psi^-\rangle^\dagger\right] = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{A.29})$$

Singlet states are form invariant with respect to arbitrary unitary transformations in the single-particle Hilbert spaces and thus also rotationally invariant in configuration space, in particular under the rotations  $|+\rangle = e^{i\frac{\varphi}{2}} \left(\cos\frac{\theta}{2}|+\rangle' - \sin\frac{\theta}{2}|-\rangle'\right)$  and  $|-\rangle = e^{-i\frac{\varphi}{2}} \left(\sin\frac{\theta}{2}|+\rangle' + \cos\frac{\theta}{2}|-\rangle'\right)$  in the spherical coordinates  $\theta, \varphi$  defined earlier [e. g., Ref. <sup>20</sup>, Eq. (2), or Ref. <sup>21</sup>, Eq. (7–49)].

The Bell singlet state is unique in the sense that the outcome of a spin state measurement along a particular direction on one particle “fixes” also the opposite outcome of a spin state measurement along *the same* direction on its “partner” particle: (assuming lossless devices) whenever a “plus” or a “minus” is recorded on one side, a “minus” or a “plus” is recorded on the other side, and *vice versa*.

Results:

We now turn to the calculation of quantum predictions. The joint probability to register the spins of the two particles in state  $\rho_{\Psi^-}$  aligned or antialigned along the directions defined by  $(\theta_1, \varphi_1)$  and  $(\theta_2, \varphi_2)$  can be evaluated by a straightforward calculation of

$$\begin{aligned} P_{\Psi^- \pm_1 \pm_2}(\hat{\theta}, \hat{\varphi}) &= \text{Tr} [\rho_{\Psi^-} \cdot \mathbf{F}_{\pm_1 \pm_2}(\hat{\theta}, \hat{\varphi})] \\ &= \frac{1}{4} \{1 - (\pm_1 1)(\pm_2 1) [\cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)]\}. \end{aligned} \quad (\text{A.30})$$

Again, “ $\pm_i$ ,”  $i = 1, 2$  refers to the outcome on the  $i$ 'th particle.

Since  $P_+ + P_- = 1$  and  $E = P_+ - P_-$ , the joint probabilities to find the two particles in an even or in an odd number of spin-“ $-\frac{1}{2}$ ”-states when measured along  $(\theta_1, \varphi_1)$  and  $(\theta_2, \varphi_2)$  are in terms of the expectation function given by

$$\begin{aligned} P_+ &= P_{++} + P_{--} = \frac{1}{2} (1 + E) \\ &= \frac{1}{2} \{1 - [\cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)]\}, \\ P_- &= P_{+-} + P_{-+} = \frac{1}{2} (1 - E) \\ &= \frac{1}{2} \{1 + [\cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)]\}. \end{aligned} \quad (\text{A.31})$$

<sup>20</sup> Günther Krenn and Anton Zeilinger. Entangled entanglement. *Physical Review A*, 54:1793–1797, 1996. DOI: 10.1103/PhysRevA.54.1793. URL <http://dx.doi.org/10.1103/PhysRevA.54.1793>

<sup>21</sup> L. E. Ballentine. *Quantum Mechanics*. Prentice Hall, Englewood Cliffs, NJ, 1989

Finally, the quantum mechanical expectation function is obtained by the difference  $P_{=} - P_{\neq}$ ; i.e.,

$$E_{\Psi^{-} -1, +1}(\theta_1, \theta_2, \varphi_1, \varphi_2) = -[\cos\theta_1 \cos\theta_2 + \cos(\varphi_1 - \varphi_2) \sin\theta_1 \sin\theta_2]. \quad (\text{A.32})$$

By setting either the azimuthal angle differences equal to zero, or by assuming measurements in the plane perpendicular to the direction of particle propagation, i.e., with  $\theta_1 = \theta_2 = \frac{\pi}{2}$ , one obtains

$$\begin{aligned} E_{\Psi^{-} -1, +1}(\theta_1, \theta_2) &= -\cos(\theta_1 - \theta_2), \\ E_{\Psi^{-} -1, +1}(\frac{\pi}{2}, \frac{\pi}{2}, \varphi_1, \varphi_2) &= -\cos(\varphi_1 - \varphi_2). \end{aligned} \quad (\text{A.33})$$

The general computation of the quantum expectation function for operator (A.26) yields

$$\begin{aligned} E_{\Psi^{-} \lambda_1 \lambda_2}(\hat{\theta}, \hat{\varphi}) &= \text{Tr} \left[ \boldsymbol{\rho}_{\Psi^{-}} \cdot R_{\frac{1}{2} \frac{1}{2}}(\hat{\theta}, \hat{\varphi}) \right] = \\ &= \frac{1}{4} \{ (\lambda_- + \lambda_+)^2 - (\lambda_- - \lambda_+)^2 [\cos\theta_1 \cos\theta_2 + \cos(\varphi_1 - \varphi_2) \sin\theta_1 \sin\theta_2] \}. \end{aligned} \quad (\text{A.34})$$

The standard two-particle quantum mechanical expectations (A.32) based on the dichotomic outcomes “−1” and “+1” are obtained by setting  $\lambda_+ = -\lambda_- = 1$ .

A more “natural” choice of  $\lambda_{\pm}$  would be in terms of the spin state observables (A.23) in units of  $-\hbar$ ; i.e.,  $\lambda_+ = -\lambda_- = \frac{1}{2}$ . The expectation function of these observables can be directly calculated *via*  $S_{\frac{1}{2}}$ ; i.e.,

$$\begin{aligned} E_{\Psi^{-} -\frac{1}{2}, +\frac{1}{2}}(\hat{\theta}, \hat{\varphi}) &= \text{Tr} \left\{ \boldsymbol{\rho}_{\Psi^{-}} \cdot \left[ S_{\frac{1}{2}}(\theta_1, \varphi_1) \otimes S_{\frac{1}{2}}(\theta_2, \varphi_2) \right] \right\} \\ &= \frac{1}{4} [\cos\theta_1 \cos\theta_2 + \cos(\varphi_1 - \varphi_2) \sin\theta_1 \sin\theta_2] = \frac{1}{4} E_{\Psi^{-} -1, +1}(\hat{\theta}, \hat{\varphi}). \end{aligned} \quad (\text{A.35})$$

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